BP 1: Protein Structure and Dynamics

Time: Monday 9:30–13:00 Location: H 1028

Invited Talk BP 1.1 *(3)* Mon 9:30 H 1028

Thermodynamics and kinetics of protein aggregation from atomistic simulations — •Birgit Strodel — Institute of Complex Systems: Structural Biochemistry, Forschungszentrum Jülich, Germany — Institute of Theoretical and Computational Chemistry, Heinrich Heine University, Düsseldorf

I will present two different techniques developed by my group, which allow the extraction of the thermodynamics and kinetics of protein aggregation from molecular dynamics data. The first technique uses transition networks (TNs) to characterize the aggregation pathways, as will be demonstrated for the formation amyloid β-protein (Aβ) oligomers, which are connected to the development of Alzheimer's disease. The TNs reveal that the oligomers leading to the size distributions observed in experiments originate from metastable compact conformations, while extended oligomers are the ones driving the aggregation process. It is further elucidated how changes in the sequence of Aβ, a pH change or the presence of Cu(II) ions lead to different aggregation pathways, which is of direct relevance to the toxicity of Aβ oligomers. In the other technique, we extended the idea of automated Markov state models (MSM) to protein self-assembly by constructing reaction coordinates from descriptors that are invariant to permutations of the molecular indexing. I will demonstrate the power of this technique for the identification of kinetically relevant aggregation pathways for the KFFE peptide. Both the TN and MSM formalism developed by us are quite general and can therefore be used for the automated analysis of any other self-assembling molecular system.

BP 1.2 *(128)* Mon 10:00 H 1028

Short-time self-dynamics of immunoglobulin under biomimicking crowding conditions — •Marco Grimaldo[1], Beck Christian[1,2], Felix Roosen-Runge[3], Fajun Zhang[2], Frank Schreiber[2], and Tilo Seydel[1] — [1]Institut Laue-Langevin, Grenoble, France — [2]IAP- Universität Tübingen, Tübingen, Germany — [3]Division for Physical Chemistry, Lund University, Lund, Sweden

Approximately 10-40% of the intra- and extracellular fluids of living organisms are occupied by macromolecules such as proteins. This macromolecular crowding condition was shown to influence reaction rates, and to lead to anomalous diffusion. We present a neutron backscattering study on the pico- to nanosecond self-diffusion and internal motion of the antibody proteins immunoglobulins (Ig) in aqueous environment. To systematically investigate the effect of macromolecular crowding on protein dynamics we vary the concentration of cellular lysate, mimicking a cellular environment. The dynamics of Ig in lysate is then compared with that of Ig in pure (heavy) water as a function of its own concentration (self-crowding) [1]. Despite the high polydispersity and the not easily predictable variance in lysate composition, both the measured diffusion and the localized internal atomic motion of Ig as a function of the overall volume fraction are in rather good agreement with those of Ig in the self-crowded environment at comparable volume fraction, suggesting a crucial role of hydrodynamic interactions on short-time protein dynamics even in a cell-like environment.
[1] Grimaldo M., Roosen-Runge F., Zhang F., Seydel T., Schreiber F. JPCB 118 (2014): 7203.

BP 1.3 *(230)* Mon 10:15 H 1028

Dramatic influence of anisotropic interaction and shape on short-time protein diffusion — Jin Suk Myung[1], •Felix Roosen-Runge[1], Roland G. Winkler[2], Gerhard Gompper[2], Peter Schurtenberger[1], and Anna Stradner[1] — [1]Division of Physical Chemistry, Lund University, Sweden — [2]Theoretical Soft Matter and Biophysics, Forschungszentrum Jülich, Germany

Diffusion of proteins in cells is an essential process, strongly influencing the cellular machinery through numerous processes such as signal transmission or reactions between proteins. We present a combined experimental and computational study on effects of anisotropic interactions and shape on the initial step of structural relaxation on nearest-neighbor distance, i.e. short-time cage diffusion. Using neutron spin echo spectroscopy in crowded solutions of crystallin proteins, cage diffusion for α crystallin follows predictions for hard spheres, while the cage diffusion of the weakly attractive γ crystallin shows a dramatical slowing down at comparably low volume fractions [1]. In mesoscale hydrodynamic simulations employing multiparticle collision dynamics (MPC), we observe a significant dynamical slowing down due to attractions, which is strongly enhanced due to anisotropy in protein interactions [1] and shape [2]. These results particularly demonstrate that simplistic spherical models for globular proteins can be severely misleading when studying effects of crowding on structural relaxation and diffusion.
[1] S Bucciarelli, JS Myung et al. Sci. Adv. (2016) 2:e1601432
[2] JS Myung, F Roosen-Runge et al. in preparation

BP 1.4 *(334)* Mon 10:30 H 1028

Stochastic modeling of multiprotein complex formation — •Stefanie Förste, Reinhard Lipowsky, and Sophia Rudorf — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The formation of a multiprotein complex, arising from the assembly of multiple peptide chains inside the crowded cell environment, is subject of ongoing research. In contrast to the canonical view that protein assembly is a post-translational process, recent experiments show that protein complexes can also assemble co-translationally, i.e., the different chains may assemble before translation has finished. Here, we investigate under which conditions post translational and/or co-translational assembly can occur. We analyze the influence of different parameters - such as the spatial distance of the translation sites - on the assembly dynamics using a combination of Gillespie simulations and analytical Markov modeling. In particular, we study the cross-over from a co-translational to a post-translational assembly regime.

BP 1.5 *(353)* Mon 10:45 H 1028

Characterisation of binding interaction of the influenza virus proteins Hemagglutinin and Neuraminidase with a synthetic sialic acid receptor by single molecule force spectroscopy — •Valentin Reiter-Scherer[1], Sumati Bhatia[2], Jose Luis Cuellar-Camacho[2], Daniel Lauster[1], Rainer Haag[2], Andreas Herrmann[1], and Jürgen P. Rabe[1] — [1]HU Berlin — [2]FU Berlin

The influenza virus is causing annual epidemics. In the first step of the infection, the virion binds to a host cell through multivalent attachment, mediated by the major virus spike protein hemagglutinin (HA) and sialic acid (SA) receptors of the glycocalyx of epithelial cells of the respiratory tract [1]. Neuraminidase (NA) on the other hand is known to cleave SA from the glycoproteins enabling the release of newly formed virions. A common strategy to inhibit infection, is the use of drugs that bind specifically to the binding pockets of the viral proteins to prevent SA binding [2]. Here we introduce a ligand architecture (LAPEG-SA) ideally synthesized to test the tensile strength between individual SA units and recombinant HA and NA of influenza H1N1. Individual binding strength and affinity at the single molecular level, being of central importance for the development of novel potent inhibitors, are characterized by scanning force microscope based single molecule force spectroscopy. Rupture forces of the SA protein binding are measured for several rates of force loading and the dissociation parameters off-rate as well rupture length are derived from the single barrier model [3]. - [1] Sieben et al., PNAS 2012. [2] Bhatia et al., J. Am. Chem. Soc. 2016. [3] Evans et al., Biophys. Journal 1997.

15 min. break

BP 1.6 *(247)* Mon 11:15 H 1028

Exploring protein structure with cryogenic optical localization in three dimensions — Daniel Boening, •Franz Ferdinand Wieser, and Vahid Sandoghdar — Max Planck Institute for the Science of Light, Erlangen, Germany

Super-resolution optical microscopy has considerably advanced the study of cellular processes, but optical access to the molecular structure of proteins and biomolecular assemblies remains very limited. We have recently exploited the enhanced photostability of fluorophores at cryogenic temperatures to increase the number of detected photons, thus reaching a significantly higher signal-to-noise ratio compared to room-temperature measurements. Using this approach, cryogenic optical localization in three dimensions (COLD) is capable of determining the positions of several fluorescent sites within a single protein at Angstrom resolution [1]. We present results on imaging DNA Origami, the four binding sites of streptavidin and the conformational state of

the Per-ARNT-Sim domain of the histidine kinase CitA. With its high spatial resolution COLD opens new possibilities for obtaining quantitative structure information from small to medium sized biomolecules and for correlative measurements with established imaging methods.

[1] S. Weisenburger et al., Nature Methods 14, 141-144 (2017).

BP 1.7 *(358)* Mon 11:30 H 1028

The relevance of conformational entropy for ligand-protein interactions: The case of biotin and streptavidin — •Mona Sarter[1,2], Andreas Stadler[1], Doreen Niether[1], Bernd König[1], Simone Wiegand[1,3], Jörg Fitter[1,2], Michaela Zamponi[1], Wiebke Lohstroh[4], and Niina Jalarvo[5] — [1]FZJ Jülich — [2]RWTH Aachen — [3]Universität zu Köln — [4]TUM München — [5]SNS Oak Ridge

Molecular dynamics play a vital role for the biological function of proteins. For protein ligand interactions changes of conformational entropy of the protein and the hydration layer are relevant for the binding process. In an experimental study we investigated the relevance of conformational entropy for the binding of biotin to the protein streptavidin. In order to investigate the proteins conformational entropy and dynamics quasi elastic neutron scattering (QENS) was used, for the protein and hydration layer isothermal titration caliometry (ITC) was used and for the hydration layer thermodiffusion (TDFRS) was used.

QENS results show that the conformational entropy of streptavidin is reduced upon biotin binding, while ITC results show that the conformational entropy of the hydration layer increases upon biotin binding. TDFRS results also indicate an increased entropy of the hydration layer. This leads to the conclusion that the hydration layer plays an important role in stabilising the binding of biotin to streptavidin. The internal streptavidin dynamics before and after biotin binding were compared. This showed that the flexibility of streptavidin is greatly reduced upon biotin binding leading to the complex being more rigid.

BP 1.8 *(371)* Mon 11:45 H 1028

Hydration behaviour of collagen — •Philip Loche[1], Lise Thornfeldt Hansen[1], Lorena Ruiz[2], Jan Daldrop[1], Alexander Schlaich[1], Emanuel Schneck[2], Luca Bertinetti[2], Kerstin G. Blank[2], and Roland R. Netz[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg, 1 OT Golm, Germany

Collagen is a key protein in the extraceullar matrix of connective tissues such as bones, skin, cartilage, tendons and muscles. Materials such as leather or parchment are known to shrink upon dehydration. An important component in these materials is collagen. The fact that water has an effect on the properties of collagen is well known, but the reasons for this are not. Here we use classical molecular dynamics simulations to obtain insights into the structure and behaviour of collagen. By comparison with x-ray scattering experiments, we show that the choice of the forcefield used in simulations is crucial to reproduce correct hydration effects. From our simulations we reproduce the experimental scattering intensities as well a experimental osmotic pressures. We also calculate the energetic and entropic contributions to the osmotic pressure for different collagen types.

BP 1.9 *(372)* Mon 12:00 H 1028

Protein assemblies of hGBP1 studied with Time Resolved-Small Angle Scattering — •Charlotte Lorenz and Andreas Stadler — Jülich Centre for Neutron Science (JCNS-1), Forschungszentrum Jülich

The human Guanylate Binding Protein 1 belongs to the family of dynamin-like proteins and is activated by addition of nucleotides which lead to protein oligomerization and stimulated GTPase activity. Standard protein expression and purification from bacterial E.coli cells leads to hGBP1 without the posttranslational attachment of farnesyl. With an integrative approach using analytical ultracentrifugation (AUC), dynamic light scattering (DLS) and on-line size exclusion chromatography (SEC-SAXS) we investigated intermediate states during the hydrolysis cycle of hGBP1. We were able to show that farnesylation prevents hGBP1 in the inactive monomeric form in nucleotide free solution, whereas the unmodified hGBP1 (nf-hGBP1) consists of monomers and dimers in nucleotide free solution. Furthermore, the nf-hGBP1 assembles to mostly dimers and tetramers after nucleotide induction. Contrary, the farnesylated hGBP1 assembles after nucleotide addition to large macromolecular structures. The polymer growth and composition is analyzed in solution using time resolved SAXS (TR-SAXS). This study shows the importance of posttranslational modifications regarding the signaling regulation and controlled growth of macromolecular complexes.

BP 1.10 *(389)* Mon 12:15 H 1028

High spatial and temporal resolution study of biological processes in a live cell via interferometric scattering microscopy (iSCAT). — Richard Taylor[1], Reza Gholami[1], Verena Rauschenberger[2], •Anna Kashkanova[1], Alexandra Schambony[2], and Vahid Sandoghdar[1] — [1]Max Planck Institute for the Science of Light, Erlangen, 91058, Germany — [2]Developmental Biology Unit, Friedrich-Alexander University Erlangen-Nuremberg, Erlangen, 91058, Germany

Transmembrane proteins on a live cell exhibit a variety of dynamic behaviors, such as diffusion on the cell membrane, transport into the cell and trafficking along filaments. Those processes have been studied using standard technologies, however real-time visualization with nanoscopic resolution is a challenge, with fluorescent microscopy as the primary workhorse.

However, fluorescent microscopy has a critical limitation: fluorophores emit a limited number of photons in their lifetime, which limits spatial and temporal resolution, and the observation time. Interferometric scattering microscopy (iSCAT), uses gold nanoparticles in place of fluorophores. The scattered light is imaged interferometrically and the measurement can be performed indefinitely with spatial (temporal) resolution of several nanometers (microseconds).

We present an experiment in which the epidermal growth factor receptor (EGFR) protein in a live HeLa cell was labeled with a 50 nm gold nanoparticle and its life cycle observed. Our precise 3D information provides exciting new insights into the dynamics of the receptor.

BP 1.11 *(406)* Mon 12:30 H 1028

Validation of reaction coordinates describing protein functional motion: combining equilibrium and non-equilibrium MD methods — •Matthias Ernst, Steffen Wolf, and Gerhard Stock — Biomolecular Dynamics, University of Freiburg

Finding low-dimensional reaction coordinates that concisely describe mechanistic details of protein motion is a fundamental and crucial step to understand (and, at a later stage, to manipulate) protein dynamics. Statistical methods like Principal Component Analysis are often used and well understood, but usually not able to causally disentangle local rearrangements that drive some motion and others that are merely correlated or follow it. In my presentation, I will outline a strategy to combine non-equilibrium methods with equilibrium results to challenge and validate reaction coordinates: we use Targeted MD[1] as "molecular tweezer" to induce local rearrangements and explain causal relations between and the overall functional motion. Investigating the prominent PacMan-like hinge-bending motion of T4 Lysozyme, with 2600 atoms a rather small but extensively studied protein, we could show[2] that a so far unrecognized reorientation of actually one single side chain acts as a lock to stabilize and distinguish the open from the closed state and is the cause of the rather long ($\approx 10\mu$s) timescale. We propose and verify a 4-state model for the hinge-bending motion of T4 Lysozyme, which is supported by mutation studies and higher temperature runs.

[1] J.Schlitter, M.Engels, P.Krüger, *J.Mol Graph.* **1994**, *12*, 84.
[2]M.Ernst,S.Wolf,G.Stock,*J.Chem.Theory Comput.***2017**,*13*(10),5076.

BP 1.12 *(121)* Mon 12:45 H 1028

Elucidation of light-induced structural changes of aureochrome and its recovery kinetics by small-angle X-ray scattering — •Saskia Bannister, Elena Herman, Thomas Hellweg, and Tilman Kottke — Bielefeld University, Germany

Aureochromes function as blue-light-regulated transcription factors in algae. Their basic region leucine zipper (bZIP) effector domain binds DNA specifically while a light-, oxygen-, or voltage-sensitive (LOV) domain acts as the sensor. Due to the inversed arrangement of sensor and effector, aureochromes are interesting for studying their mechanism and for the engineering of new optogenetic tools.

By applying small-angle X-ray scattering (SAXS) we pursue two main targets, namely the elucidation of light-induced structural changes of the receptor in solution and the analysis of the recovery kinetics from its light state back to its dark state. However, SAXS on photoreceptors is challenging. First, dark conditions need to be absolutely strict to avoid conversion of the highly sensitive receptor. Second, the analysis under illumination needs to ensure full conversion. Therefore we have established SAXS experiments under rigorous

control of light. Here, we reveal light-induced structural changes of the photoreceptor and its recovery kinetics.

Banerjee, A., Herman, E., Serif, M., Maestre-Reyna, M., Hepp, S., Pokorny, R., Kroth, P. G., Essen, L.-O., Kottke, T. (2016), *Nucleic Acids Res.* 44(12), 5957-5970.

BP 2: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Monday 9:30–13:00 Location: H 1058

BP 2.1 *(189)* Mon 9:30 H 1058

PFG-NMR studies of ATP diffusion in PEG-DA hydrogels and aqueous solutions of PEG-DA polymers — •Günter Majer[1] and Alexander Southan[2] — [1]MPI für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Institut für Grenzflächenverfahrenstechnik und Plasmatechnologie IGVP, Universität Stuttgart, Nobelstraße 12, 70569 Stuttgart, Germany

Adenosine triphosphate (ATP) is the major carrier of chemical energy in cells. The diffusion of ATP in hydrogels, which have a structural resemblance to the natural extracellular matrix, is therefore of great importance for understanding many biological processes. A powerful tool to determine the diffusion coefficients of ATP and other solutes directly, i.e. without the need for a fluorescent label and independent of any diffusion-model assumptions, is pulsed field gradient nuclear magnetic resonance (PFG-NMR). We present precise PFG-NMR measurements of ATP diffusion in PEG-DA hydrogels of various mesh sizes as well as in aqueous solutions of PEG-DA polymers, which are not cross-linked to a three-dimensional network. A major result of this work is that the diffusion coefficients are determined by the polymer volume fraction only, regardless of whether the polymers are cross-linked or not. Obviously, the ATP diffusion takes place only in the aqueous regions of the systems, with the volume fraction of the polymers, including a solvating water layer, being blocked for the ATP molecules. This modified obstruction model is most appropriate to correctly describe ATP diffusion in PEG-DA hydrogels.

BP 2.2 *(96)* Mon 9:45 H 1058

Ion and Molecule Transport Bulk and in Nanopores - a NMR study — •Sarah Schneider and Michael Vogel — TU Darmstadt Institut fuer Festkoerperphysik, Darmstadt, Germany

We analyze ion and molecule transport in aqueous salt solutions confined to nanopores as part of a project that aims to develop a new generation of nanosensors by combining biological and synthetic nanopores. While being highly selective and sensitive, biological ion channels lack the robustness for technological applications. Contrarily silica pores are well-proven in industrial and clinical environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favorable properties of both fields.

To optimize such pores, it is of strong interest to understand the influence of the confinement on the T-dependent ion and molecule transport inside. We vary the pore parameters systematically and study their effects on the dynamics by NMR. Using ^{1}H and ^{2}H NMR we can selectively investigate water dynamics whereas ^{7}Li and ^{23}Na NMR analyze the local and long-range dynamics of ionic species. Analyzing the local ion and water dynamics reveals a slowdown with increasing salt concentration, which may differ in bulk and confinement due to altered prospensity for crystallization. At a given concentration there is a slowdown in confinement with more heterogenious dynamics. Both can be explained by a slower layer at the pore walls and bulk-like dynamics in the pore center. Field-gradient NMR is applied to measure self-diffusion. The extent of the effect and the relation between short- and long-range dynamics depend on the confinement properties.

BP 2.3 *(286)* Mon 10:00 H 1058

Fluoridation of hydroxyapatite - time dependence and protective properties — •Thomas Faidt[1], Andreas Friedrichs[1], Christian Zeitz[1], Samuel Grandthyll[1], Michael Hans[2], Matthias Hannig[3], Frank Müller[1], and Karin Jacobs[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Functional Materials, Saarland University, Saarbrücken, Germany — [3]Clinic of Operative Dentistry, Periodontology and Preventive Dentistry, Saarland University Hospital, Homburg, Germany

The application of fluoride containing products to protect tooth enamel from caries is daily practice for many decades. However, to this day little is known about the time dependence of fluoride uptake in hydroxyapatite (HAP) which is the mineral component of human enamel. In our study, we used highly dense HAP pellet samples as a model system for the crystallites of tooth enamel. To investigate the time dependence of the fluoride uptake, samples were exposed to a fluoride solution (NaF, 500 ppm) for different times. XPS depth profiling revealed a saturation behavior both for the overall amount of fluoride taken up by the sample and for the thickness of the formed fluoridated layer. We found that the maximum thickness of the fluoridated layer is about 13 nm. To explore the efficacy of such an ultrathin layer as a protective shield against acid attacks, we used AFM to determine the etching rates of untreated and fluoridated HAP samples. In spite of very low fluoride concentrations in the fluoridated samples, our results show a strong reduction of the etching rate after fluoride treatment.

BP 2.4 *(92)* Mon 10:15 H 1058

Flexoelectricity in bones — •Fabian Vasquez-Sancho[1,2], Amir Abdollahi[3], Dragan Damjanovic[4], and Gustau Catalan[1,5] — [1]Institut Catala de Nanociencia i Nanotecnologia, Barcelona, Catalunya — [2]CICIMA, Universidad de Costa Rica, San Jose, Costa Rica — [3]Laboratori de Calcul Numeric, Universitat Politecnica de Catalunya, Barcelona, Catalunya — [4]Ecole Politechnique Federale de Lausanne (EPFL), Lausanne, Switzerland — [5]Institut Catala de Recerca i Estudis Avançats (ICREA), Barcelona, Catalunya

Bones have been known to generate electricity under pressure since Fukada and Yasuda's seminal measurement of bone piezoelectricity in 1957. This piezoelectricity is thought to be essential for bone's self-repair and remodelling properties, and its origin is attributed to the piezoelectricity of collagen (the main structural protein of bones). However, since the discovery of flexoelectricity, it is known that strain gradients can also generate voltages in materials of any symmetry. Here we have detected and quantified the flexoelectricity of bone and bone mineral (hydroxyapatite), and determined that flexoelectricity can account for bone's electrical response to inhomogeneous deformations. In addition, we have used the flexoelectric coefficient of hydroxyapatite to calculate the (flexo)electric fields generated by cracks in bone mineral. Crack-generated electricity has been found to be large enough to be able to induce osteocyte apoptosis and thus initiate the crack-healing process, indicating a central role of flexoelectricity in bone damage repair and remodelling.

Invited Talk BP 2.5 *(17)* Mon 10:30 H 1058

Light-based tools for investigating cell-ECM and cell-cell interactions — •Aranzazu del Campo — INM-Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany

Cells are able to sense and respond to biochemical and mechanical signals of their microenvironment. Despite impressive progress in the field of mechanotransduction, we still lack precise biophysical tools to dynamically regulate receptors and forces at the cell-ECM and cell-cell interfaces at molecular scale. In this context, novel tools based on phototriggers, light-driven molecular motors and optogenetics will be presented.

15 min. break

BP 2.6 *(329)* Mon 11:15 H 1058

Quantitative Prediction of Multivalent Ligand-Receptor Binding Affinities for Influenza, Cholera and Anthrax Inhibition — •Susanne Liese[1,2] and Roland R. Netz[1] — [1]Freie Universität Berlin, Fachbereich Physik — [2]University of Oslo, Department of Mathematics

Multivalency achieves strong, yet reversible binding by the simultaneous formation of multiple weak bonds. It is a key interaction principle in biology and promising for the synthesis of high-affinity inhibitors of pathogens. We present a model for the binding affinity of synthetic multivalent ligands onto multivalent receptors consisting of n receptor units arranged on a regular polygon. Ligands consist of a rigid polygonal core to which monovalent ligand units are attached via flexible

linker polymers. The calculated binding affinities quantitatively agree with experimental studies for cholera toxin (n=5) and anthrax receptor (n=7) and allow to predict optimal core size and linker length. Maximal binding affinity is achieved for a core that matches the receptor size and for linkers that are slightly longer than the difference between receptor size and core size. We construct an enhancement diagram that quantifies the multivalent binding affinity compared to monovalent ligands. We conclude that multivalent ligands against influenza viral hemagglutinin (n=3), cholera toxin (n=5) and anthrax receptor (n=7) can outperform monovalent ligands only for a monovalent ligand affinity that exceeds a core-size dependent threshold value. Thus multivalent drug design needs to balance core size, linker length as well as monovalent ligand unit affinity.

BP 2.7 *(320)* Mon 11:30 H 1058

Are there knots in chromosomes? — Jonathan Siebert[1], Alexey Kivel[1], Tim Stevens[2], Ernest Laue[2], and •Peter Virnau[1] — [1]JGU Mainz, Institut für Physik — [2]Cambridge University, Department of Biochemistry

Recent developments have for the first time allowed the determination of three-dimensional structures of individual chromosomes and genomes in nuclei of single haploid mouse embryonic stem (ES) cells based on Hi-C chromosome conformation contact data. Although these first structures have a relatively low resolution, they provide the first experimental data that can be used to study chromosome and intact genome folding. Here we further analyze these structures and provide the first evidence that G1 phase chromosomes are knotted [1], consistent with the fact that plots of contact probability vs sequence separation show a power law dependence that is intermediate between that of a fractal globule and an equilibrium structure.

[1]J.T. Siebert et al., Are There Knots in Chromosomes?, Polymers 9:8 (2017)

BP 2.8 *(194)* Mon 11:45 H 1058

Small-angle X-ray scattering on gold nanoparticle-decorated DNA-origami nanostructures — •Kilian Frank[1,2], Caroline Hartl[1], Amelie Heuer-Jungemann[1], Tim Liedl[1], and Bert Nickel[1] — [1]Faculty of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Germany — [2]present address: Georg-August-Universität, Institute for X-ray Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The DNA origami technique is a robust method for positioning guest molecules at the nanoscale, allowing for 3D crystalline assembly from monomeric building blocks. We report on synchrotron small-angle X-ray scattering (SAXS) experiments on DNA origami with guest gold nanoparticles. Geometric models were applied to investigate the particle placement and the lattice parameters of crystalline superstructures. In collaboration with Heinz Amenitsch (TU Graz) the model-free pair distance distribution function (PDDF) from the scattering data was analyzed. The PDDF reveals interparticle distances with nanometer resolution and is thus a valuable tool in the study of DNA-templated particle assemblies. The structure of a DNA-based lattice was confirmed to be rhombohedral with a spacing of 65 nm (T. Zhang, C. Hartl, S. Fischer, K. Frank, P. Nickels, A. Heuer-Jungemann, B. Nickel and T. Liedl. arXiv: 1706.06965). In situ SAXS confirmed previously found melting temperatures of the structures. These results help to optimize future designs of monomeric building blocks regarding lattice type and size.

BP 2.9 *(336)* Mon 12:00 H 1058

Magnetic collecting of malaria pigment crystals by magnetized thin films — •Szilvia Mucza[1], Tamas Prok[1], Agnes Orban[1], Adrienne Furedi[2], Peter Furjes[2], and Istvan Kezsmarki[1] — [1]Dept. of Physics, Budapest Uni. of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, HU — [2]Inst. of Technical Physics and Materials Science, Centre for Energy Research, HAS, 1121 Budapest, HU

Malaria pigment (hemozoin) crystals are the by-product of the hemoglobin metabolism and are unique indicators of the malaria infection. These micrometer-sized, needle-like, paramagnetic crystals have low crystal symmetry, thus show optical and magnetic anisotropy. Our group has been developing a malaria diagnostic device based on their linear dichroism and we aim to integrate a magnetic prefilter to increase the method's efficiency.

For this reason we started to investigate the behaviour of hemozoin crystals in their liquid suspension under magnetic field. To enhance the magnetic field gradient we designed micron-sized magnetizable periodic structures by lithography, and we observed the behaviour of synthetically prepared hemozoin crystals in liquid over these structures. We explained our observations theoretically, with the modeling of the magnetic properties near the surface of the periodic structure. We performed measurements under flow using an aligned microfluidic system to optimize different geometric parameters of magnetic structures.

BP 2.10 *(310)* Mon 12:15 H 1058

Fibers and glasses: the complex behavior of protein droplets — •Louise Jawerth[1,2], Elisabeth Fischer-Friedrich[3], Supriya Saha[1], Anthony Hyman[2], and Frank Jülicher[1] — [1]MPI for the Physics of Complex Systems. Dresden — [2]MPI of Molecular Cell Biology and Genetics, Dresden — [3]Biotec, TU Dresden

Liquid-like protein droplets are intracellular compartments that segregate material without the use of a physical barrier such as a membrane. Such compartments are important in a wide array of biological processes ranging from embryonic development to pathological fiber formation during neurodegenerative disease. The existence of many of these compartments has been known for decades; however, only recently has it become clear that these compartments exhibit liquid-like properties. In this talk, I will discuss our efforts to characterize and quantify these new materials in vitro. I will preset our recent work on quantifying the mechanical properties of these droplets using a combination of active and passive microrheology. We find that these droplets are not simple liquids, but become increasingly elastic as the droplets age. This appears to be a universal behavior shared by many protein varieties that form droplets. Furthermore, this and other characteristics are strikingly similar to behaviors observed in glass-like materials suggesting that protein droplets are in fact not simple liquids but, rather, a type of glass.

BP 2.11 *(221)* Mon 12:30 H 1058

Light-driven biomolecule electrophoresis by asymmetric photochemistry — •Michael Kiess, Friederike Möller, and Dieter Braun — LMU Munich, Amalienstrasse 54, 80799 München, Germany

Ion and pH gradients across membranes are widespread in biology and are decisive for cell metabolism and signal transmission. We recreate such gradients in bulk water by local photolysis of photodissociable compounds. Focused light creates a non-equilibrium between photoproducts of different charges. Similar to pattern formation in biology, the differential diffusion of the photoproducts generates a radial electric field on a micrometer scale. Charged biomolecules move in this field through electrophoresis, which reaches a steady state within seconds in proportion to $\exp(-\mu/\mathrm{D}\ \Phi)$. The complete description and theoretical analysis of this phenomenon allows us to analyse and manipulate molecules in water. We call this effect photochemical microscale electrophoresis (PME) and use it as a fast, purely optical tool for the simultaneous determination of electrophoretic mobilities, diffusion coefficients and charges of biomolecules ($\mathrm{Q}\propto\mu/\mathrm{D}$) such as DNA and proteins as well as the quantification of binding probabilities. We expect that the presented photochemically induced, electrokinetic reaction-diffusion-migration system will be a versatile playground for further research. It can be a valuable tool for the investigation of electrokinetic effects and for the development of optical methods such as zeta potential measurements or isoelectric focusing. Furthermore, it is likely that the optically controlled interaction of electrical fields with pH and ion gradients may lead to a novel testbed for intracellular processes.

BP 2.12 *(199)* Mon 12:45 H 1058

Thermal gradients, a natural choice to support the origins of life — •Christof Mast[1], Lorenz Keil[1], Friederike Möller[1], Michael Kiess[1], Patrick Kudella[1], Mara Heinlein[1], Matthias Morasch[1], Hannes Mutschler[2], and Dieter Braun[1] — [1]LMU Munich, Amalienstrasse 54, 80799 München, Germany — [2]Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Martinsried, Germany

Life is a non-equilibrium system, which is nowadays maintained by a highly developed energy conversion machinery. Four billion years ago, other non-equilibrium mechanisms were needed to kick-start living processes. We propose ubiquitous heat fluxes as suitable driving force: Thermal gradients across water filled pores lead to a concurrent fluid convection and directed movement of dissolved charged molecules along the temperature difference. Combined, both effects accumulate the dissolved biomolecules in a length dependent manner. Oligonucleotides are pushed into a hydrogel phase, depending on their sequence

and chirality: A mixture of strands with different sequence demixes into sequence-pure and homochiral hydrogels upon thermal accumulation, possibly selecting for interacting strands during the origin of life. The thermal non-equilibrium also creates and maintains a pH gradient over two units by the selective accumulation of charged buffer molecules, which shifts the local equilibrium in pH. In this system, early compartments of life may have cycled between different external pH conditions, implementing an important boundary condition for a primordial metabolism. [1] Keil et al. Nat Com, 2017, 10.1038/s41467-017-02065-3

BP 3: Cell Adhesion and Migration, Multicellular Systems I

Time: Monday 9:30–13:00 Location: H 2013

BP 3.1 *(27)* Mon 9:30 H 2013

Molecular motors govern liquid-like ordering and fusion dynamics of bacterial colonies — •Tom Cronenberg, Anton Welker, Robert Zöllner, Claudia Meel, Enno R. Oldewurtel, Katja Siewering, and Berenike Maier — Department of Physics, University of Cologne, Zülpicher Str. 77, 50539 Köln, Germany

Bacteria can adjust the structure of biofilms to enhance their survival rate under external stress. Here, we explore the link between bacterial interaction forces and colony structure. We show that the activity of extracellular pilus motors enhances local ordering and accelerates fusion dynamics of bacterial colonies. The radial distribution function of mature colonies shows local fluid-like order. The degree and dynamics of ordering are dependent on motor activity. At a larger scale, the fusion dynamics of two colonies shows liquid-like behavior whereby the ratio between surface tension and viscosity decreases with decreasing motor activity.

BP 3.2 *(64)* Mon 9:45 H 2013

Organization of Fibronectin and NIH/3T3 Fibroblasts on Bulk Microgrooved TiO2 — •Astrid Weidt[1,2], Mareike Zink[1], and Stefan G. Mayr[2,3] — [1]Junior Research Group Biotechnology and Biomedicine, Peter-Debye-Institute for Soft Matter Physics, Leipzig University, Germany — [2]Leibniz Institute of Surface Engineering (IOM) e.V., Leipzig, Germany — [3]Division of Surface Physics, Leipzig University, Germany

The choice of suitable nano- and microstructures of biomaterials is crucial for successful implant integration within the body. In particular, surface characteristics affect the adsorption of various extra cellular matrix proteins. This work illustrates the interaction of protein adsorption and early cell adhesion on bulk microstructured titanium surfaces with parallel grooves of 27 to 35 micron widths and 15 to 19 micron depths, respectively. In contact with low concentrations of fibronectin solutions, distinct adsorption patterns are observed on the edges of the ridges. Moreover, NIH/3T3 fibroblasts cultured in serum-free medium for 1 h, 3 h and 1 d show enhanced early cell adhesion on fibronectin coated samples compared to uncoated ones. In fact, early adhesion and cell contacts occur mainly on the groove edges where fibronectin adsorption was preferentially detected. Such adsorption patterns also support cellular contact guidance on short time scales which is hardly seen for uncoated samples. Thus, surface structures can promote directed adsorption of low concentrated fibronectin which facilitates early cell adhesion. These results may give rise to new developments in surface engineering of biomedical implants for improved osseointegration.

BP 3.3 *(107)* Mon 10:00 H 2013

Mechanics and Dynamics of Dictyostelium discoideum Adhesion — •Nadine Kamprad[1,2], Christian Westendorf[1], Albert Bae[1], Lyova Mamoyan[2], and Marco Tarantola[1] — [1]Max-Planck-Institut for Dynamic and Self-Organization, Göttingen, Germany — [2]University of Göttingen, Germany

Motile cells exert traction on the substratum in order to extend anterior pseudopodia and retract the rear. While the cytoskeleton generates protrusive and contractile forces, interaction of the ventral cell surface with the underlying support is necessary for force transmission. Here we focus on substrate adhesion of Dictyostelium discoideum (D.d), an integrin-free cellular model system. The amoeba adheres to substrates using actin foci; the latter are actin-rich areas, believed to be involved in non-specific adhesion processes. We perform co-localization studies of actin and known adhesion mediators like Talin, SCAR, Arp2/3 and the D.d. specific transmembrane adhesion protein Sad A. Coincidence is assessed using Total Internal Reflection Fluorescence Microscopy of single cells in an early developmental stage with considerably reduced motility. Current opposing hypotheses view actin foci as byproducts of endocytosis and not as adhesive areas. Thus, we examine colocalization of a protein coating endocytotic vesicles, Clathrin, to discern endocytosis from adhesion. In addition, we study cell lines with impaired adhesion based on knock out approaches for the aforementioned proteins and assess their influence on contact area morphology and adhesion forces.

BP 3.4 *(118)* Mon 10:15 H 2013

Confinement and topography control 3D motility of crawling cells — •Benjamin Winkler[1], Igor S. Aranson[2,3], and Falko Ziebert[1,4] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany — [2]Department of Biomedical Engineering, Pennsylvania State University, University Park, USA — [3]Materials Science Division, Argonne National Laboratory, USA — [4]Institute for Theoretical Physics, Ruprecht-Karls-University Heidelberg, Germany

The natural environment of motile cells are heterogeneously-shaped, three-dimensional geometries, often inducing also strong confinement effects. In turn, it is of great importance to model the role substrate topography and confinement play in cellular movement. We have developed a three-dimensional computational model, based on the so-called phase field approach, to study lamellipodium-driven crawling cells in arbitrarily shaped surroundings. We then studied several well-defined scenarios, such as a systematic variation of substrate curvature (from cells on thin fibers to the movement inside a capillary), vertical confinement between two plates, as well as topographically structured substrates. The derived, purely physical, guiding principles for motile cells should help discerning effects from truly specific biochemical cues and/or regulatory activity from the cell itself.

BP 3.5 *(143)* Mon 10:30 H 2013

Bacterial adhesion under flow condition — •Johannes Mischo[1], Friederike Nolle[1], Christian Spengler[1], Nicolas Thewes[1], Markus Bischoff[2], and Karin Jacobs[1] — [1]Department of Experimental Physics, Saarland University, Saarbruecken — [2]Institute for Medical Microbiology and Hygiene, Saarland University, Homburg/Saar

Bacterial biofilm formation reduces the effect of antibiotics, which is one of the main reasons for the mandatory removal of infected implants from the body. Therefore, the prevention of biofilm formation or material specifications that result in the death of adhering bacteria without harming somatic cells is considered key in medical implant development. Our flow chamber experiments, as a first step towards *in vivo* situations, aim at characterizing bacterial adhesion and viability of *S. aureus* on silicon surfaces. While surface chemistry and subsurface composition of the silicon surfaces are consistent, bacterial adhesion rate and viability on nano-rough silicon can be ascribed to geometry constraints, as changes in the adhesion strength due to a variation of the long-range van der Waals force can be neglected. Comparing adhesion rate and viability on hydrophobic and hydrophilic substrates of identical roughness reveals the influence of short-range, e.g. hydrophobic, forces. The data obtained from our flow chamber measurements can be compared to our single cell force spectroscopy data on the same surfaces.

BP 3.6 *(144)* Mon 10:45 H 2013

Patterning of adhesion mediated by binders of multiple types — •Josip Vlajčević[1] and Ana-Sunčana Smith[1,2] — [1]Rudjer Bošković Institute, Division of Physical Chemistry, Zagreb — [2]PULS Group, Institut für Theoretische Physik, Univesität Erlangen-Nürnberg

Cellular adhesion is mediated by binding of multiple proteins of different lengths, flexibilities and binding affinities. However, in most modelling efforts so far, only one type of molecular binding has been considered. These studies showed that the membrane, which in the absence of specific molecular forces resides in a non-specific potential,

deforms upon molecular complexation. This in turn introduces cooperative effects that promote further binding.

Building on a coarse grained Monte Carlo framework that quantitatively captures the dynamics of adhesion mediated by a single type of ligand-receptor pairs, we study a complete phase behaviour and the dynamics in the system containing two types of molecular binders which differ in molecular flexibilities, lengths, binding energies and densities.

By including ligand-receptor pairs and flexible polymers that can crosslink both adherent interfaces, we can capture the behaviour observed in experiments with artificially produced DNA-oligomers or the adhesion of T-lymphocyte cells induced by binding of TCR to pMHC and LFA-1 to ICAM-1 proteins during the formation of the immune synapse.

15 min. break

Invited Talk BP 3.7 *(9)* Mon 11:15 H 2013

Morphology control by active fluid flows — •Karen Alim — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Fluid flows can induce long-ranged interactions and propagate information on large scales. Especially during the development of an organism, coordination on large scales in short time is essential. What are the principal mechanisms of how fluid flows induce, transmit and respond to biological signals and thus control morphology? The role of fluid flows in patterning and morphing is particularly prominent during the growth and adaptation of transport networks like vascular networks. Here, the network-forming slime mould *Physarum polycephalum* emerged as a model to study the complex dynamics of transport networks. Investigating the pivotal role of fluid flows in this live transport network we find that flows are patterned in a peristaltic wave across the network thereby optimising transport. In fact, flows are hijacked by signals to propagate throughout the network promoting their own transport by invoking a propagating front of increased flow. These simple non-linear dynamics are sufficient to explain surprisingly complex dynamics of the network-like organism as adapting into the shortest path through a maze.

BP 3.8 *(163)* Mon 11:45 H 2013

Stochastic Dynamics of Cell Migration in Complex Environments — •David B. Brückner[1], Alexandra Fink[2], Christoph Schreiber[2], Peter J. F. Röttgermann[2], Joachim O. Rädler[2], and Chase P. Broedersz[1] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, München — [2]Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-Universität, München

The migration of cells is crucial in a variety of biological processes, including development, homeostasis, and cancer. In all these cases, cells migrate in complex and confined environments. To elucidate the physics of such confined migration in a standardised manner, we study cancer cells (MDA-MB-231) migrating on dumbbell-shaped micropatterns consisting of two square adhesion sites connected by a thin guidance cue. We observe that these cells stochastically migrate back and forth between the adhesion sites. We reconstruct equations of motion directly from the experimentally determined short time-scale dynamics, allowing us to decompose the migration into deterministic and stochastic contributions. This equation of motion captures the full dynamics of the confined cell and accurately predicts the long time-scale transitions between the sites. Our findings unveil the non-linear dynamics that governs cell migration in such environments. This approach could provide a basis for the understanding of the microscopic processes driving cell migration as well as the collective dynamics of many cells.

BP 3.9 *(326)* Mon 12:00 H 2013

Time-Resolved Force Spectroscopy of Flagella-Surface Contacts — •Anni Röse, Christian Titus Kreis, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, D-37077 Göttingen, Germany

Cellular appendages such as cilia and flagella are important tools for microbes to sense their environment, to propel themselves and also for mediating cell adhesion to surfaces. Despite the fact that the flagella axoneme represents a universal building block in cell biology, the biological mechanisms and characteristics of flagella mediated adhesion remains elusive so far. Recently, we discovered that *Chlamydomonas*, a unicellular biflagellated microalga, can actively switch the flagella adhesiveness on and off by light [1]. This rapid adaptation to environmental conditions within seconds distinguishes the adhesion mechanism of microalgae (eukaryotes) from bacteria (prokaryotes). In order to obtain a quantitative understanding of the characteristics of microalgal adhesion, we study flagella-substrate interactions by means of time-resolved in vivo force spectroscopy. Our micropipette-based force measurements allow us to correlate adhesion forces with optical images of flagella configuration during the rupture of the adhesive contact. These experiments indicate that each flagellum forms multiple adhesive contacts with the substrate. We identify the spatial distribution of the contacts on the flagella and also measure the strength of the individual contacts. These characteristic signatures of microalgal adhesion represent a remarkable difference compared to bacterial adhesion.

[1] Kreis et al., Nature Physics, 2017.

BP 3.10 *(359)* Mon 12:15 H 2013

Universal kinetics for the engagement of mechanosensing pathways in cell adhesion — •Samuel Bell and Eugene M. Terentjev — Cavendish Laboratory, 19 JJ Thomson Ave, Cambridge, CB3 0HE, United Kingdom

When plated onto a 2D substrate, cells will adhere and then spread, before becoming polarised. It is well known that cells plated onto surfaces with lower elastic moduli spread to a smaller final area than on stiffer surfaces. We studied the time of onset of spreading for two cell lines, endothelial cells (EA.hy927) and fibroblasts (NIH/3T3) onto a large range of substrates, and, remarkably, found that the dynamics of early spreading are the same over a wide range of stiffnesses (460Pa-30GPa). Instead, the dynamics were found to be greatly influenced by temperature. The long-time probability of onset displays an exponential activation, $P(t) \sim \exp(-kt)$ for both cell lines, with an Arrhenius-type rate constant $k \propto \exp(-G/k_BT)$. The energy barrier was found for both cell lines to be $G \approx 19$kcal/mol, and tallies with a recent study on the activation of focal adhesion kinase (FAK). Further to this, the short-time probability of having spread by time t follows a universal power law scaling, much as in nucleation theory, $Q(t) \propto t^5$. This is evidence for the onset of spreading being governed by the assembly of focal complexes with 5 major steps of building followed by FAK activation.

BP 3.11 *(116)* Mon 12:30 H 2013

Flow rate of transport network controls uniform metabolite supply to tissue — •Felix J. Meigel and Karen Alim — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Functioning of higher organisms depends on the continuous supply of metabolites to tissue and organs. What are the requirements on the transport network pervading the tissue to provide a uniform supply of metabolites? We consider the transport dynamics of metabolites in a vascular network of connected tubes. On a single tube level, we describe metabolite spread by diffusion and advection as well as absorption at the tube wall. Applying our theoretical model of metabolite supply to the example of xylem vasculature in leaves, we find that on the network level, the flow rate is the key factor for uniform supply. While at low inflow rate metabolites are already exhausted near the flow inlet, too high inflow flushes metabolites through the network. We identify a scaling law, predicting the optimal inflow rate providing uniform metabolite supply. We identify how overall change in network topology compensates sub-optimal inflow rates in numerical simulations.

BP 3.12 *(154)* Mon 12:45 H 2013

Collective cell migration in embryogenesis follows the laws of wetting — •Bernhard Wallmeyer[1], Sarah Trinschek[2], Sargon Yigit[1], Uwe Thiele[2], and Timo Betz[1] — [1]Institute of Cell Biology, ZMBE, Münster, Germany — [2]Institute for Theoretical Physics, Münster, Germany

Collective cell migration is a fundamental process during embryogenesis and its initial occurrence, called epiboly, is an excellent *in vivo* model to study the physical processes involved in collective cell movements that are key to understand organ formation, cancer invasion and wound healing. In zebrafish, epiboly starts with a cluster of cells at one pole of the spherical embryo. These cells are actively spreading in a continuous movement towards its other pole until they fully cover the yolk. Inspired by the physics of wetting we determine the contact angle between the cells and the yolk during epiboly. Similar to the case of a liquid drop on a surface one observes three interfaces that carry me-

chanical tension. Assuming that interfacial force balance holds during the quasi-static spreading process, we employ the physics of wetting to predict the temporal change of the contact angle. While the experimental values vary dramatically, the model allows us to rescale all measured contact angle dynamics onto a single master curve explaining the collective cell movement. Thus, we describe the fundamental and complex developmental mechanism at the onset of embryogenesis by only three main parameters: the offset tension strength α, the tension ratio δ and the rate of tension variation λ.

BP 4: Active Matter DY I (joint session DY/CPP/BP)

Time: Monday 10:00–13:15 Location: BH-N 243

See DY 8 for details of this session.

BP 5: Systems Biology & Gene Expression and Signalling

Time: Monday 15:00–16:45 Location: H 1028

BP 5.1 *(435)* Mon 15:00 H 1028

Mathematical modeling of drug-induced receptor internalization in breast cancer cells — •Mirjam Fehling-Kaschek[1], Diana Peckys[2], Jens Timmer[1], and Niels de Jonge[3] — [1]University of Freiburg — [2]Department of Biophysics, Saarland University — [3]Leibniz Institute for New Materials, Saarbrücken

About 20% of breast cancer tumors over-express the HER2 receptor. Trastuzumab, an approved drug to treat this type of breast cancer, is an antibody directly binding at the HER2 receptor and inhibiting cell growth. The goal of our study was to understand the early impact of trastuzumab on HER2 internalization and recycling in the HER2-positive SKBR3 cell line. To this end, single cell fluorescence microscopy, monitoring the state of HER2 expression on the membrane, was combined with mathematical modeling to derive the flux of HER2 receptors from and to the membrane. We constructed a dynamic multi-compartment model based on ordinary differential equations to account for intracellular HER2 production and distribution of HER2 receptors between membrane ruffles and flat regions of the cell by internalization and recycling processes. To account for the heterogeneity in cell size and HER2 expression in SKBR3 cells, the dynamic model was expanded to a mixture model. The model describes the experimental observation that drug induced receptor internalization occurs preferentially in cells containing membrane ruffles, while internalization in non-ruffled cells happens at a much smaller rate. Our analysis shows that the common hypothesis of constitutive HER2 recycling back to the plasma membrane is not supported by the data.

BP 5.2 *(377)* Mon 15:15 H 1028

Effect of ultra small carbon nanodots on the gene expression of primary human hematopoietic stem cells — Stefan Fasbender[1], Lisa Zimmermann[1], Ron-Patrick Cadeddu[2], Rainer Haas[2], and •Thomas Heinzel[1] — [1]Experimental Condensed Matter Physics, Heinrich-Heine-University Dusseldorf — [2]Department of Haematology, Oncology and Clinical Immunology, University Hospital Dusseldorf

Carbon nanodots (CDs) are often considered as nontoxic alternative to inorganic quantum dots. They show potential in a wide range of biomedical applications like long term imaging of normal and malignant cells in vivo and in vitro, cancer diagnostics and therapeutic tumor cell targeting. Here we prepare fluorescent CDs by thermal decomposition of citric acid and diethylentriamine [1] using microwave irradiation. Primary human hematopoietic stem cells (CD34+) obtained from the leukapheresis products of four healthy donors are exposed to a concentration of 500 ug/ml CDs for 36 hours. Via flow cytometry we demonstrate a significant uptake of the particles into the cells and the effect on the gene expression is studied using the Clariom S microarray.

[1] Qu et al., Light: Science & Applications, 2015, 4, e364

BP 5.3 *(232)* Mon 15:30 H 1028

Computational analysis on the regulation of σ/anti-σ factor operons — •Hao Wu and Georg Fritz — LOEWE Center for Synthetic Microbiology, Phlipps University Marburg, Germany

Bacterial alternative σ factors are subunits of RNA polymerase that determine its promoter specificity, thereby regulating crucial processes like cell homeostasis and stress responses. In the absence of input signals, σ factors are sequestered by their cognate anti-σ factors. Meanwhile, many σ/anti-σ factor pairs are co-expressed in operons, most of them are auto-regulated by the σ factor, implying a regulation module with a positive and a negative feedback at the same time. Strikingly, there are two distinct mechanisms to activate this module: One involves the active degradation of anti-σ factors upon input signal detection, constituting a non-equilibrium sensing mechanism, while the other one relies on a reversible conformational change of the anti-σ factor to a non-functional form, resembling an equilibrium sensing mechanism. Here we conducted a comprehensive computational study on the quantitative properties of this important regulatory module. While many characteristics prove independent of the sensing mechanism, we identified some major differences between their dynamical properties. Interestingly, in the responsive regime the activation of σ factor level becomes very slow for the non-equilibrium sensing mechanism, while it remains fast for the equilibrium sensing mechanism. These results deepen our understanding of the σ/anti-σ factor regulation module and help us to explain the choice of the two distinct sensing mechanisms in different physiological contexts.

BP 5.4 *(108)* Mon 15:45 H 1028

Self-organised homeostasis of stem cells through competition for mitogens — Yu Kitadate[1,2], •David J. Jörg[3,4], Benjamin D. Simons[3,4,5], and Shosei Yoshida[1,2] — [1]Division of Germ Cell Biology, National Institute for Basic Biology, National Institutes of Natural Sciences, Okazaki, Japan — [2]Department of Basic Biology, School of Life Science, Graduate University for Advanced Studies (Sokendai), Okazaki, Japan — [3]Cavendish Laboratory, Department of Physics, University of Cambridge, United Kingdom — [4]The Wellcome Trust/Cancer Research UK Gurdon Institute, University of Cambridge, UK — [5]The Wellcome Trust/Medical Research Council Stem Cell Institute, University of Cambridge, UK

How stem cell populations self-organise to control their density and maintain robust homeostasis is in many cases still elusive. Especially challenging to understand are facultative niche environments, in which stem cells lie dispersed among their progeny and only sporadically make contact with signal-releasing regions. How do such stem cells sense and control their density over large distances? We conjecture that stem cells compete for a limited supply of mitogens: by adjusting their fate behaviour according to the local mitogen abundance, a constant cell density is maintained throughout the tissue. Using the murine germ line as an example, we developed a theoretical model that quantitatively captures both the key features of stem cell density regulation and the regeneration kinetics after injury. This "mitogen competition model" provides a generic and robust mechanism of self-organised stem cell homeostasis in a facultative niche.

BP 5.5 *(368)* Mon 16:00 H 1028

Proliferation rate inference with continuous labelling assays — Rode Julian[1], Brusch Lutz[1], and •Rost Fabian[1,2] — [1]Technische Universität Dresden, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Precise estimates of proliferation rates are crucial for quantitative models of the development and maintenance of tissues. Continuous labelling assays are a popular approach to infer proliferation rates *in vivo*. In these assays, proliferating cells take up a label, e.g. BrdU, when synthesizing DNA for cell division. Intuitively, more cells take up the label per time if they proliferate faster. So far, the experimental and theoretical study of continuous labelling assays focused on the dynamics of the mean labelling-fraction but not on the labelling-fraction distribution dynamics. To study this distribution dynamics, we developed a stochastic model of continuous labelling assays. With the

model, we study the effects of cell and sample level noise in the distribution of cell cycle lengths. Using simulated data as ground truth, we show that current inference methods give biased proliferation rate estimates. Therefore, we derive analytical results for the Likelihood for our model that can be used to achieve unbiased estimates of the proliferation rates *in vivo*.

Invited Talk BP 5.6 *(19)* Mon 16:15 H 1028

Synchronization of synthetic gene oscillators — •Lev Tsimring — BioCircuits Institute, University of California, San Diego

One of the defining characteristics of life is the ability to keep time, which organisms often achieve by using internal genetic "clocks" to govern fundamental cellular behavior. While the gene networks that produce oscillatory expression signals are typically quite elaborate, certain recurring network motifs are often found at the core of these biological clocks. One common motif which leads to oscillations in many natural biological clocks is delayed auto-repression. We designed and constructed several synthetic gene circuits that use this motif, and observed robust "degrade-and-fire" oscillations of gene expression in bacteria E. coli. When gene oscillators in different cells are coupled by fast-diffusing chemical signals, they exhibit population-wide synchronization. We also predicted and observed intra-cellular synchronization of different gene oscillators indirectly coupled by a common degradation enzyme.

BP 6: Cytoskeletal Filaments I

Time: Monday 15:00–17:30 Location: H 1058

BP 6.1 *(288)* Mon 15:00 H 1058

Glassy Dynamics in Composite Biopolymer Networks — •Tom Golde[1], Constantin Huster[1], Martin Glaser[1,2], Tina Händler[1,2], Harald Herrmann[3,4], Josef A. Käs[1], and Jörg Schnauss[1,2] — [1]University of Leipzig, Leipzig, Germany — [2]Fraunhofer IZI, Leipzig, Germany — [3]German Cancer Research Center, Heidelberg, Germany — [4]University Hospital Erlangen, Erlangen, Germany

The cytoskeleton is a highly interconnected meshwork of strongly coupled filament systems providing mechanical stability as well as dynamic functions to cells. To elucidate the underlying biophysical principles it is central to investigate not only one distinct functional subsystem but rather their interplay as composite biopolymer structures. Here, we show that composite networks of actin and vimentin filaments can be fully described by a superposition of two non-interacting scaffolds. We demonstrate arising effects in a scale-spanning frame connecting single filament dynamics to macro-rheological network properties and show that linear and non-linear bulk mechanics of actin and vimentin filament networks are captured within the glassy wormlike chain model. Our findings clearly disagree with previous studies reporting emergent effects in these composite networks. These new insights pave the way to deterministically predict the mechanics of the cytoskeleton in distinct cell types based on the properties of its single structural components.[1]

[1] Golde et al., Submitted

BP 6.2 *(31)* Mon 15:15 H 1058

The mitotic spindle is chiral due to torques generated by motor proteins — •Maja Novak[1], Bruno Polak[2], Juraj Simunic[2], Zvonimir Boban[1], Andreas W. Thomae[3], Iva M. Tolic[2], and Nenad Pavin[1] — [1]Faculty of Science, University of Zagreb, Zagreb, Croatia — [2]Rudjer Boskovic Institute, Zagreb, Croatia — [3]University of Munich, Munich, Germany

Mitosis relies on forces generated in the spindle, a micro-machine composed of microtubules and associated proteins. Forces are required for the congression of chromosomes to the metaphase plate and their separation in anaphase. However, torques may also exist in the spindle, yet they have not been investigated. Here we show that the spindle is chiral. Chirality is evident from the finding that microtubule bundles follow a left-handed helical path, which cannot be explained by forces but rather by torques acting in the bundles. STED super-resolution and confocal microscopy of human spindles revealed that the average helicity of the bundles with respect to the spindle axis is about -2°/μm. Inactivation of kinesin-5 (Kif11/Eg5) abolished the chirality of the spindle. We introduce a theoretical model, which predicts that torques generate curved shapes of bundles, where the twisting component of the torque is required for the helical component of the shape. By comparing the model with experiments, we find that the twisting moment is roughly -10 pNμm. We conclude that torques generated by motor proteins, in addition to forces, exist in the spindle and determine its architecture.

Reference: bioRxiv 167437, https://doi.org/10.1101/167437

BP 6.3 *(146)* Mon 15:30 H 1058

Metaphase kinetochore movements are regulated by kinesin-8 motors and microtubule dynamic instability — •Agneza Bosilj[1], Anna Klemm[2], Iva Tolic[2,3], and Nenad Pavin[1] — [1]Department of Physics, Faculty of Science, University of Zagreb, Bijenicka cesta 32, 10000 Zagreb, Croatia — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany — [3]Division of Molecular Biology, Ruder Boskovic Institute, Bijenicka cesta 54, 10000 Zagreb, Croatia

During metaphase, sister chromatids are connected to microtubules (MTs) extending from the opposite spindle poles via kinetochores, protein complexes on the chromosome. Kinetochores congress to the equatorial plane of the spindle and oscillate around it, with kinesin-8 motors restricting these movements. Yet, the physical mechanism underlying kinetochore movements is unclear. We show that kinetochore movements in the fission yeast Schizosaccharomyces pombe are regulated by kinesin-8-promoted MT catastrophe, force-induced rescue and MT dynamic instability. A candidate screen showed that only kinesin-8 motors Klp5/Klp6 are required for kinetochore centering. Our theoretical model with Langevin description of MT dynamic instability shows that kinesin-8 motors are required for kinetochore centering, whereas sensitivity of rescue to force is necessary for the generation of oscillations. We found that irregular kinetochore movements occur for a broader range of parameters than regular oscillations. Thus, our work shows how regulation of MT dynamic instability contributes to kinetochore congression and the accompanying oscillations.

Invited Talk BP 6.4 *(5)* Mon 15:45 H 1058

Broken detailed balance in active biopolymer assemblies — •Chase Broedersz — Ludwig-Maximilians-Universitaet München, Munich, Germany.

We present a non-invasive approach to identify and quantify non-equilibrium dynamics in living systems based on broken detailed balance. With this approach, we study the dynamics of beating flagella, primary cilia, and cytoskeletal networks. In particular, we use stochastic time traces of the system's dynamics to infer the probability currents in a phase space of the mesoscopic configurational coordinates of a biological assembly. In addition, we will present a more general theoretical framework to investigate what information about the system's non-equilibrium state can be extracted from such phase space currents. For example, we will discuss how to extract the entropy production rate - a measure of the dissipated power in a driven system - from measured current cycles. Next, we present predictions for the scaling behavior of the entropy production rate with the distance between measurement points in the system. Our results provide insight in to how internal driving by enzymatic activity generates non-equilibrium dynamics on different scales in a variety of biological systems, including biopolymers and their assemblies.

BP 6.5 *(29)* Mon 16:15 H 1058

Stress-Strain Behavior of Vimentin Intermediate Filaments — Johanna Block[1], Hannes Witt[2], Andreas Janshoff[2], Sarah Köster[1], and •Anna Schepers[1] — [1]Institute for X-Ray Physics, University of Goettingen, 37077 Göttingen, Germany — [2]Institute of Physical Chemistry, University of Goettingen, 37077 Göttingen, Germany

It is widely accepted that the cytoskeleton, which is composed of three filamentous protein structures - microfilaments (MFs), microtubules (MTs) and intermediate filaments (IFs) - plays a major role for cell mechanics. Whereas MFs and MTs are conserved between cell types, at least 70 different genes in humans code for IFs, which are expressed in a cell type specific manner. So far, it was not possible to infer the

mechanical properties found on length scales of protein superstructure, cells and beyond, from the peculiar molecular architecture of IFs. Using optical tweezers, combined with microfluidics and fluorescence microscopy, we directly probed the stress-strain behavior of single vimentin IFs under physiological buffer conditions in a highly controlled fashion. We found a strong loading-rate dependent behavior, indicating that vimentin IFs act as a "safety belt" for cells. Further, our results provide evidence that single vimentin IFs act as an intracellular shock absorber using a balance of classical energy dissipation and storage of potential energy. By theoretical modelling and Monte Carlo simulations we are able to directly attribute filament mechanics to a molecular mechanism and reveal an intriguing non-equilibrium phenomenon leading to pronounced energy dissipation and mechanical adaption.

BP 6.6 *(177)* Mon 16:30 H 1058

Actin dynamics deform membrane in and out mimicking filopodia and endocytosis — •Camille Simon[1], Remy Kusters[1], Valentina Caorsi[1], Jean-François Joanny[2], Clément Campillo[3], Julie Plastino[1], Pierre Sens[1], and Cécile Sykes[1] — [1]Institut Curie, Paris, France — [2]ESPCI, Paris, France — [3]Université Evry Val d'Essonne, Evry, France

The cell membrane is able to deform inward, as in endocytosis intitiation, or outward, as in filopodia formation. Interestingly, both deformations are generated by the same branched, Arp2/3-based, polymerizing actin network. How an inward or an outward deformation can result from the same network structure? What are the physical parameters that will trigger the direction of membrane deformation? To address these questions, we use a reconstituted membrane system of liposomes and purified actin. A dynamic branched actin network is generated at the liposome surface. We investigate the conditions under which the actin cytoskeleton induces inward or outward membrane deformations. We reveal that actin dynamics is the sole player of membrane deformations by photo-damaging the actin structure that relaxes membrane shape. Lowering membrane tension is key to produce filopodia-like structures. Oppositely, endocytic-like structures are robust features that only weakly depend on membrane tension. A pulse-chase two color actin experiment reveals the details of network growth during inward or outward membrane deformation. Our results, supported by theoretical models, explain how such deformations depend on a mechanical balance between the membrane and the actin network.

BP 6.7 *(167)* Mon 16:45 H 1058

Dynactin stabilises microtubules to establish their uniform orientation in neuronal axons — •Maximilian Jakobs and Kristian Franze — Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

The microtubule (MT) cytoskeleton in neuronal axons is highly oriented with almost all MTs pointing with their growing end (+end) away from the cell body (+end out). Motor proteins rely on this orientation to move cellular cargo to the distal regions of the axon. Despite 30 years of research, the mechanism that establishes MT orientation remains unknown. We here analysed MT growth with supervised machine learning in *D. melanogaster* neurons, complemented by an analytical model of MT growth. We found that +end out MTs grow for longer times than oppositely oriented MTs (−end out). According to our model, this leads to dramatic differences in average MT lengths, so that −end out MTs are short and unstable. Additionally, we found evidence that dynactin is responsible for the differences in growth times by promoting growth at the axonal tip through a molecular gradient. These findings suggest a simple mechanism that organises axonal MTs. First, +end out MTs are stabilized by distally located dynactin. Subsequently, the short −end out MTs depolymerize or reorient, leaving only +end out MTs in the axon. Our results pave the way towards a deeper understanding of how the cytoskeleton in neurons orients to support molecular transport, potentially shedding light on pathologies that are characterized by axonal transport deficiencies such as Alzheimers disease.

BP 6.8 *(382)* Mon 17:00 H 1058

A field-theoretic approach to microtubule growth — •Johannes Pausch and Gunnar Pruessner — Department of Mathematics, Imperial College London, United Kingdom

Microtubule filaments are a major part of the cytoskeleton. They influence the shape and movement of the cell and are used for transport processes inside the cell. Microtubules grow and shrink by polymerising and depolymerising, that is by absorbing and emitting tubulin which diffusively spread in the cytoplasm. Here, we model the stochastic process of microtubule growth as a field theory.

In our model, we recover the classic diffusion and diffusion-convection results. Furthermore, we are able to model the tubulin-absorption-induced spatially discrete growth of the microtubule filament and find analytic real space results for expected assembly speed and variance. Our approach produces analytic expressions in Fourier space that require a short-length scale cutoff in two dimensions and above. It is particularly flexible to incorporate more complex interactions between microtubules and tubulin. In one dimension, our results are easily compared to corresponding results using probabilistic techniques.

BP 6.9 *(30)* Mon 17:15 H 1058

Investigations on the cell morphology of oral mucosa cancer and non-cancer cells — •Nina Bartels[1], Maja Strugacevac[1], Constanze Wiek[2], Julia Kristin[2], Marcel Glaas[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Heinrich-Heine-Universität Düsseldorf, Institute of Applied Physics, Universitätsstr. 1, 40225 Düsseldorf, Germany — [2]Düsseldorf University Hospital, Department of Othorinolaringology, Moorenstrasse 5, 40225 Düsseldorf, Germany

In order to develop new cell-selective treatment strategies for head and neck squamous cell carcinoma, our group is investigating the differences of the cell morphology and physical properties of different oral cancer cells and oral keratinocytes. The cell lines originate from different locations of the oral mucosa and are investigated using a fluorescence microscope.

To obtain more information about cell morphology, the cells were stained using CellMask Green (cell membrane) and Hoechst (cell nuclei) staining kits. By the confocal laser-scanning microscope three-dimensional images of the cells were made to compare the different cell lines in size, volume and shape.

A staining kit for active mitochondria (MitoTracker) enables us to compare the aerobic metabolism of tumor and non-cancer cells to verify the Warburg hypothesis. Additionally, actin filaments and microtubules were stained to observe differences in the cytoskeleton which is specific for cell elasticity. This contribution will show and discuss our latest results.

BP 7: Focus Session: Statistical Physics-Based Methods in Molecular Evolution - organized by Alexander Schug and Martin Weigt (joint session BP/DY)

Time: Monday 15:00–17:00 Location: H 2013

Invited Talk BP 7.1 *(21)* Mon 15:00 H 2013

Evolution of quantitative traits and non-equilibrium matrix ensembles — Simone Pompei, Torsten Held, and •Michael Lässig — Institute for Theoretical Physics, University of Cologne

Evolution affects molecular quantitative phenotypes, such as stability, binding affinities, and metabolic activities of cellular proteins. Linking sequence data to phenotypic and functional changes remains a critical gap in our understanding of evolutionary processes. In this talk, we present new methods to infer *a priori* unknown quantitative phenotypes from their correlation signature in time-resolved sequence data, using non-equilibrium statistical mechanics and random matrix theory. We use these methods to map the phenotypic evolution of the human influenza virus.

BP 7.2 *(300)* Mon 15:30 H 2013

Big Data in Structural Biology: Predicting Protein and RNA Structures by inferring residue co-evolution — •Alexander Schug — John von Neumann Institute for Computing, Jülich Supercomputer Centre, Forschungszentrum Jülich

To gain any detailed understanding of biomolecular function, one needs to know their structure. The structural characterization of many important biomolecules and their complexes remains experimentally challenging. Novel statistical tools based on statistical physics such as Direct Coupling Analysis (DCA) take advantage of the explosive growth of sequential databases and trace residue co-evolution to infer secondary and tertiary contacts for proteins [1] and RNAs [2]. These contacts can be exploited as spatial constraints in structure prediction methods leading to excellent quality predictions [1,2,3]. Going beyond anecdotal cases of a few protein families, we have applied our methods to a systematic large-scale study of nearly 2000 PFAM protein families of homo-oligomeric proteins [4]. Also, we can apply DCA to infer mutational landscapes by capturing epistatic couplings between residues and can assess the dependence of mutational effects on the sequence context where they appear [5].

[1] Weigt M et al., PNAS (2009); F. Morcos et al., PNAS (2011)
[2] E. De Leonardis et al., NAR (2015)
[3] Schug A et al., PNAS (2009); Dago A et al., PNAS (2012)
[4] G. Uguzzoni et al., PNAS (2017)
[5] M. Figliuzzi et al., MBE (2016)

BP 7.3 *(87)* Mon 15:45 H 2013

Coevolution based inference of allosteric architectures — •Barbara Bravi[1], Carolina Brito[2], Riccardo Ravasio[1], and Matthieu Wyart[1] — [1]Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland — [2]Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil

We analyze maximum entropy approaches to infer the functional design of elastic materials exhibiting allostery, i.e. the property of highly specific responses to ligand binding at a distant active site. To guide and inform protocols of de novo drug design, it is fundamental to understand what architectures underlie such a transmission of information and whether their features can be predicted from sequence data alone. We consider the functional designs of in silico evolved allosteric architectures which propagate efficiently energy (including shear, hinge, twist) or strain (resulting in a less-constrained trumpet-shaped region between the allosteric and the active site). We show that maximum entropy approaches, built to capture statistical properties such as conservation and correlations, can provide predictive information on the cost of single and double mutations while their performance at reproducing the original allosteric fitness is strongly design-dependent. We benchmark existing maximum entropy inference methods on these computationally evolved functional architectures and we propose an improved framework accounting for a multiplicity of co-evolutionary factors which is aimed at disentagling allostery-based correlations from extrinsic ones.

BP 7.4 *(117)* Mon 16:00 H 2013

Architecture of allosteric materials — Carolina Brito[1], Solange Flatt[2], •Riccardo Ravasio[2], Matthieu Wyart[2], and Le Yan[3] — [1]Universidad Federal do Rio Grande do Sul, CP 15051, 91501-970 Porto Alegre RS, Brazil — [2]Ecole Polytechnique Federale de Lausanne, CH-1015, Lausanne, Switzerland — [3]Kavli Institute for Theoretical Physics, Santa Barbara, CA 93106, USA

Allosteric proteins transmit a mechanical signal induced by binding a ligand. However, understanding the nature of the information transmitted and the architectures optimising such transmission remains a challenge. We show using an in-silico evolution scheme and theoretical arguments that architectures optimised to be cooperative, which propagate efficiently energy, qualitatively differ from previously investigated materials optimised to propagate strain. Although we observe a large diversity of functioning cooperative architectures — including shear, hinge and twist designs, they all obey the same principle of nearly displaying a mechanism, i.e. an extended zero mode with a predicted optimal frequency. Overall, our approach leads to a natural explanation for several observations in allosteric proteins, and suggests a path to discover new ones. On this line, we study the extended soft modes of hessians defined from 46 couples of proteins for which the active and inactive structures are available and compare them with the aforementioned principle. Moreover, the set of architectures that are evolved through the in-silico scheme defines a well controlled ground where to benchmark the results of co-evolutionary methods, usually applied to protein sequences.

BP 7.5 *(304)* Mon 16:15 H 2013

Direct Coupling Analysis on the genome scale — •Erik Aurel — Royal Institute of Technology in Stockholm, Sweden

Direct Coupling Analysis (DCA) is a powerful tool to find pair-wise dependencies in large biological data sets. It amounts to inferring coefficients in a probabilistic model in an exponential family, and then using the largest such inferred coefficients as predictors for the dependencies of interest. A main success story has been predicting spatially proximate residues in protein structures from sequence data.

From a population genetics point of view DCA should be viewed as inferring epistasis, synergistic effects on fitness, from samples. I will discuss applications of DCA to the genome scale in bacteria and how that allows to find unexpected (and expected) dependencies between genes in trans i.e. that are not close on the genome.

This is joint work with many people, most recently with Chen-Yi Gao and Hai-Jun Zhou, available as arXiv:1710.04819.

BP 7.6 *(441)* Mon 16:30 H 2013

Interprotein coevolution: bridging scales from residues to genomes — Giancarlo Croce[1], Thomas Gueudre[2], Hendrik Szurmant[3], Matteo Figliuzzi[1], and •Martin Weigt[1] — [1]Université Pierre & Marie Curie, Sorbonne Université, Paris, France — [2]Human Genetics Foundation, Turin, Italy — [3]Western University of Health Sciences, Los Angeles, USA

Interacting proteins coevolve at multiple but interconnected scales, from the residue-residue over the protein-protein up to the family-family level. The recent accumulation of enormous amounts of sequence data allows for the development of novel, data-driven computational approaches. Notably, these approaches can bridge scales within a single statistical framework [1,2], which is built upon idea from the inverse statistical physics [3,4]. While being currently applied mostly to isolated problems on single scales, their immense potential for an evolutionary informed, structural systems biology is steadily emerging.

[1] H. Szurmant and M. Weigt, Current Opinion in Structural Biology 50, 26-32 (2017).

[2] G. Croce, T. Gueudre, MV Ruiz Cuevas, H. Szurmant, M. Figliuzzi, M. Weigt, submitted (2017).

[3] S. Cocco, C. Feinauer, M. Figliuzzi, R. Monasson, M. Weigt, Rep. Prog. Phys. (2017), https://doi.org/10.1088/1361-6633/aa9965.

[4] H. Chau Nguyen, Riccardo Zecchina, Johannes Berg, Advances in Physics, 66 (3), 197-261 (2017)

BP 7.7 *(324)* Mon 16:45 H 2013

The evolutionary consequences of population spread on curved surfaces — Daniel A. Beller[1], Kim M. J. Alards[2], Ricardo A. Mosna[3], Federico Toschi[2], and •Wolfram Möbius[4] — [1]Brown University, Providence, RI, USA — [2]TU Eindhoven, Eindhoven, The Netherlands — [3]Universidade Estadual de Campinas, Campinas, SP, Brazil — [4]University of Exeter, Exeter, United King-

dom

We investigate the evolutionary dynamics of populations growing and expanding on curved surfaces. Using a combination of individual-based simulations and theory we characterize the effect of individual features (cones and spherical caps) on the shape of the population front and the genetic composition of an expanding population. We find that, on sufficiently large scales, geodesics allow us to describe both population and evolutionary dynamics quantitatively. Using these findings, we characterize the consequences of large-scale surface roughness on genetic diversity and compare to the case of heterogeneous but flat environments.

BP 8: Active Matter DY II (joint session DY/BP/CPP)

Time: Monday 15:30–18:45 Location: BH-N 243

See DY 16 for details of this session.

BP 9: Postersession I

Topics: Protein Structure and Dynamics (9.1–9.10), Single Molecule Biophysics (9.11–9.20), Biomaterials and Biopolymers (9.21–9.36), Systems Biology & Gene Expression and Signalling (9.37–9.42).

Time: Monday 17:30–19:30 Location: Poster A

BP 9.1 *(37)* Mon 17:30 Poster A

Internal Dynamics of Unfolded Apo-myoglobin — •Livia Balacescu[1,3], Tobias Erich Schrader[1], Andreas Stadler[2], and Jörg Fitter[2,3] — [1]Jülich Centre for Neutron Science, Forschungszentrum Jülich GmbH, Outstation at MLZ, Garching, Germany — [2]Jülich Centre for Neutron Science JCNS & Institute for Complex Systems ICS, Forschungszentrum Jülich GmbH, Jülich, Germany — [3]1.Physikalisches Institut (IA), RWTH Aachen, Aachen, Germany

As a model for the well-characterized protein systems in different folding states we chose apo-myoglobin.[1,2,3] We investigated internal dynamics of its unfolded and folded form on a time-scale up to several hundred nanoseconds and in the nanometer length-scale using neutron spin echo spectroscopy (NSE) [4]. Aggregation state and center of mass diffusion were monitored in parallel with dynamic light scattering. Our first NSE data show a polymer like behavior of the unfolded protein. This indicates that the powerful polymer models may be used for characterization of protein systems.

[1] J. Phys. Chem. B, 2015, 119 (1), 72 [2] J Mol. Biol., 1996, 263(4), 531 [3] J. Am. Chem. Soc., 2014, 136 (19), 6987 [4] Richter D. et al., 2005, Neutron Spin Echo in Polymer Systems. Advances in Polymer Science, vol 174. Springer, Berlin, Heidelberg

BP 9.2 *(44)* Mon 17:30 Poster A

Performance of genetically encoded FRET-based biosensors investigated on single molecule level — •Henning Höfig[1,2], Martina Pohl[3], Julia Otten[3], Arnold Boersma[4], and Jörg Fitter[1,2] — [1]RWTH Aachen University, I. Physikalisches Institut (IA), AG Biophysik, Aachen, Germany — [2]Research Centre Juelich, ICS-5, Juelich, Germany — [3]Research Centre Juelich, IGB-1, Juelich, Germany — [4]University of Groningen, Department of Biochemistry, Groningen, Netherlands

Genetically encoded FRET-based biosensors consist of two fluorescent proteins (donor and acceptor) and a sensing domain. The readout of FRET-based biosensors usually utilizes the ratio of fluorescence emission intensities of the donor and the acceptor upon donor excitation. We carried out single-molecule measurements on a confocal microscope for two types of CFP-YFP biosensors, one sensitive to glucose concentration [1] and another one monitors macromolecular crowding [2]. From our measurements we obtained FRET efficiencies histograms dissecting the different subpopulations of the sensor under varying environmental conditions. In order to demonstrate the capability of utilizing transfer efficiency histograms for judging the performance of FRET-based sensor constructs we analyze various glucose sensor constructs. The obtained smFRET histograms display specific fingerprints of the respective sensor properties and provide a valuable basis for a rational design of FRET-based biosensors.

[1] R. Moussa et al., J. Biotechnol., 191, 250-259 (2014); [2] A. J. Boersma et al., Nat. Methods, 12, 227-229 (2015)

BP 9.3 *(113)* Mon 17:30 Poster A

Dielectric spectroscopy of bovine serum albumin at GHz frequencies — Eva-Maria Laux, Jessica Gibbons, Elena Ermilova, Frank F. Bier, and •Ralph Hölzel — Fraunhofer Institute for Cell Therapy and Immunology, Branch Bioanalytics and Bioprocesses, Potsdam, Germany

In recent years electronic components have become available reaching the upper GHz range. This makes this frequency range accessible for novel biomedical applications. Still, detailed knowledge about the properties of biological materials at these frequencies is missing, and the interaction mechanisms with such electromagnetic fields are often unclear. Here we present an experimental system based on a vector network analyser for the temperature controlled determination of the dielectric properties of biomolecules. The influence of protein concentration, of temperature and of denaturing agents on aqueous solutions of bovine serum albumin (BSA) is presented between 10 MHz and 110 GHz. Further work aims at reducing sample size and improving accuracy.

BP 9.4 *(207)* Mon 17:30 Poster A

Analysis of dynamics of membrane-protein microdomains in bacteria — Daniella Lucena[1,3], •Marco Mauri[1,2], Felix Schmidt[1,4], Bruno Eckhart[1,4], and Peter L. Graumann[1,3] — [1]SYNMIKRO, Marburg — [2]INRIA Grenoble, France — [3]Department of Chemistry, Philipps University, Marburg — [4]Department of Physics, Philipps University, Marburg

Cell membrane has a remarkably intricate temporal and spatial organization that is central for the maintenance of fundamental processes in bacteria. While early models often envisioned proteins freely and homogeneously diffusing on the membrane, there is nowadays growing evidence in support of lipid microdomains. To date there has been no broad study to evaluate how protein size, number of transmembrane domains, and temperature affect the diffusion of membrane proteins. In this work, we have undertaken a systematic study of the effects of these factors on membrane protein diffusion and investigate the dynamics of membrane organization in live B. subtilis cells by mean of single-molecule tracking, physical modelling and computer aided visualization methods. We found that diffusion coefficients do not correlate with protein molecular weight, but decrease with increased transmembrane radius. Moreover, diffusion coefficients are anomalous and are better described by discriminating diffusion rates into two protein populations. Also, we observed that temperature can influence the spatiotemporal organization of membrane proteins and significantly impact their dynamics. We think that data analysis methods here introduced can be valuable for membrane protein studies in any bacteria.

BP 9.5 *(257)* Mon 17:30 Poster A

Unraveling the effects of an oscillating electric field on Amyloid-beta (1-40) conformational dynamics using G-PCCA, a generalized Markov state modeling method — •Bernhard Reuter[1], Marcus Weber[2], and Martin E. Garcia[1] — [1]Theoretical Physics II, Institute of Physics, University of Kassel, Kassel, Germany — [2]Zuse Institute Berlin (ZIB), Berlin, Germany

We have studied the influence of a strong oscillating electric field on the Amyloid-beta (1-40) peptide, associated with Alzheimer disease. To this end we conducted extensive molecular dynamics (MD) simulations utilizing the GROMACS v5.1.2 program package. Typically Markov state models (MSMs) are very well suited for the identification and analysis of metastabilities and related kinetics. However, the state-of-the-art methods and tools require the fulfillment of a detailed balance condition, violated in the non-equilibrium case. To date, they

are unsuitable to deal with more general dominant data structures including cyclic processes, which are essentially associated with the effects of an oscillating electric field. Instead, for this purpose we utilized a generalization of the common robust Perron cluster cluster analysis (PCCA+) method, termed generalized Perron cluster cluster analysis (G-PCCA). Applying G-PCCA we identified and analyzed, by comparison to equilibrium simulations in the absence of an external electric field, significant non-thermal effects on the conformational dynamics of Amyloid-beta, imposed by the oscillating electric field.

BP 9.6 *(273)* Mon 17:30 Poster A

Studies of bio-molecular dynamics in aqueous solutions using 147Nd nuclear probe — •Sardool Singh Ghumman — Department of Physics, Sant Longowal Institute of Engineering & Technology, Deemed University, Longowal 148 106 Punjab, India

Conventional perturbed angular correlation technique is employed to investigate molecular dynamics in aqueous solutions of biomolecules of TES (Ntris[hydroxymethyl]methyl 2-Amino ethane sulphonic acid), BSA (Bovine Serum Albumin), Oxine (1,4-Benzodioxane-6-boronic acid pinacol ester) and EDTA (ethylenediaminetetraacetic acid) using 147Nd nuclear probe. In addition to the use of 147Nd radioactive probe that it proves to be helpful tool for perturbed angular correlation studies it also emerges out to understand the dynamics of molecules of bio-molecular compounds in aqueous environments. Considerable decrease in attenuation coefficient with higher molar concentrations is noticed for EDTA complexes while the attenuation effect has been found to be more pronounced for macromolecules of BSA and chelates of Oxine. Applications of this isotope are outlined for future non-biomolecular materials too.

BP 9.7 *(369)* Mon 17:30 Poster A

A computational approach to study signal transduction in coiled-coil structures — •Judit Clopés Llahí[1], Jaeoh Shin[2], Marcus Jahnel[3,4], Stephan Wolfgang Grill[1,3,4], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Chemistry, Rice University, Houston 77005 TX, USA — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany — [4]Biotechnology Center, Technical University Dresden Tatzberg 47/49, 01309 Dresden, Germany

The Early Endosome Antigen 1 (EEA1) is a fibrous protein mediating the tether and fusion of vesicles in the early endosome. Its functionality is related to an allosteric switch between two configurations with different stiffnesses. Recent experiments have shown that the transition from the stiff to the soft state in EEA1 is triggered right after its interaction with Rab5, a small signalling protein that binds to the free end of EEA1. Structurally, the EEA1 folds as a homodimeric coiled-coil in almost its total length, which spans up to 200 nm. In this work, we propose a computational description of the hydrophobic interactions stabilising a coiled-coil structure that could model the underlying mechanism behind the signal transduction of the Rab5:EEA1 interaction. For this, we mapped the hydrophobic interactions by means of a one-dimensional Frenkel-Kontorova model. Using this description, we analyzed how the energy introduced by a register shift in one of the extremes propagates along the chain.

BP 9.8 *(419)* Mon 17:30 Poster A

Simulating the ADP release of the PKAC cycle with different Magnesium quantities approximated by static charge and dummy-atom models — •Robert C. König, Alexander Lipskij, Bernhard Reuter, and Martin E. Garcia — Theoretische Physik II, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

The modification of biomolecules by addition of phosphates (phosphorylation/dephosphorylation) is essential for the regulation of vital cell processes as growth, division or morphogenesis. The protein kinase A (PKA) is responsible for important phosphorylation processes. The rate limiting process in the catalytic cycle of PKA is the release of ADP and the so-called Mg2 magnesium ion. The details and actual molecular dynamics of the ADP release are not well resolved. To observe the sub-millisecond behavior of the ADP release, we performed molecular dynamics (MD) simulations utilizing GROMACS v2016.3, with the AMBER03 and AMBER99SB-ILDN force-fields, based on the crystallized structure of PKAC with ADP and Mg2. This structure is already in an intermediate state between the open and the closed conformation, depending on the positions of the Gly-rich loop and C-terminal tail. While simulating the ADP release we investigated the influence of the Mg quantity by running the simulations (i) without any Mg ions, (ii) with one Mg ion and (iii) with two Mg ions, with the second magnesium ion added at the position of the linchpin magnesium ion, termed Mg1. To approximate the effect of the Mg charge we used both a standard static charge and a dummy-atom model, imitating the coordination number of Mg.

BP 9.9 *(424)* Mon 17:30 Poster A

Scaling rules for vibrational energy transport in proteins — •Luis Valino, Adnan Gulzar, Sebastian Buchenberg, and Gerhard Stock — Biomolekulare Dynamik Physik Uni-Freiburg

Computational studies of vibrational energy flow in biomolecules require the inspection of possible energy pathways on a case by case basis[1]. Though these studies succesfully elucidate the energy flow, the interpretation of the underlying processes driving energy transport is still missing. One alternative to these techniques is a master equation approach that simulates the transfer of energy from one amino acid to another and to the solvent on the basis of transition rates[2]. These transition rates can be determined through the fitting of the master equation to the energy profiles of nonequilibrium MD simulations. The scaling rules arising from this fit reveal a set of simple quantities that govern energy flow in proteins. We apply this model to various systems with different secondary structures and compare the relevant quantities and their scaling rules. Some of the scaling rules are conserved in all cases, whereas some others are dependent on the particular secondary structure.

[1] P. H. Nguyen, S. Park, and G. Stock. Journal of Chemical Physics 132, 025102 (2010)

[2] S. Buchenberg, D. M. Leitner, and G. Stock. J. Phys. Chem. Lett. 7, 25 (2016)

BP 9.10 *(425)* Mon 17:30 Poster A

Nonequilibrium computational study of vibrational energy transport in proteins — •Adnan Gulzar, Luis Valino Borau, Sebastian Buchenberg, and Gerhard Stock — Biomolekulare Dynamik Physik Uni-Freiburg

Vibrational energy transport is thought to play an important role in numerous processes essential to protein function, including kinetics of ligand binding and dissociation, charge transfer, enzyme kinetics and allosteric mechanisms. Time resolved spectroscopies developed to study vibrational energy flow[1] have elucidated the nature and rate of energy transport through a number of peptides and proteins. To provide a theoretical description of these experiments, extensive nonequilibrium molecular dynamics simulations of the energy transport in various systems, including TrpZip2 and PDZ3, have been performed. To mimic the experimental heating processes we employ computational heating methods such as T-jump- and photo-excitation. These nonequilibrium techniques of introducing energy into the system closely reproduce the observed experimental timescales. Additionally, the high resolution of MD simulations allows an in-depth analysis of vibrational energy transport. As a result, we have found out that energy flows not only through the backbone and β-stabilizing hydrogen bonds, but also through stacking contacts of the peptide with the heater.

[1] V. Botan, E. H. G. Backus, R. Pfister, A. Moretto, M. Crisma, C. Toniolo, P. H. Nguyen, G. Stock, and P. Hamm Energy transport in peptide helices PNAS 2007 104: 12749-12754

BP 9.11 *(25)* Mon 17:30 Poster A

Ectoine protects biomolecules from ionizing radiation: Molecular mechanisms — •Marc Benjamin Hahn[1,2], Tihomir Solomun[2], Maria-Astrid Schröter[2], Hans-Jörg Kunte[2], Susann Meyer[2], and Heinz Sturm[2,3] — [1]Freie Universität Berlin — [2]Bundesanstalt für Materialforschung und -prüfung — [3]Technische Universitäat Berlin

The compatible solute and osmolyte ectoine is an effective protectant of biomolecules and whole cells against heating, freezing and high salinity. The protection of cells (human Keratinocytes) by ectoine against ultraviolet radiation was also reported by various authors, although the underlying mechanism is not yet understood. We present results[1] on the irradiation of biomolecules (DNA) with ionizing radiation (high energy electrons) in fully aqueous environment in the presence of ectoine and high salt concentrations. The results demonstrate an effective radiation protection of DNA by ectoine against the induction of single strand breaks by ionizing radiation. The effect is explained by an increased in low-energy electron scattering at the enhanced free-vibrational density of states of water due to ectoine, as well as the action of ectoine as an OH-radical scavenger. This was demonstrated by Raman spectroscopy, electron paramagnetic resonance (EPR) and

Monte-Carlo simulations (Geant4).

[1] Hahn *et al. Phys. Chem. Chem. Phys.*, 2017, **19**, 25717-25722

BP 9.12 *(76)* Mon 17:30 Poster A

Preferential binding of urea to single-stranded DNA structures: a molecular dynamics simulation study — •Ewa Anna Oprzeska-Zingrebe and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

In nature, a wide range of biological processes, such as transcription termination or intermolecular binding, depend on the formation of specific DNA secondary and tertiary structures. These structures can be both stabilized or destabilized by different co-solutes, coexisting with nucleic acids in the cellular environment. In our molecular dynamics simulation study, we investigate the binding of urea at different concentrations to short 7-nucleotide single-stranded DNA structures in aqueous solution. The local concentration of urea around native DNA hairpin in comparison to an unfolded DNA conformation is analyzed by preferential binding model in the light of Kirkwood-Buff theory. All our findings indicate a pronounced accumulation of urea around DNA, which is driven by a combination of electrostatic and dispersion interactions and accomplished by a significant replacement of water molecules in terms of a dehydration effect. The outcomes of our study can be regarded as a first step into a deeper mechanistic understanding towards co-solute-induced effects on nucleotide structures in general.

BP 9.13 *(156)* Mon 17:30 Poster A

Dielectrophoretic Immobilization of Nanoobjects as Singles — •Xenia Knigge[1], Christian Wenger[2], Frank F. Bier[1], and Ralph Hölzel[1] — [1]Fraunhofer Institute for Cell Therapy and Immunology IZI, Branch Bioanalysis and Bioprocesses, Potsdam (IZI-BB), Germany. — [2]IHP GmbH - Leibniz Institute for Innovative Microelectronics, Frankfurt (Oder), Germany.

For the construction of a biosensor the immobilization of the bioreceptor is a key element. Here we demonstrate the immobilization of fluorescently labeled nanospheres as a model system applying dielectrophoresis (DEP). DEP is a phenomenon in which a dipole is induced in a polarizable particle in an inhomogeneous AC electric field. By the right choice of frequency, this particle can be moved and immobilized. Also an alignment of the biomolecules is advantageous to get a strong signal, which is achieved by DEP. The nanoobjects have been immobilized as individual objects on electrodes of a regular array consisting of many thousands of vertical silicon or tungsten based nanoelectrodes. Immobilization and singling is proved by fluorescence microscopy in combination with scanning electron microscopy. Owing to the large number of electrodes being observed simultaneously, occupation numbers of submicroscopical particles could be determined with good statistics applying histograms. Occupation numbers and patterns were determined as a function of particle size (down to 50nm) and electrode diameter (50nm and 500nm).

BP 9.14 *(165)* Mon 17:30 Poster A

Polymer brushes in motion – measuring flow with nanometre resolution — •Jan Christoph Thiele, Sebastian Isbaner, Narain Karedla, Ingo Gregor, and Jörg Enderlein — III. Institute of Physics – Biophysics, Georg August University Göttingen, Germany

Polymer brushes are a versatile method to tailor surface properties. These include wetting behaviour, friction and interactions with colloids and biomolecules. Coating a surface with polymer brushes changes its hydrodynamic properties in a complex way. Experiments on brush coated capillaries showed an unexpected large flow reduction by the brush, while recent simulations are predicting a backflow within the brush layer.

Our aim is to measure how the brushes impact the flow at the surface and to verify the predicted backflow. For this, we will use fluorescence lifetime correlation spectroscopy (FLCS) in combination with metal induced energy transfer (MIET). FLCS enables a precise and non-invasive measurement of the flow speed, while MIET causes a modulation of the dye's lifetime in close proximity to a gold surface underneath the brush. This modulation allow us to section the volume into different layers based on their lifetime. We will use a fluorescence dye dissolved in the liquid or the brush and measure the movement of the dye molecules and their distance from the gold surface. This way we can obtain a high resolution flow profile in the range of 0 to 100 nm distance to the surface.

BP 9.15 *(215)* Mon 17:30 Poster A

Organelle-specific density measurements of the V-ATPase using atomic force microscopy — Elisabeth Eilers[2], •Julia Teckentrup[1,2], Katharina Schiller[2], Volker Walhorn[1], Thorsten Seidel[2], Karl-Josef Dietz[2], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanoscience, Bielefeld University, Germany — [2]Plant Biochemistry and Physiology, Bielefeld University, Germany

The V-ATPase functions as a membrane-embedded rotational proton pump, which creates a proton motif force and thus drives secondary active transport of solutes across endomembranes. Therefore, these enzymes are essential for cellular pH- and ion homeostasis.

V-ATPases are located in the endomembranes of the endoplasmic reticulum, the Golgi apparatus as well as the vacuolar membrane in plants, which we could show using molecular biology techniques and fluorescence microscopy. In atomic force microscopy (AFM) images, V-ATPases showed prominent structures with a height of roughly 10 nm corresponding to the hexameric arrangement of their catalytic head. Using AFM we aim to investigate the differences in the number of V-ATPases between different compartments of plant cells. We will further apply AFM-based single molecule force spectroscopy to test the stability of the complexes. The latter is driven by the observation, that the vacuolar enzyme shows a diffuse organization of its stabilizing stalk proteins in the presence of desoxyglucose as observed by FRET-microscopy (Schnitzer et al., 2011, Plant Cell Physiol.).

BP 9.16 *(234)* Mon 17:30 Poster A

Quantifying the association of the chemotherapeutic drug mitoxantrone to DNA by magnetic tweezers — •Dennis Kreft, Ying Wang, Helene Schellenberg, Katja Tönsing, and Dario Anselmetti — Experimental Biophysics and Applied Nanoscience, Bielefeld Institute for Nanoscience (BINAS), Bielefeld University, Bielefeld, Germany

Chemotherapeutic agents (anti-cancer drugs) are small cytotoxic molecules that often bind to double-stranded DNA (dsDNA) and thus interfere with the cell division process (mitosis). For medical regulation and optimization issues of these pharmaceutical products, it is inevitable to identify/quantify their binding mechanism. Therefore, we investigated the anthraquinone compound mitoxantrone that is used for treating certain cancer types like leukemia and lymphoma. We employed magnetic tweezers (MT) to investigate the association of mitoxantrone with dsDNA and conducted force-extension and rotation-extension experiments with a sensitivity from some piconewtons down to tens of femtonewtons. We found a concentration-dependent bimodal binding behavior, where mitoxantrone associates to dsDNA either as a groove binder at low concentrations and as an intercalator at high concentrations.

BP 9.17 *(238)* Mon 17:30 Poster A

Investigation of sea cucumber proteoglycans by atomic force microscopy — •Niklas Biere[1], Pierre Piel[1], Volker Walhorn[1], Xavier Fernàndez-Busquets[2], Paulo A. S. Mourão[3], Eduardo Vilanova[3], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanosciences, University of Bielefeld, Germany — [2]Nanoscience and Nanotechnology Institute (IN2UB), University of Barcelona, Spain — [3]Hospital Universitário Clementino Fraga Filho and Instituto de Bioquímica Médica, Universidade Federal do Rio de Janeiro, Brazil

Sea cucumbers belong to the echinoderm family and are a widely spread marine life form in the world's oceans, yet not all aspects of their biology are well researched. As such, they possess remarkable properties, like the catch connective tissue, whose mechanical stiffness can be adapted without the use of muscles. In this work, we investigate the proteoglycan molecules from the sea cucumber species *Isostichopus badionotus* which make up part of its body wall. These proteoglycans, which exhibit antimalarial and anticoagulant properties, are studied in detail with atomic force microscopy to gain insights in the structure and chemical morphology of their polysaccharide components, namely fucosylated chondroitin sulfates and sulfated fucans. We will discuss their role in maintaining the adaptive elasticity of the tissue and show that this ability is related to the concentration of Ca^{2+} ions, which subsequently influences the tissue's capability to store water.

BP 9.18 *(278)* Mon 17:30 Poster A

Label-free detection and trapping of individual nanosystems — •Larissa Kohler — KIT, Karlsruhe, Deutschland

The label-free detection of nanosystems provides the opportunity to

understand biomolecular dynamics and interactions without undesired modifications of the system. To achieve the high sensitivity required for studying individual nanosystems, we use signal enhancement in a fiber-based Fabry-Perot cavity with high finesse ($F \approx 10^5$), which is integrated in a microfluidic channel. Dispersive interaction between the sample and the cavity field is used to detect the presence and the dynamics of individual nanoobjects. The tight focus of the cavity mode ($w_0 \approx 1\,\mu m$) can be furthermore harnessed to trap individual particles between the fibers far away from surfaces. At the same time, a polarizable particle shifts the resonance frequency and thereby the intracavity laser power, such that particle motion couples back to the trapping potential. In this so-called self-induced back-action regime, trapping of sub-100 nm is predicted to become possible at biocompatible low intensity levels. We show first results on the detection of 150 nm silica nanoparticles and report the current status of the experiment.

BP 9.19 *(316)* Mon 17:30 Poster A

DNA origami mold-based wires: Synthesis long metallic wires and its temperature dependent charge transport mechanism — •Türkan Bayrak[1,2], Seham Helmi[3], Jingjing Ye[2,3], Jeffrey Kelling[1], Tommy Schönherr[1], Artur Erbe[1,2], and Ralf Seidel[2,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden,Germany. — [2]Technische Universität Dresden, cfaed, 01062 Dresden, Germany. — [3]Universität Leipzig, Ritterstraße 26, 04109 Leipzig, Germany

The DNA origami method provides a programmable bottom up approach for creating nanostructures of any desired shape, which can be used as scaffolds for nanoelectronics and nanophotonics device fabrications. This technique enables the precise positioning of metallic and semiconducting nanoparticles along the DNA nanostructures. In this study, DNA origami nanoMOLDS are used for the fabrication of nanoelectronic devices. To this end, electroless gold deposition is used to grow the AuNPs within the DNA origami nanoMOLDS and create eventually continues nanowires. In order to contact the fabricated nanostructues electrically, a method using electron-beam lithography was developed. Temperature-dependent characterizations for four wires exhibiting different conductance at RT were performed in order to understand the dominant conductance mechanisms from RT to 4.2K. Two of these nanowires showed metallic conductance. The other two wires deviated from pure metallic behavior and they showed thermionic, hopping and tunnelling conductance.

BP 9.20 *(387)* Mon 17:30 Poster A

Towards video rate imaging of IFT at nanoscale resolution using the Atomic Force Microscope — •Renata Garces and Christoph F. Schmidt — Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen

Atomic force microscopy is a powerful tool for characterizing single molecules with nano-scale spatial resolution. The improvement of image acquisition rates render possible to access dynamical processes having place at nano-scale, such as the ones driving the highly dynamic traffic in the cell. Here we present the advances in the implementation of an experimental in vitro model system to study the dynamics of molecular motors involved in Intra Flagellar Traffic (IFT) keeping high spatial resolution. Our system consist of Chlamydomonas reinhardtii axonemes adhered to a hard substrate. Topographic images from the atomic force microscope allows to distinguish doublets of microtubules and tubulin dimers from axoneme surfaces. Adding high concentrations of immobilized dimeric kinesin-1 motor in presence of nonhydrolyzable ATP analog (AMP-PNP) results in fully decorated axoneme surfaces. Addition of ATP at different concentrations results in differentiated motor activity.

BP 9.21 *(82)* Mon 17:30 Poster A

Smart Gelatin Hydrogels: Modification by Electron Irradiation towards Stimuli-Responsive Elements — •Stefanie Riedel[1,2], Benedikt Heyart[1], Katharina Apel[1], Emilia Wisotzki[1], and Stefan Mayr[1,2] — [1]Leibniz Institute of Surface Engineering (IOM) Leipzig — [2]Felix Bloch Institute, Faculty of Physics and Earth Sciences, University Leipzig

Stimuli responsive materials have attracted considerable interest during the past years due to their potential use in sensor and actuator applications. They are designed to transform small external stimuli e.g. temperature and humidity changes into a significant response. While a large number of alloys or synthetic polymers are well-established at this point, we explore the potential of the biomaterial gelatin to respond to temperature and humidity for possible use as biological active control elements or as switchable scaffolds. To tailor the stimuli responsiveness of gelatin, it is crosslinked by high energy electron irradiation which is nontoxic and thus enables biomedical applications. Thereby, a temperature dependent shape memory is introduced which can be utilized to develop a temperature-responding system. Furthermore, we will show that electron irradiated gelatin has a high potential as a biocompatible and stimuli responsive demonstrator responding to humidity. By adaption of environmental parameters such as irradiation dose, gel concentration, pH-value and salt concentration, the response of the responsive element can be precisely tuned.

BP 9.22 *(136)* Mon 17:30 Poster A

Uptake and release of proteins in microgels studied on single particle level — •Farzaneh Vaghefikia[1], Julia Kratz[1], Julia Walter[1], Wenjing Xu[2], Andrij Pich[2], and Jörg Fitter[1] — [1]RWTH Aachen University, I. Physikalisches Institut (IA), AG Biophysik, Aachen, Germany — [2]DWI-Leibniz Institut for Interactive Materials, Aachen, Germany

For efficient drug delivery, a smart network of polymers called microgel particles can be used. These particles with an ability to swell and deswell in response to environmental changes, allow uptake and release of drugs in a controlled manner. Their sensitivity to environmental changes along with biocompatibility make it a good candidate for a drug carrier, especially for therapeutic proteins. An impact of environmental conditions on proteins outside the cell often causes protein denaturation and aggregation [1]. We studied the uptake and release of the positively charged cytochrome c, in and from microgel particles. The loading of the microgels took place at pH 8, a value at which microgels are charged negatively [2]. By employing wide-field fluorescence microscopy we made a reliable characterization of single particles, e.g. the maximum loading of the particles, the stability of the loading, and the amount of proteins to be released at the target location.

[1] Antosova et al. Trends Biotechnol. 2009
[2] Ricarda Schröder et al, Macromolecules, 2015.

BP 9.23 *(168)* Mon 17:30 Poster A

A novel water soluble iron phthalocyanine as a redox mediator integrated to multifunctional hydrogel based graphene nanoplatelet for glucose monitoring — •hadi al-sagur, komathi shanmugasundaram, and aseel hassan — Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, United Kingdom

Herein, we report a novel sensing platform for glucose biosensor applications. A three-dimensional multifunctional hydrogel interconnected network of water-soluble iron phthalocyanine (FePc) in single-layer graphene nanoplatelet (SLGNPs) for glucose oxidase (GOx) immobilization (PAA-FePc-SLGNPs/PANI /GOx-MFH) has been reported. Structural and morphological studies for (PAA-FePc-SLGNPs/PANI -MFH) were carried out using scanning electron microscopy (SEM), Fourier-Transform Infrared (FTIR), transmission electron microscopy, (TEM), X-ray diffraction (XRD), Raman spectroscopy and UV*Visible absorption spectroscopy. The electrochemical biosensor was fabricated utilizing PAA-FePc-SLGNPs/PANI -MFH as the enzyme immobilizing matrix coated on a screen-printed carbon electrode, and glucose oxidase (GOx) was used as a model enzyme. The electrical conductivity of the detection electrode was studied using electrochemical impedance spectroscopy (EIS). The modified electrodes were studied by amperometry and cyclic voltammetry. The PAA-FePc-SLGNPs/PANI /GOx-MFH was designed towards glucose monitoring with high sensitivity, good selectivity and low detection limit. Our biosensor could potentially be a valuable tool at the clinical uses for monitoring diabetes.

BP 9.24 *(217)* Mon 17:30 Poster A

Exposure of mesenchymal stromal cells to graphene quantum dots — •Sibel Tezkan[1], Stefan Fasbender[1], Tim Ebbecke[2], Katharina Raba[2], Johannes Fischer[2], and Thomas Heinzel[1] — [1]Experimental Condensed Matter Physics, Heinrich Heine University, Düsseldorf — [2]Transplantation Diagnostics and Cell Therapeutics, University Hospital Düsseldorf

Fluorescent graphene quantum dots (GQDs) are prepared by the slightly modified method of Qu et al. [1] via thermal decomposition of citric acid and diethylenetriamine with subsequent dialysis to obtain a pure GQD solution. The obtained aqueous solution is analyzed with fluorescence spectroscopy. Mesenchymal stromal cells are exposed to GQDs and a high uptake is determined using flow cytometry. The number of incorporated GQDs is estimated by comparing the fluorescence of cells with GQDs and without GQDs. In addition, the uptake

of GQDs into exosomes is investigated.

[1] Qu et al., Light: Science & Applications, 2015, 4, e364

BP 9.25 *(218)* Mon 17:30 Poster A

Effects of changing the Zeta potential of Graphene Quantum Dots for Biological Applications — •Stefanie Berger[1], Stefan Fasbender[1], Sebastian Bauer[2], Stephan Schmidt[2], Laura Hartmann[2], and Thomas Heinzel[1] — [1]Heinrich Heine Universität Düsseldorf, Institut für Experimentelle Physik der kondensierten Materie — [2]Heinrich Heine Universität Düsseldorf, Institut für Organische und Makromolekulare Chemie

Fluorescent graphene quantum dots (GQDs) are prepared by thermal decomposition of citric acid and diethylenetriamine slightly modifying the method of Qu et al. [1]. The concentration dependent fluorescence properties are studied with fluorescence spectroscopy and the Zeta potential is measured using dynamic light scattering. Both is compared to GQDs with modified features. Possible modifications include the binding of a positive charged amide or a slight change of the GQD recipe. In order to analyse the particles' properties for biological applications, their uptake into primary human blood cells and their nucleus is investigated using flow cytometry and visualised via confocal microscopy.

[1] Qu et al., Light: Science & Applications, 2015, 4, e364

BP 9.26 *(223)* Mon 17:30 Poster A

Cellular uptake of graphene quantum dots into murine precision-cut liver slices and MMTV-PyMT mammary carcinoma cells — •David Kersting[1], Stefan Fasbender[1], Angelika Hallenberger[2], Johanna Naskou[3], Katharina Raba[4], Johannes Fischer[4], Hans Neubauer[3], and Thomas Heinzel[1] — [1]Experimental Condensed Matter Physics, Heinrich-Heine-University Dusseldorf — [2]Institute for Anatomy II, University Hospital Dusseldorf — [3]Department of Obstetrics and Gynecology, University Hospital Duesseldorf — [4]Institute for Transplantation Diagnostics and Cell Therapeutics, University Hospital Dusseldorf

Precision-cut liver slices were produced from outbred C57BL/6 mice liver lobes and incubated under cultural conditions for 1 or 2 days supplementing their growth medium with a defined concentration of N-doped graphene quantum dots (GQDs). The slices were examined using flow cytometry, confocal microscopy and fluorescence spectroscopy clearly indicating a quantum dot uptake into the cultivated tissue, which might decay with increasing penetration depth. These experiments constitute to our knowledge the first incubation of GQDs on precision-cut tissue slices (PCTS), which display a versatile in vitro tool for probing drug effects on cells in a molecular environment close to their in vivo intra-organ situation. In a second approach the GQDs were incubated in two concentrations over a period up to two days on cultured cell lines of the murine MMTV-PyMT mammary carcinoma model. Our first data obtained by flow cytometry hint at a proposed uptake depending linearly on the incubation time.

BP 9.27 *(224)* Mon 17:30 Poster A

Comparing the properties of graphene quantum dots prepared in a microwave and graphene quantum dots prepared on a hot plate — •Alexandra Steina, Stefan Fasbender, and Thomas Heinzel — Experimental Condensed Matter Physics, Heinrich-Heine-University Dusseldorf

Fluorescent graphene quantum dots (GQDs) are prepared by the method of Wu et al. [1] via hydrothermal treatment (3 hours, 180° C) of citric acid and dicyandiamide on a hot plate (hGQDs). The fluorescence properties of these GQDs (quantum yield: 29 %, emission maximum around 450 nm at 360 nm excitation) are compared to GQDs prepared in a microwave oven (mGQDs) using the same recipe and the same synthesis temperature. The duration of the microwave synthesis is varied and the highest fluorescence quantum yield amounts to 29 % after a synthesis time of 2 minutes. The mGQDs show a nearly identical fluorescence spectrum compared to the hGQDs with the same emission maximum around 450 nm at 360 nm excitation. XPS data reveals that hGQDs are composed of 52 % carbon, 23 % nitrogen and 25 % oxygen whereas mGQDs are composed of 43 % carbon, 26 % nitrogen and 31 % oxygen.

[1] Wu et al., Nanoscale, 2014, 6, 3868

BP 9.28 *(226)* Mon 17:30 Poster A

Studying the fluorescence properties of graphene quantum dots — •Maren Sakowski[1], Stefan Fasbender[1], Ralf Kühnemuth[2], Bekir Bulat[2], Claus Seidel[2], and Thomas Heinzel[1] — [1]Experimental Condensed Matter Physics, Heinrich-Heine-University Dusseldorf — [2]Molecular Physical Chemistry, Heinrich-Heine-University Dusseldorf

Fluorescent graphene quantum dots (GQDs) are prepared by thermal decomposition of citric acid and diethylentriamine slightly modifying the method of Qu et al. [1]. The particles are purified with HPLC and the fluorescence properties are studied using fluorescence spectroscopy, UV-vis, fluorescence correlation spectroscopy (FCS) and time-correlated single photon counting (TCSPC). The GQDs show an absorption maximum around 360 nm with an emission maximum around 450 nm (25 % quantum yield) and a second absorption maximum around 480 nm with an emission maximum around 560 nm (6 % quantum yield). TCSPC reveals a fluorescence lifetime of 9.92 ns at 360 nm excitation and 1.78 ns at 480 nm excitation. The Stokes radius is identified to be 0.6 nm using FCS.

[1] Qu et al., Light: Science & Applications, 2015, 4, e364

BP 9.29 *(229)* Mon 17:30 Poster A

Uptake of fluorescent graphene quantum dots into human breast cancer cell lines — •Rabea Pilch[1], Stefan Fasbender[1], André Franken[2], Marina Willibald[2], Katharina Raba[3], Johannes Fischer[3], Hans Neubauer[2], and Thomas Heinzel[1] — [1]Experimental Condensed Matter Physics, Heinrich-Heine-University Dusseldorf — [2]Department of Obstetrics and Gynecology, University Hospital Dusseldorf — [3]Institute for Transplantation Diagnostics and Cell Therapeutics, University Hospital Dusseldorf

Fluorescent graphene quantum dots (GQDs) are prepared by thermal decomposition of citric acid and diethylentriamine referring to the method of Qu et al. [1]. The breast cancer cell lines MCF-7 and MDA-MB-231 and the non-tumor cell line MCF-10A are exposed to various concentrations of GQDs for various times. The MTT viability assay shows a decrease of the viability of all three cell lines to 60 % compared to cells without GQDs, when exposed to a maximum concentration of 1 mg/ml GQDs for 72 hours. Flow cytometry is used to analyse the time dependent uptake of the GQDs into the cells. The number of incorporated GQDs per cell is estimated to be 5 billion for the tumor cell lines (MCF-7 and MDA-MB-231) and 43 billion for the non-tumor cell line (MCF-10A) by measuring the fluorescence intensity of cells exposed to GQDs for 48 hours with fluorescence spectroscopy.

[1] Qu et al., Light: Science & Applications, 2015, 4, e364

BP 9.30 *(252)* Mon 17:30 Poster A

Secondary structure analysis of xanthan using atomic force microscopy — •Jenny Fjodorova[1], Volker Walhorn[1], Julia Voss[2], Vera Ortseifen[2], Karsten Niehaus[2], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience, Bielefeld University, Germany — [2]Proteome and Metabolome Research, Bielefeld University, Germany

Xanthan is an extracellular polysaccharide, secreted by the microorganism *Xanthomonas campestris*. Due to its unique viscosifying properties, xanthan has numerous industrial applications. Therefore, the optimization of xanthan production and its rheological properties is of particular interest. Targeted genetic modification of the *Xanthomonas* metabolism can be a powerful tool to optimize shear-thickening potency and to improve the xanthan production efficiency.

Using atomic force microscopy (AFM) imaging and single molecule force spectroscopy (SMFS), we analyzed the structure and the elastic characteristics of single xanthan polymers, which were produced by different *Xanthomonas* strains. We identified structures ranging from single-stranded coiled networks to branched double-strands. Taking into account the varying ability to form double-strands and differences in the bending stiffness, we observed a correlation between the formation of secondary structures and its resulting different viscosifying properties. Our results enable a better understanding of relevant metabolic pathway modifications for an optimized xanthan synthesis.

BP 9.31 *(298)* Mon 17:30 Poster A

Gas bubbles in thermal gradients accumulate DNA and trigger wet-dry cycles — •Matthias Morasch, Jonathan Liu, Christof Mast, and Dieter Braun — LMU Munich, Amalienstr. 54, 80799 München, Germany

Life has developed in water, but dry steps are essential for many prebiotically plausible syntheses and polymerization processes [1,2]. This posits the question how dry-wet cycles can be combined with an underwater scenario without diluting the reaction products into the ocean. We found that a nonequilibrium system in form of a temperature gra-

dient across a gas bubble in water creates an efficient accumulation setting. In addition to the known thermophoretic trap, molecules hereby strongly accumulate at the water-gas interface [3]. Movements of the gas bubble thereby trigger continuous drying and re-hydration steps, while maintaining high local concentrations of ca. 1000-fold near the interface. Here, we show the underlying mechanisms for the accumulation process at the water-air interface, which also exhibits a length-selectivity e.g. for DNA strands. In addition, we demonstrate the precipitation and redilution of RNA monomers that polymerize only under dry conditions [2]. This mechanism allows reaction pathways such as the formation, phosphorylation, or polymerization of nucleotides that require both aqueous and dry conditions.

[1] Powner et al., (2009) Nature 459:239-242. [2] Morasch et al (2014) ChemBioChem 15:879-883. [3] Braun et al. (in submission)

BP 9.32 *(340)* Mon 17:30 Poster A

Nanoscale properties of polymer micro-moulds studied by a combination of AFM and SICM — •Annelie Marx, Regina Lange, Ingo Barke, and Sylvia Speller — University of Rostock, Institute of Physics, 18059 Rostock, Germany

PDMS (polydimethylsiloxane) is a versatile material for creating micro-moulds or stamps. We prepared PDMS moulds as test samples for scanning ion conductance microscopy (SICM) and as prospective substrates for cell adhesion experiments. We focus on the achievable level of detail on the nanoscale by producing moulds from dry eched glass structures exhibiting equidistant grids and pillars of different aspect ratios with vertical side walls. We also report on attempts to produce moulds from metallic nanostructures (Fischer samples) and multichannel plates (MCPs). Both the moulds and the original samples were studied by AFM and SICM. With SICM the topography of a soft sample placed in a (conducting) liquid is measured on the nanoscale, largely avoiding direct forces between the sample and the probe. A decent reproduction quality was obtained on samples with 2 μm deep grooves and unity aspect ratio. We discuss general properties and benefits of PDMS micro-moulds for applications in Biophysics (e.g. with live cells), including the possibility to produce artificial replica by creating a second mould from an initial one.

[1] Y. Xia, G.M. Whitesides, Annu. Rev. Mater. Sci. 28, 153 (1998)

BP 9.33 *(388)* Mon 17:30 Poster A

Investigating Compression of Single DNA Molecules in a Thermophoretic Trap — •Tobias Thalheim, Marco Braun, and Frank Cichos — Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany

We report on the trapping of single DNA molecules in liquids with the help of a force-free trapping method utilizing feedback-driven dynamic temperature gradients. These temperature gradients, that are obtained by spatially and temporally vary the temperature at a circular plasmonic nano-structure, induce thermophoretic drift velocities which prevent the randomization of the positions and conformations of the DNA molecules due to Brownian motion. Because of the generated inhomogenous temperature profiles, drift velocities in the outer regions of the thermophoretic trap are larger than those in the center forcing the elongated DNA molecules into more compressed states of their conformation compared to freely diffusing molecules. A model-free statistical tool called principal-components analysis as introduced by Cohen and Moerner [1] is employed to assess these distortions of the DNA's conformation and conformation dynamics.

References
[1] A. E. Cohen, and W. E. Moerner, PNAS 104 (31), 12622-12627 (2007)

BP 9.34 *(403)* Mon 17:30 Poster A

Dilute molecular crowders enhance activity of ligase ribozyme — •Mrityunjoy Kar, Juan Manuel Iglesias Artola, Oliver Beutel, Alf Honigmann, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

The RNA world hypothesis remains a hallmark in *origin of life* research despite very poor robustness and low reactivity of most model replicators studied so far. A frequently used trick to enhance ribozyme activity is the use of high concentration molecular crowders (M to mM) to increase RNA concentrations by excluded volume effects. Here we show, that excluded volume effect is not strictly required to enhance ribozyme activity using R3C ligase as a model ribozyme and polyethylene glycol (PEG) as a model crowding agent. As observed in other systems before, we find that also for the R3C system reactivity is increased in presence of crowder. However, our data shows higher affinity (lower Km) at lower concentrations of crowder (1% wt/v). This suggests that excluded volume might not be the only effect. If so, enhanced activity should also be seen at even lower concentrations of crowder. Indeed, we find in our experiments a remarkable enhancement of R3C ligase activity at concentrations down to 50ppm (wt/v). With this, we suggest a beneficial role of polymeric crowders (impurities) during the origin of life.

BP 9.35 *(404)* Mon 17:30 Poster A

Self-Assembled Protein Hybrid Nanofibres — •Christian Helbing[1], Tanja Deckert-Gaudig[2], Gang Wei[3], Volker Deckert[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science, Otto-Schott-Institute of Materials Research, Faculty of Physics and Astronomy, Friedrich Schiller University Jena, Germany — [2]Institute for Photonic Technology, Jena, Germany — [3]Hybrid Materials Interfaces Group, Faculty of Production Engineering, University of Bremen, Germany

Over the last years, the interest in materials consisting of biomolecules arranged in nanofibers increased. There is a special focus on plasma proteins for applications in nanofiber materials because of their high biocompatibility. An easy feasible strategy to create these nanofibers is the self-assembly mechanism of protein molecules. Here we test the hypothesis that novel self-assembled hybrid protein nanofibers (PNF) can consist of two different proteins. In this work, we present self-assembled plasma hybrid PNF consisting of two different plasma proteins. Further, long-time CD-measurements provide information about the fiber formation dynamics. Especially, for the PNNF hybrid it confirmed interactions between both molecules. We confirmed the existence of a novel PNF hybrid by tip enhanced Raman spectroscopy and immunolabeling. Also, differences in the mechanical behaviour were shown by force spectroscopy. These results lay the foundation for a novel biomaterial based on these (h)PNNFs.

BP 9.36 *(423)* Mon 17:30 Poster A

Peptide heterogeneity enhances genetic identity and fluidity of RNA rich complex coacervates — •Juan M. Iglesias-Artola[1], Mrityunjoy Kar[1], Anatol W. Fritsch[1], Bjorn Drobot[1], Hannes Mutschler[2], Dora Tang[1], and Moritz Kreysing[1] — [1]MPI-CBG, Dresden, Germany — [2]MPIB, Munich, Germany

Complex coacervates have been proposed as a model system for protocells, and we found that they spontaneously assemble in temperature gradients. We have formed complex coacervates from short cationic peptides and an enzymatic RNA molecule. The coacervation process that we observe occurs through the interaction of a positively charged peptide and a negatively charged RNA. As a result, neutral complexes are formed, which phase separate from the surrounding medium to generate droplets. We characterized the physical properties of the RNA inside these compartments. The mobility of the RNA inside these droplets can be tuned by changing the peptide-RNA interaction strength and by the presence of other components in the surrounding medium. These droplets sequester RNA efficiently and can maintain genetic identity for long periods of time. Currently, we are working on rescuing RNA enzymatic activity inside these compartments. Here, we provide evidence on how a rudimentary identity of fluid protocells, necessary for the onset of natural selection, could have arisen when only simple components were available.

BP 9.37 *(147)* Mon 17:30 Poster A

Modelling the cell-cycle dependent regulation of p21 after DNA damage — •Isabella-Hilda Mendler and Barbara Drossel — TU Darmstadt, Germany

Ionizing radiation causes DNA double strand breaks and hence threatens the successful division or even the survival of a cell. For this reason, cells react to DNA damages by upregulating the tumor suppressor protein p53, which shows multiple pulses after the occurrence of the damage and activates numerous target proteins. One of the most important target proteins of p53 is p21, a potent cyclin-dependent kinase inhibitor that regulates cell-cycle arrest after DNA damage. Recent single-cell experiments showed that the timing and rate of its induction after DNA damage is heterogeneous, with the cell-cycle stage playing a crucial role.

We present a minimalistic nonlinear delay differential equation model for the regulation of p21 by p53 that reproduces the main features of the cell-cycle dependent dynamical behavior of p21 in response to the p53 oscillations following DNA damage. The p53 measurement

data are input to the model, and the p21 response is modelled by including cell-cycle dependent protein production and degradation rates. These features enable us to reproduce the observed delay of p21 response in cells that experience the damage in the S phase, as well as the prompt pulse-like response of p21 in cells that are irradiated in G1 and progress to S phase.

BP 9.38 *(188)* Mon 17:30 Poster A

Clocks and timers in genetic networks. — •Jose Negrete JR[1,2], Ivan M. Lengyel[1,3], Laurel A Rohde[2], Andrew C. Oates[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [3]Instituto de Investigación en Biomedicina de Buenos Aires CONICET of, Argentina

Genetic oscillations are noisy and in many cases, as in embryo development, short lived. We present a model of a noisy transcription factor that controls the timing and amplitude of an stochastic genetic oscillator. The transcription factor determines how long the oscillator is on and it is denominated as a timer, while the genetic oscillator is denominated as a clock due to its repetitive nature. The model is given by a single delay differential equation, and we show analytically the set of measurable parameters that characterises it. The predictions of the model were tested by analysing two different cases: self sustained genetic oscillations from cycardian rhythms and in the transient oscillatory gene expression from cells extracted from the presomitic mesoderm of zebrafish embryos.

BP 9.39 *(279)* Mon 17:30 Poster A

Modelling the Single Photon Response in Rods — •Charlotte J. Beelen[1], Karl-Wilhelm Koch[1], and Daniele Dell'Orco[2] — [1]Dept. Neuroscience, Biochemistry, University of Oldenburg — [2]Department of Neurosciences, Biomedicine and Movement Sciences, Sect. of Biological Chemistry, University of Verona

Rod cells are responsible for vision in dim light. After the activation of the pigment molecule rhodopsin, a complex signal transduction cascade leads to an electrical signal, which can then be transmitted further through the retina. This phototransduction cascade can be modelled using differential equations for the molecular species involved, mainly with mass-action kinetics [1,2]. The model can reproduce rods' behaviour across a vast range of experiments and mutations.

Rod cells are extremely sensitive: they have a reproducible response to single photons, thus operating at the physical sensing limit [3]. It is astonishing that the response to a single photon is very uniform, since a fluctuating signal would be expected.

To explain the uniformness of the single photon response and investigate which reactions are essential for its reproducibility, we modify the deterministic model of the phototransduction cascade in rods to also include stochasticity and spontaneous activation of the effector. We investigate how the reproducibility of the single photon response comes about and study the effect of multiple phosphorylations of rhodopsin.

[1] D. Dell'Orco et al, Mol. BioSyst. **5** 1232-1246 (2009)
[2] B.M. Invergo et al, Mol. BioSyst. **10** 1481-1489 (2014)
[3] R.D. Hamer et al, J. Gen. Physiol. **122** 419-444 (2003)

BP 9.40 *(285)* Mon 17:30 Poster A

Time distribution of mRNA delivery mediated by lipoplexes determined from single cell expression onsets — •Anita Reiser[1,2], Neha Mehrotra[1], Rafal Krzyszton[1,2], Daniel Woschée[1], Helmut H. Strey[3], and Joachim O. Rädler[1,2] — [1]Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-University, Munich, Germany — [2]Graduate School of Quantitative Biosciences (QBM), Ludwig-Maximilians-University, Munich, Germany — [3]Department of Biomedical Engineering and Laufer Center for Quantitative Biology, Stony Brook University, Stony Brook, NY, USA

Nucleic acid (NA) based therapies require efficient delivery systems. New Methods are required to assess uptake and release kinetics in living cells in order to improve the internalization of NA carriers. Here we employ automated time-lapse microscopy to study the delivery-time distribution of lipid based mRNA vectors. We determine the protein expression onset-times after transfection from single cell time courses of eGFP reporter fluorescence. We show how maximum likelihood fitting yields best estimates of individual onset times from hundreds of individual time courses in a robust and automated manner. The distribution of delivery dwell-times is found to be log-normal distributed in all cases with the mean depending on the transfection agent. For cationic lipid formulation containing various amounts of cholesterol the delivery timing correlates with efficiency. The profile of delivery timing might be a valuable indicator for the development of nanocarriers with improved uptake activity and endosomal release kinetics.

BP 9.41 *(295)* Mon 17:30 Poster A

Single-cell kinetics of siRNA-mediated mRNA degradation — •Rafał Krzyszton[1,2], Daniel Woschée[1], Anita Reiser[1,2], Gerlinde Schwake[1], Helmut Strey[3], and Joachim O. Rädler[1,2] — [1]Ludwig-Maximilians-Universität Munich (LMU), Geschwister-Scholl-Platz 1, Munich — [2]Graduate School of Quantitative Biosciences (QBM), Geschwister-Scholl-Platz 1, Munich — [3]Stony Brook University, Stony Brook, NY

RNA interference (RNAi) is a natural mechanism of post-transcriptional gene regulation and is underlying the therapeutic action of small interfering RNA (siRNA) directed against disease-related genes. Quantitative assessment of the siRNA knockdown efficiency is typically carried out at the population level. In contrast, direct measurement of the siRNA induced mRNA degradation requires time-resolved studies. Here we report on life cell imaging of the time-resolved expression and knockdown level after delivery of two mRNA reporter genes (eGFP, CayenneRFP) and delayed delivery of siRNA duplexes. Thousands of single cell time traces were recorded in parallel using micro-pattern assisted time-lapse microscopy (MPA-TLM) combined with automated image analysis. With the help of maximum likelihood fits to a mathematical translation model we yield scatter-plots of individual mRNA life-times and determine the siRNA meditated RISC activity as fold-change of mRNA degradation rate. Time-lapse imaging proves faster (<24hours) and more accurate (+/-1%) measurement of mRNA degradation and hence will allow new sensitive studies of sequence dependence RNAi

BP 9.42 *(434)* Mon 17:30 Poster A

Network coherences - a universal approach to quantify the match between "omics" data and a biological network — •Piotr Nyczka[1], Marc-Thorsten Hütt[1], Kristina Schlicht[2], Carolin Knecht[2], and Michael Krawczak[2] — [1]Departement of Life Sciences and Chemistry, Jacobs University, Bremen, Germany — [2]Institute of Medical Informatics and Statistics, Christian-Albrechts-University Kiel, Germany

Network-based analyses of "omics" data are a cornerstone of systems medicine. Their goal is to quantify and statistically evaluate the clustering of biological signals (e.g., co-expression of genes) in a network (e.g., a metabolic network or a protein-interaction network). Network coherences are topological indices evaluating the connectivity of subnetworks spanned by the "omics" signal of interest [1,2]. They have been used very successfully to identify scientifically relevant patient subgroups in disease cohorts [2-4].

Here, we aim at a deeper theoretical understanding of network coherence. Using various random walk models on graphs, we test, refine and calibrate this method. In this way, the dependence of a given network coherence upon the number of (e.g., disease-associated) genes, the topology of the underlying biological network or the fragmentation of the functional signal in the network can be studied numerically and compared to analytical predictions.

Our method allows us to detect functional signal even in very noisy data. The main novelty of this approach lies in taking into account collective expression profiles of the whole group of patients and contrast it with individual ones. In order to find relevant signals we "tune" parameters of the collective expression extraction procedure with respect to maximization of the network coherence. This allows us to pick up structures which are not detectable when dealing with individual patients separately.

Based upon our results, we also present a range of applications of (in particular metabolic) network coherence to the analysis of transcriptome profiles in chronic inflammatory diseases. This investigation seems to have huge potential for further development and following applications also outside of this specific field.

[1] Sonnenschein et al. (2011) BMC Systems Biology 5, 40.
[2] Sonnenschein et al. (2012) BMC Systems Biology 6, 41.
[3] Knecht et al. (2016). Scientific Reports, 6.
[4] Häsler et al. (2016). Gut, gutjnl-2016-311651.

BP 10: Postersession II

Topics: Cytoskeletal Filaments (10.1–10.8), Cell Mechanics (10.9–10.33), Cell Adhesion and Migration, Multicellular Systems (10.34–10.58), Neurosciences (10.59–10.61).

Time: Monday 17:30–19:30 Location: Poster C

BP 10.1 *(46)* Mon 17:30 Poster C

Mechanical Properties of Intermediate Filaments — Johanna Block[1], Hannes Witt[2], Julia Kraxner[1], Charlotta Lorenz[1], •Anna Schepers[1], Andreas Janshoff[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, Georg-August-Universität, Göttingen, Germany — [2]Institute of Physical Chemistry, Georg-August-Universität, Göttingen, Germany

Different cell types exhibit different mechanical properties which are determined by the cytoskeleton. Microtubules and microfilaments are conserved throughout all metazoan cell types, whereas different intermediate filaments (IFs) are expressed in a cell-type specific manner. Therefore, IFs are believed to play a major role in determining the mechanical properties of the different cell types. Using optical tweezers, combined with microfluidics and fluorescent microscopy, we directly probed the stretching behavior of single IFs. Under physiological buffer conditions and due to varying stretching protocols we found a strong loading rate dependent behavior as well as a tensile memory and a pronounced energy dissipation for the IF vimentin. By theoretical modeling and Monte Carlo simulations we are able to fit our data and link the results to the molecular structure of vimentin.

BP 10.2 *(48)* Mon 17:30 Poster C

Comparison of the cytoskeleton of squamous cells using fluorescence microscopy — •Mona Plettenberg[1], Maja Strugacevac[1], Constanze Wiek[2], Julia Kristin[2], Marcel Glaas[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany — [2]Düsseldorf University Hospital, Department of Othorinolaringology, Moorenstrasse 5, 40225 Düsseldorf, Germany

Our group's aim is to investigate the mechanical properties of benign and malign squamous cells. The fluorescence microscopy is one of the group's essential experimental techniques to gain new knowledge.

The cell's mechanical properties are mainly determined by the cytoskeleton. Especially the microtubule and actin filaments are key features for the cell's elasticity. In cancerous squamous cells, the cytoskeleton structures are changing. To investigate the differences, we compared the cytoskeleton of four cell lines extracted from tumors of different states in the head-neck area. By staining the cytoskeleton filaments with SiR-Actin and SiR-Tubulin, they could be observed under the fluorescence microscope. For this purpose, we optimized the staining process for our used cell lines.

The higher the tumor state is, the more the cytoskeleton is unorganized and the cells show more motility characteristics. We also could observe a decline of the actin-skeleton as well as of the microtubules. These facts lead us to the assumption that our investigated cells are more elastic in a higher tumor state.

BP 10.3 *(246)* Mon 17:30 Poster C

FRAP traces of immobile self-assembled complexes from Monte-Carlo simulations — •Justin Grewe[1,2] and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg — [2]Bioquant, Heidelberg

Non-muscle myosin II plays an important role in many essential cellular processes, including adhesion, migration and cytokinesis. Because myosin II is a non-processive motor, it cannot generate appreciable levels of force by itself, but needs to work in larger ensembles. In non-muscle cells, it assembles into myosin II minifilaments, which are approximately 300 nm large and contain around 30 myosin II molecules. As shown by experimental FRAP studies, this supramolecular complex is very dynamic, exchanging myosin monomers with a typical half time of 70 seconds. Using Monte-Carlo methods, we study the interplay between assembly and force generation in a spatial model for minifilaments. Our simulated FRAP-traces show the signature of different time scales, in contrast to the standard analysis of experimental FRAP-traces, which uses only one time scale.

BP 10.4 *(264)* Mon 17:30 Poster C

DNA based molecular force sensors in reconstituted actin networks — •Christina Jayachandran[1], Max Wardetzky[2], Florian Rehfeldt[1], and Christoph F. Schmidt[1] — [1]1Drittes Physikalisches Institut, Fakultät für Physik, Georg-August-Universität, Göttingen — [2]Institut für Numerische und Angewandte Mathematik, Georg-August-Universität, Göttingen

Actin, among the other bio-polymers present in cells, is largely responsible for cellular shape and mechanical stability. The actin cytoskeleton which self-assembles into networks of crosslinked filaments and bundles is responsible for active cellular processes ranging from migration, division and intracellular transport to morphogenesis. Crucial for these processes is the spatial and temporal regulation of the structure and dynamics of the network and of the generation of forces, mostly by myosin motors. To understand basic phenomena in such active networks, we investigate model networks comprised of semi-flexible actin filaments crosslinked by custom designed dsDNA constructs as flexible cross linkers. We also utilize these DNA constructs as force sensors in order to map stress distributions in the networks. We characterized the FRET-based stress sensors with a spectrophotometer. We study the rheological properties of the actin/DNA networks with a bulk rheometer and by high-bandwidth and high-resolution microrheology aiming to understand network failure mechanisms beyond linear response.

BP 10.5 *(282)* Mon 17:30 Poster C

Stretching Adherent Cells with Light — •Tobias Neckernuss, Daniel Geiger, Jonas Pfeil, Irina Schrezenmeier, and Othmar Marti — Institute of Experimental Physics, Ulm University

The mechanical properties of cells are important parameters in natural science and medicine. Over the years various techniques have been developed to assess parameters like stiffness, creep and relaxation constants of all kinds of cells. Often the investigation relies on the interaction of the cells with a probe like in AFM or micropipette aspiration. However, these techniques always measure properties of the joint system cell and probe.
In 2001 Guck et al. demonstrated a new method to trap and stretch cells in a microfluidic channel with laser light. To the best of our knowledge this technique has only been applied to suspended cells so far. We will present a novel setup to stretch and measure adherent cells - that is the majority of cells in the human body - with a laser. This represents the first non contact opportunity to deform cells perpendicular to the substrate. A demonstration of the capability of the technique to determine overall cellular stiffness is given. Furthermore, we show a selection of models for the viscoelastic response as well as a glimpse of further applications.

BP 10.6 *(292)* Mon 17:30 Poster C

Dynamic Actin Structures in Frog Egg Extract — •Jianguo Zhao and Christoph F. Schmidt — Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen

The actin cytoskeleton in eukaryotic cells undergoes continuous turnover, which is of crucial importance for various functions, e.g. cell motility and division. While components are constantly exchanged, the concentrations and distributions of components, including monomeric and polymeric actin often maintain a steady-state. On the other hand, cytoskeletal structures are also quite adjustable when needed, and different steady states can be accessed in response to regulatory signals. Given the complexity of cells, it is desirable to be able to study such dynamic rearrangements in reconstituted model systems. We employed water-in-oil emulsion droplets composed of Xenopus laevis egg cytoplasmic extract as a model system. In preliminary experiments, we observed local actin network clusters in the presence of Arp2/3 complex. The size of aggregated clusters was dependent on droplet dimensions, concentration of extract, nucleation protein and MgCl2. Small clusters were quite active and transported stress over a relatively long-distance inside the droplet.

BP 10.7 *(312)* Mon 17:30 Poster C

Failure of biological networks with dynamic cross-links — •Mareike Berger, David Brückner, and Chase Broedersz — Ludwig-Maximilians-Universität, Munich, Germany

The cytoskeleton is a complex network of crosslinked biopolymers, which is crucial for cellular rigidity and cell motility. To achieve such a variety of functions, it is important that these cytoskeletal networks can both withstand stress and adapt to external forces by remodeling. Rheological experiments with reconstituted crosslinked actin filament networks have revealed that these systems exhibit a complex viscoelastic response, which depends sensitively on the external stress imposed on the system: Under stress the network can behave either more fluid-like or more solid-like, depending on the configuration of the system. To investigate this behavior, we introduce a simple model of dynamically cross-linked networks. With this model we can study both these nonlinear viscoelastic properties as well as the failure of these networks under stress.

BP 10.8 *(396)* Mon 17:30 Poster C

Tug of War and Coordination in Bidirectional Transport by Molecular Motors — •Omar Munoz and Stefan Klumpp — Institut für Nichtlineare Dynamik, Universität Göttingen

Intracellular cargo transport is known to be bidirectional and mediated by molecular motors that bind to the cargoes and cytoskeletal filaments. Theoretical models for bidirectional transport include a tug-of-war between the motors and motor coordination through a mediator. Here, a tug-of-war model is extended to include motor activation and inactivation as a mechanism for biochemical coordination. Stochastic simulations provide an understanding of the dynamics of this system and of the effect of this additional coordination. The proposed coordination model is successful in describing the experimental observations of unexpectedly long unidirectional runs as well as memory of the direction after forced unbinding. These results and the recent experimental findings suggest that models of bidirectional transport should be cargo specific and combine features of both coordination and tug-of-war.

BP 10.9 *(40)* Mon 17:30 Poster C

Is the size of a cell nucleus an indicator for cancer? — •Lisa Rohde[1], Maja Strugacevac[1], Nina Bartels[1], Constanze Wiek[2], Julia Kristin[2], Marcel Glaas[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Heinrich-Heine-Universität Düsseldorf, Institute of Applied Physics, Düsseldorf, Germany — [2]Düsseldorf University Hospital, Department of Otorhinolaryngology

Identifying characteristics of cancer cells is still one of the main topics of recent research. Due to that our group is investigating properties of head and neck squamous cell carcinoma cells and dysplastic oral keratinocytes by fluorescence microscopy. The live cell imaging gives detailed information about single organelles, which is necessary for comparing the cell differences.

The nucleus is involved in the mitosis, contains the DNA and is therefore responsible for important physiological processes. As the mitosis rate is increased cancer cell nuclei hold much more chromatin than healthy cells do. This potential indicator for cancer motivates the comparison of the size of the different cell nuclei.

The cell nucleus is marked with Hoechst 33342, a blue fluorescent staining kit. The used laser scanning fluorescence microscope allows us three-dimensional cell nuclei observation. Different cancer cell lines and oral keratinocytes were compared to investigate whether the size of cell nuclei is an indicator for cancer.

BP 10.10 *(49)* Mon 17:30 Poster C

Stress fiber network organization during cell spreading on micropatterned substrates — •Dimitri Probst[1], Julia Jäger[1], Elena Kassianidou[2], Anne-Lou Roguet[3], Sanjay Kumar[2], and Ulrich S. Schwarz[1] — [1]Institute for Theoretical Physics and BioQuant, Heidelberg University, Heidelberg, Germany — [2]Department of Bioengineering, University of California, Berkeley, USA — [3]École Polytechnique, Palaisaeu, France

Cell spreading, adhesion and migration are strongly modulated by both biochemical and physical cues from the environment. The latter is particularly evident for the actomyosin system, whose organization is strongly determined by adhesive geometry, stiffness and topography of the extracellular environment. In order to understand how the actomyosin system dynamically responds to the adhesive geometry of its environment, we have studied cell spreading onto rectangular fibronectin frames with varying gap locations that determine final cell shape. We find that the global spreading dynamics onto a given pattern can be well predicted with a Cellular Potts Model describing the interplay between adhesion and tension, and that the distribution of stress fiber (SF) orientations can be predicted by establishing that discrete SFs form tangentially behind the advancing lamellipodium at spatial intervals of approximately 2.0 μm and temporal intervals of approximately 15 minutes. Because these times are comparable with the overall spreading times, cells have a memory of their spreading history through the organization of the SF network, despite the fact that their final shape is mainly dictated by the pattern geometry.

BP 10.11 *(54)* Mon 17:30 Poster C

Cytoskeletal morphology of oral keratinocytes and oral carcinoma cells — •Nina Bartels[1], Maja Strugacevac[1], Niklas Ullrich[1], Julia Kristin[2], Constanze Wiek[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, Heinrich-Heine-University Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany — [2]Department of Otorhinolaryngology, Düsseldorf University Hospital, Moorenstrasse 5, 40225 Dusseldorf, Germany

Our group is investigating the differences in cell morphology and physical properties of head and neck squamous cell carcinoma cells (HNSCC) and oral keratinocytes. As the cytoskeleton plays an important role in elasticity and mechanical properties of the cell, it is a significant part of our research. The cell lines, originating from different locations of the oral mucosa are investigated using a confocal laser scanning fluorescence microscope. To obtain more information about the cell morphology with a focus on the cytoskeleton, the cells were stained using SiR-Actin (actin filaments) and SiR-Tubulin (microtubules) staining kits. Three-dimensional images of the cells were used to compare the cytoskeleton of the different cell lines in size, volume and shape. The cytoskeleton of cell lines originating from the same area show similar properties whereas cell lines from other head and neck areas show differences. Our latest results will be presented and discussed.

BP 10.12 *(58)* Mon 17:30 Poster C

Characterization of a piezoelectric actuator for output power and thermal behaviour — •Tobias Löffler[1], Stefan Krüger[1], Maja Strugacevac[1], Julia Kristin[2], Constanze Wiek[2], Marcel Glaas[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf — [2]Düsseldorf University Hospital, Department of Otorhinolaryngology, Moorenstrasse 5, 40225 Düsseldorf, Germany

Our group is investigating the influence of acoustic waves on squamous cell carcinoma cells of the head-neck area in order to to determine their mechanical properties. A piezoelectric actuator with a sharp tip is used to produce sound waves in the range from 0,5 to 10 kHz. A detailed characterization of the acoustics is necessary for a better understanding of the interaction between the sound waves and the cells.

Temperature measurements at different distances in direction of oscillation and additional as a function of time have been performed in order to determine the temperature-profile in the vicinity of the probe. Additionally, the output energy was characterized. The experimental setup and the probe's characteristics will be presented in detail.

Furthemore, we observed the behaviour of the cancer cells on acustic waves at various frequencies and sound intensities. These results will be presented as well.

BP 10.13 *(70)* Mon 17:30 Poster C

Time Resolved Measurements of Force Evolution in Platelets Under Flow Condition — •Jana Hanke, Anna Zelena, and Sarah Köster — Institute of X-Ray Physics, University of Göttingen, Göttingen, Germany

Force generation plays an important role for numerous biological processes like contraction, spreading and motility. In vivo, both chemical and physical cues influence this process. For cells like e.g. endothelial cells and blood cells, an important physical factor is external shear flow. Blood platelets, in particular, generate strong forces while constantly being subject to shear. Hence, studying the impact of shear on their contractile behaviour is important for the understanding the mechanics of blood clotting. Here, we present a method combining microfluidics with time-resolved traction force microscopy to mimic blood flow. We study the adhesion and contraction of human blood platelets under low shear rate conditions as found in veins and compare the results to data recorded without flow. We can reveal that the spatial traction force distribution and the total force remains unchanged with increasing shear flow. Similarly, the force dipoles show no difference in the degree of anisotropy between static and flow conditions. Interestingly, however, when studying the preferred orientation of contraction with respect to the flow direction, we observe adaptation of the platelets to the flow. With increasing shear rate, the angle rises from 45° to 90°. Our microfluidic chamber can be easily reproduced and adapted to mimic various different physiological conditions,

enabling the study of other cell types.

BP 10.14 *(102)* Mon 17:30 Poster C

How filaments density impacts force generation and protrusion rate of lamellipodium in motile cells — •Setareh Dolati and Martin Falcke — Max delbrück center for molecular medicine(MDC), Berlin, Germany.

In Migrating cells, the Arp2/3-complex is thought to be responsible for formation and maintenance of the lamellipodium. However, studies show in addition to Arp2/3 activity formins also contribute to actin filament nucleation and elongation in the lamellipodium of B16-F1 melanoma cells and their activity strongly impacts force generation. Loss of formins reduces actin density, lamellipodium width and protrusion velocity of B16-F1 melanoma cells, while Arp2/3 activity and the actin network assembly rate are not affected by the absence of formins. Knocking out FMNL2 and FMNL3 individually and both together shows a correlation between actin filament area density and protrusion rates. Also, by manipulating Arp2/3 activity in B16-F1 melanoma cells, the same correlation between the protrusion rate and the filament area density in the lamellipodium has been observed.

Here, we mathematically model the lamellipodium as a viscoelastic gel representing an actively polymerizing and cross linked network of actin filaments. Taking the density of filaments as a control parameter, we suggest a mechanism that explains how the formins contribution to the actin area density leads to their corresponding contribution to the protrusion rate in the lamellipodium and how the structure of the actin network and properties like assembly rate of the network affect the dynamics of the lamellipodium.

BP 10.15 *(131)* Mon 17:30 Poster C

Cellular Forces under Altered Gravity Conditions — •Julia Eckert[1,2,3], Stefano Coppola[2], Thomas Schmidt[2], Lukas M. Eng[1], Robert Lindner[3], and Jack J.W.A. van Loon[3,4] — [1]School of Science, Department of Physics, Technische Universität Dresden, Dresden, Germany — [2]Physics of Life Processes, Leiden Institute of Physics, Leiden University, Leiden, The Netherlands — [3]Life & Physical Science, Instrumentation and Life Support Laboratory (TEC-MMG), ESA/ESTEC, Noordwijk, The Netherlands — [4]VU Medical Center/ACTA, Amsterdam, The Netherlands

During future long-term space missions, the human organism will be exposed to microgravity and other gravitational levels for extended periods of time. Hence, it is of vital importance to develop a basic understanding of mechanobiology and mechanosensing under such conditions.

Here, we introduce a measuring approach based on a micropillar array technology. Different cell types, like bone and fibroblast cells, were placed on polydimethylsiloxane pillars with controlled stiffness allowing to examine cell traction forces. Further, they were exposed to altered gravity in the Large Diameter Centrifuge and in the Random Positioning Machine of the European Space Agency in The Netherlands. We found that cells respond to the new gravitational environment and their behavior depend on g-force into or away from the pillar array, substrate stiffness and their cell type. Our approach is suitable to study biological response to changing gravity conditions at the cellular level.

BP 10.16 *(132)* Mon 17:30 Poster C

Design and construction of a magnetic trap for microrheological measurements — •Jonas Pfeil, Irina Schrezenmeier, Tobias Neckernuss, Daniel Geiger, Frederike Erb, Fabian Port, and Othmar Marti — Institute of Experimental Physics, Ulm University, Ulm, Deutschland

Today microrheological measurements on living cells using optical tweezers are scientific state of the art for analysis of cell mechanics. The maximum force that can be exerted on cells is limited by the maximum tolerable temperature of the cell. This limits the maximum forces to the nN range, which are too small to deform a whole cell significantly.

In contrast magnetic traps using superparamagnetic beads and high speed optical measurements do not heat the sample. Instead the limiting factors are magnetic flux and the gradient of the magnetic flux, which corresponds to the force on the beads. To achieve high gradient fields strong magnets can be used or the tip of the magnet has to be brought to the vicinity of the sample.

We will present solutions for the construction of a magnetic trap using a sharp tip and a single electromagnet using previously published designs adapted to our setup and our performance needs.

BP 10.17 *(134)* Mon 17:30 Poster C

The role of endothelial cell mechanics in leukocyte extravasation — •Matthias Brandt[1], Volker Gerke[2], and Timo Betz[1] — [1]Institute of Cell Biology (ZMBE), University of Münster, Von-Esmarch-Straße 56, D-48149 Münster — [2]Institute of Medical Biochemistry (ZMBE), University of Münster, Von-Esmarch-Straße 56, D-48149 Münster

The endothelium forms the inner surface of blood and lymphatic vessels in the human body. For the immune response of an organism, leukocytes need to transmigrate through this endothelial cell (EC) monolayer, which requires coordination and adaptation of the EC and leukocyte mechanics. We aim to investigate the effect of EC stiffness on leukocyte guidance and the role of EC mechanics in this transendothelial migration.

We use an *in vitro* model consisting of HUVEC cells cultivated on a polyacrylamide gel substrate functionalized with basement membrane proteins, and leukocytes flown in by a microfluidic setup. The impact of varying substrate stiffness on EC mechanics and the question to which extend stiffness gradients are reflected by the endothelium itself is examined. Traction force microscopy serves to measure forces applied by the ECs to the substrate and to infer force transmissions at cell-cell junctions. The stiffness of the EC cortex and intracellular forces are measured using an optical tweezer. Using optogenecic activation of Rac1, RhoA and CDC42 signaling will generate localized EC contractility allowing to correlate EC mechanics and leukocyte migration.

BP 10.18 *(137)* Mon 17:30 Poster C

Flow of a cell inside a microfluidic channel using FEM simulation — •Ralf Schuster[1], Tobias Neckernuss[1], Daniel Geiger[1], Ulrich Simon[2], Kay-Eberhard Gottschalk[1], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, D-89081 Ulm — [2]Ulmer Zentrum für Wissenschaftliches Rechnen (UZWR), Ulm University, D-89081 Ulm

From the mechanical deformation of cells conclusions, regarding type, state, size or some inherent feature, can be drawn. Variations of structure and shape of cells play an important role for cell migration and proliferation. For instance tumor and normal cells can be distinguished by elasticity, indicated by the amount of deformation under a given stress. Metastasizing cancer cells can have a softer cytoskeleton through changes in the network, leading to a reduced drag resistance when passing through narrow constrictions.

The parabolic flow profile inside a microfluidic channel causes the cells to deform, while passing through it. The deviation from circularity of the cell at steady-state conditions can be taken as a characteristic measure for the deformation (Otto et al. Nature Methods 2015). Two different finite element-modeling approaches will be shown. The composition and the values of the properties of the cell are generated according to other works and experiments, performed at our Institute. Achieving accordance between experiment and simulation will lead to numerical values for the material parameters of cells respectively cell types and will be the basis for further experiments.

BP 10.19 *(138)* Mon 17:30 Poster C

Intracellular passive and active microrheology in dividing epithelial cells — •Sebastian Hurst and Timo Betz — Institute of Cell Biology, ZMBE, University of Münster, Von-Esmarch-Straße 56, 48149 Münster

While there is a good understanding of chromosome segregation during cell division, surprisingly little is known about how the different organelles are distributed during this fundamental process. It is generally assumed that organelles are not systematic transported to the daughter cells but that their distribution relies on passive diffusion and hence stochastic transport throughout the cell. Although diffusion will provide fast mixing of small molecules, it is not clear if this can explain the even distribution of larger organelles with low copy number, especially in highly polarized cells.

Active, targeted transport of large organelles during cell division is mainly known for asymmetric cell division, and has not been reported in symmetric division. Another attractive mechanism for equal distribution of organelles during cell division is the increase of random mobility. This could be achieved by active, undirected fluctuations e.g. generated through motor protein activity. To test this hypothesis that active fluctuations help distributing organelles we perform optical tweezer based passive and active microrheology measurements with exogenous particles inside dividing MDCK cells. The results are used

to calculate the intracellular viscoelasticity and mechanical activity to pinpoint the influence of active cytosolic mixing during cell division.

BP 10.20 *(142)* Mon 17:30 Poster C

Design and characterization of mechanically tunable hyaluronic acid based hydrogels — •Martin Schilling and Florian Rehfeldt — Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany

Many aspects of cell behavior are influenced by the mechanical properties of their microenvironment. To mimic the various elastic moduli of different in vivo environments of cells, it is necessary to design and characterize hydrogels for cell culture with tunable elasticity.

Hyaluronic acid (HA), a polysaccharide consisting of disaccharide units, was chosen as base for the hydrogel system as it is biocompatible and not toxic for cells, thus allowing for 3D encapsulation.

However, native HA does not crosslink naturally so its disaccharides have to be chemically modified. Depending on the degree of modification HA can be used for different approaches. High modified HA hydrogels are tunable in a large range of elasticities and due to their degree of modification cannot be recognized by HA receptors of cells that need longer segments of unmodified disaccharides. A lower degree of modification decreases the range of elasticity but allows for cellular recognition of HA. In order to obtain a hydrogel with moderate elasticity and the properties of low modified HA both high and low modified HA are mixed in several different ratios. The gelation kinetics of the resulting hydrogels are investigated by rheology using oscillatory deformation tests. In order to analyze the viscoelastic properties of the cross-linked hydrogels the storage modulus G' and the loss modulus G" were measured.

BP 10.21 *(159)* Mon 17:30 Poster C

Mechanical and biochemical micromanipulation of individual suspended cells probed with optical tweezers — •Samaneh Rezvani[1], Todd M. Squires[2], and Christoph F. Schmidt[1] — [1]Third Institute of Physics-Biophysics, Faculty of Physics, University of Göttingen, Göttingen, Germany — [2]Department of Chemical Engineering, University of California, Santa Barbara, USA

Cells communicate with their environment through biochemical and mechanical interactions. They can respond to stimuli by undergoing shape- and, in some situations, volume changes. Key determinants of the mechanical response of a cell are the viscoelastic properties of the actomyosin cortex, effective surface tension, and osmotic pressure. It is challenging to measure the mechanical response of cells while changing environmental conditions. We here demonstrate the use of a novel microfluidic device with integrated hydrogel micro-windows to change solution conditions for cells suspended by optical traps. Solution conditions can be rapidly changed in this device without exposing the cells to direct fluid flow. We use biochemical inhibitors and varying osmotic conditions and investigate the time-dependent response of individual cells. Using a dual optical trap makes it possible to probe the viscoelasticity of suspended cells by active and passive microrheology and to quantify force fluctuations generated by the cells at the same time.

BP 10.22 *(213)* Mon 17:30 Poster C

A 2-D Continuum Model of Cell Migration — •Behnam Amiri and Martin Falcke — Max Delbrück Center for Molecular Medicine(MDC), Berlin, Germany.

Actin-based cell migration is critical for many biological processes including embryonic development and tumor metastasis. At the leading edge of the motile cells, polymerization of actin filaments creates the force necessary for protrusion. Here we present a 2-dimensional continuum model for the lamellipodia dynamics of a motile cell. The model quantitatively describes the pushing forces exerted by newly polymerized filaments in a semi-flexible layer behind the leading edge, and their effect on the retrograde flow of the cytoskeleton and the membrane protrusion. We will demonstrate that the interplay between these components can determine the most prominent aspects of the cell morphodynamics. The developed modeling framework consists of a coupled system of Reaction-Diffusion-Advection PDEs for cytoskeleton components, a stokes flow PDE for velocity profile of the cytoskeleton and a Reaction-Advection PDE for the properties of filaments in the semi-flexible region along the leading edge. All of these equations must be computed in the unsteady moving cell domain and with appropriate boundary conditions at the moving cell boundary. In order to numerically solve this hybrid continuum model, we use a moving boundary finite element scheme for free boundary problems. Our model gives insight into how actin polymerization at the leading edge can affect the overall morphodynamics of the cell.

BP 10.23 *(236)* Mon 17:30 Poster C

Near Real Time Analysis of Stress Fiber Formation in Stem Cells — •Lara Hauke, Carina Wollnik, and Florian Rehfeldt — University of Göttingen, Third Institute of Physics - Biophysics

Human mesenchymal stem cells (hMSC) can be directed to differentiate into various lineages by different matrix elasticities. While changes in lineage specific protein expression occur over a period of days to weeks, significantly different structures of stress fibers are observable within the first 24 hours of plating [1] quantified by an order parameter S. With our massively parallel live-cell imaging set-up we record cells under physiological conditions (37 °C, 5 %CO2) over a period of 24-48 hours to obtain a statistically sufficiently large data set. We aim for a full representation of filament processes over time and space allowing for statistical analysis. This unbiased classification will be represented by persistence in space and time and potential cross-talk with other cytoskeletal components. For this we developed the *FilamentSensor* [2,3] a freely available tool for near real-time image analysis of stress fibers. We present experimental data where we can distinguish the development of hMSCs on 1 kPa, 10 kPa and 30 kPa elastic substrates with 99 % confidence and are working on single filament tracking and better analysis of orientation fields. References: [1]A. Zemel, et al., Nat. Phys., 2010. [2]www.filament-sensor.de [3]B. Eltzner, et al., PLoS One, 2015.

BP 10.24 *(244)* Mon 17:30 Poster C

Elastic Response of Epithelial Model Tissues in Deformation Experiments — •Simone Gehrer[1], Sara Kaliman[1], Damir Vurnek[1], Maryam Aliee[1], Shuqing Chen[2], Andreas Maier[2], Diana Dudziak[3], Rudolf Merkel[4], and Ana-Sunčana Smith[1,5] — [1]PULS Group, Institute for Theoretical Physics I, FAU Erlangen — [2]Pattern Recognition Lab, Department of Computer Science 5, FAU Erlangen — [3]Dermatology, Universitätsklinik Erlangen — [4]ICS-7: Biomechanics, Forschungszentrum Jülich — [5]Division of Physical Chemistry, IRB Zagreb

Epithelial tissues act as barriers between different tissue types and form boundaries of the majority of organs. They are often exposed to mechanical stress to which they quickly respond by changing shape and internal organization on short time scales. On longer time scales, stress can be released by proliferation and growth.

To investigate the response of MDCK II tissues grown on PDMS substrates, we expose the cell-colonies to an uniaxial stress (10 – 30%) using a stretching device. The resulting changes are monitored for minutes to days by phase-contrast and confocal microscopy. The reversible changes in the overall shape of the cell confirm that on short time scales the tissue responds as an elastic material. This is furthermore confirmed by analysing the morphology and connectivity of individual cells before and after stress. On longer time scales, we find that the growth rate of the colony is affected by the continuous deformation, while after 24 – 48h the tissue adapts and resumes the morphological and topological characteristics as the control.

BP 10.25 *(254)* Mon 17:30 Poster C

Cell-Type Specific Mechano-Sensing Altered by Blebbistatin — •Galina Kudryasheva and Florian Rehfeldt — Göttingen University

Cells sense the mechanical properties of their surroundings with contractile acto-myosin stress fibers through focal adhesions and react to such physical stimuli by distinct pattern formation of their cytoskeleton and by altering their bio-chemical pathways. Especially striking is the mechano-guided differentiation of human mesenchymal stem cells (hMSCs). The structure and dynamics of acto-myosin stress fibers is used as an early morphological marker and theoretically modelled using classical mechanics with an active spring model. We use this approach to elucidate the mechanical cell-matrix interactions of hMSCs and several types of differentiated cells. Employing immuno-fluorescence microscopy we visualize stress fibers and analyze the global morphology of the cells cultured on elastic substrates (E_m from 1 kPa to 130 kPa). Applying the theoretical model to our experimentally obtained cell spread area we extract an effective Young's modulus of the cell (E_c). We demonstrate that E_c changes during hMSCs differentiation process and varies for different cell lines. Our experiments show that the mechanical susceptibility is cell type specific and dependent on acto-myosin contractility. Interestingly, addition of the non-muscle myosin II (NMMII) inhibitor blebbistatin at low concentrations (c =

12.5 and 25 uM) softens the cells (reduces the effective Young's modulus E_c) and facilitates cell spreading only on soft substrates through relaxing the cellular acto-myosin cortex.

BP 10.26 *(271)* Mon 17:30 Poster C

Elastic beads as in vivo tension sensors — •Arne Hofemeier, Bernhard Wallmeyer, and Timo Betz — Institute of Cell Biology, ZMBE, University of Münster

Mechanical tension has recently been recognized as a key element to understand many biological processes such as cell fate determination or collective cell migration during embryogenesis. However, direct experimental access to determine tension in vivo in a non-destructive way remains a major challenge. Here, we present a novel experimental approach that allows direct measurement of stress inside in vitro and in vivo tissue. By injecting fluorescent polyacrylamide (PAA) beads of known size and elasticity in the tissue, we are able to measure the deformation of their surface and obtain the resulting displacement vector. Solving the inverse elastic problem yields an approximation of the stress field inside the tissue. Furthermore, we show two applications of this novel technique. Firstly, PAA beads are injected into mouse muscles to examine forces exerted during muscle contraction on muscle stem cells, a cell type known to respond to changes of mechanical properties. Secondly, PAA beads are injected into zebrafish embryos to investigate the role of tissue stress in collective cell migration during embryogenesis.

BP 10.27 *(276)* Mon 17:30 Poster C

Fluid flow in curvilinear microchannels for stem cell purification- understanding the deformability-induced lift force — •Ewa Guzniczak[1], Melanie Jimenez[2], and Helen Bridle[1] — [1]Heriot-Watt University, School of Engineering and Physical Science, Department of Biological Chemistry, Biophysics and Bioengineering Edinburgh Campus, Edinburgh EH14 4AS — [2]University of Glasgow, School of Engineering, Biomedical Engineering Division, Glasgow G12 8QQ

Traditionally, fluid flow in microscale confined channels has been associated with a negligible inertia since fluid flow occurs at low Reynold's numbers. However previous work (Di Carlo 2009) has shown physical phenomena occurring at commonly neglected intermediate flow regimes, namely secondary flow and inertial migration of particles, determined by channel geometry, particle size and flow rate. The interplay between fluid flow pattern and particles, if fine-tuned, leads to particles ordering and separation, and the effect has been exploited in a range of applications. However, biological particles due to their deformable nature add complexity to the focusing mechanism and it is challenging to predict their behaviour. We exploit inertial focusing in curvilinear microchannels to purify manufactured red blood cells, which are the end-products of stem cell differentiation. Separation is based on their physical properties, namely size and deformability. Thus, we are also exploring how deformability-induced lift force affects and contributes to particles separation in the spiral microchannel.

BP 10.28 *(283)* Mon 17:30 Poster C

Measurements and Simulations with the CellMOUSE device — •Jonas Pfeil, Tobias Neckernuss, Daniel Geiger, Ralf Schuster, and Othmar Marti — Institute of Experimental Physics, Ulm University

We recently developed a tool to characterize suspended cells passing an optical sensor, the so called CellMOUSE device. With this high speed optical setup we are able to determine different parameters like shape, size and morphology of the passing particles. These are important markers to distinguish different cells.
We will show measurements of various samples using the CellMOUSE device to show the range of possible applications. Besides investigations of well known samples for validation of the measurement principle, we also observe and distinguish cells of different origins in mixtures. Due to the real time nature of the experiment, we are able to manipulate single cells according to the measurement result. The technique can be also applied to other samples like bacteria or particles of different sizes.
To complete the study, we developed a simulation system for CellMOUSE to determine the figures of merit a priori.

BP 10.29 *(296)* Mon 17:30 Poster C

Cells Modeled as Osmotically Pressurized Elastic Shells — •Behzad Golshaei, Renata Garces, Samaneh Rezvani, and Christoph F Schmidt — Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen

Animal cells, as well as bacteria, are mechanically protected by a viscoelastic envelope consisting of lipid membranes and polymer networks. External mechanical stimulation leads to responses such as deformations or flows. In order to understand the mechanical behavior of cells, we model cells as pressurized elastic shells using finite element modeling. We study how geometrical parameters (cortex thickness and cell diameter), thermodynamic effects (osmotic pressure difference), and material properties (Young*s modulus) affect the response of a cell to indentation. We focus on the time scales where cellular systems show elastic behavior in order to compare our model with experimental results. Results from two types of experimental set-ups have been used to parameterize linear elasticity equations. The first set of experiments used an optical trap to indent mammalian cells, and in the second set, bacteria were indented by beads of varying diameter using AFM.

BP 10.30 *(305)* Mon 17:30 Poster C

Mechanical Coupling of Human Embryonic Stem Cell Derived Cardiomyocytes — •Heidi Somsel[1], Wolfram-Hubertus Zimmermann[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen — [2]Institut für Pharmakologie und Toxikologie, Universitätsmedizin Göttingen, Georg-August-Universität Göttingen

In the United States, someone suffers a myocardial infarction every 40 seconds[1]. A major long-term effect of these infarctions is scar tissue with a stiffness (40 kPa) that is larger than the surrounding myocardium (15 kPa). These scars strongly interfere with heart function.

Mechanical coupling between CMs is believed to play an important role in stabilizing the global contraction of the heart[3]. In this study, we aim to understand mechanical coupling and synchronization between neighboring pairs of CMs. Human embryonic stem cell (hESC) derived CMs were plated on PDMS substrates in geometries with physiological aspect ratios. The Young's moduli of the underlying substrate were varied from those of the healthy heart (15 kPa) to infarcted tissue (45 kPa) to model the reaction of CMs in response to these different myocardial regimes. We found synchronization in frequency and phase between neighboring cells. 1] Benjamin, E., et al.(2017). 2] Riegler, J., et al.(2015). 3] Nitsan, I., et al.(2016).

BP 10.31 *(348)* Mon 17:30 Poster C

Probing C. Elegans Micromechanics in vivo — •Peter Weist, Renata Garces, Eugenia Butkevich, and Christoph F. Schmidt — Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen

To perform undulatory locomotion, C. elegans generate forces acting not only on the surrounding environment but also against its own-body bending resistance. The decoupling of body passive-active responses during the bending is crucial to quantify the forces generated by the worms muscles. To date, a direct measurement of the stresses involved in the worms deformation is lacking. In this contribution, we present an experimental set-up that monitors the global response of individual worms to bending and pulling forces in a simple geometry. Living worms are kept straight by clamping their extremities onto agar plates. We pull and move the center of the worm with a custom-made cantilever of known spring constants (values around 1 N/m). We measure the loading forces and displacement profiles. Describing the worm body as a purely elastic material, we are able to determine bending and stretching contributions to the global stiffness and to derive material parameters. Furthermore, to separate the passive response of the body from the muscle activity, we vary the contraction-relaxation state of the muscles using pharmacological treatments. We provide a synthesis of the typical range of magnitudes of the worm's material parameters for different muscles states. The characterization technique for the mechanics of wild-type worms we propose can be used as a standard test for muscle functioning, including genetically modified species.

BP 10.32 *(394)* Mon 17:30 Poster C

Elasto-Tweezers: A novel platform for high-precision cell elasticity measurements — •Sebastian Knust[1], Andy Sischka[2], Hendrik Milting[3], Bastien Venzac[4], Séverine Le Gac[4], Elwin Vrouwe[5], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University, Bielefeld, Germany — [2]Ionovation GmbH, Osnabrück, Germany — [3]Heart and Diabetes Center NRW, Ruhr University of Bochum, Bad Oeynhausen, Germany — [4]Amber, MESA$^+$ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands — [5]Micronit Microtechnologies B.V., Enschede, The Netherlands

The correct mechano-elastic properties of human cells are essential for their health and function. However, certain diseases like some cancers and cardiomyopathies alter those properties. High-throughput and high-resolution measurements of cell elasticities can therefore be used to provide insights into the pathomechanisms of these diseases.

We are able to directly measure both the forces applied to the cell with piconewton resolution and the cell deformation with submicrometre resolution by using a dual-beam optical tweezers setup with video-based force detection and coupling of functionalised beads to the cell surface. This allows all elasticity measurements with superior resolution compared to other techniques like optical stretchers.

To achieve high-throughput measurements, this novel setup will be combined with custom-designed microfluidical cartridges to facilitate automated and reliable formation of cell-bead complexes to perform completely automated measurements of up to 600 cells per hour.

BP 10.33 *(415)* Mon 17:30 Poster C

Cortical Actin Contractility of Single Suspended Cells — •Enrico Warmt, Steffen Grosser, Erik Morawetz, and Josef Käs — Universität Leipzig, Soft Matter Physics Division, Linnéstr. 5, 04103 Leipzig

Up to now cellular contractility was seen basically as a force dipole requiring adhesion sites and actin stress fibers, mainly necessary during cell migration. In this study, we investigate suspended cells regarding active contractility, lacking stress fibers and adhesion points. Epithelial cells assemble a strong acto-myosin cortex providing pretension forming round cell shape, and exhibiting more contractile behavior during long optical stretcher observation. In contrast, mesenchymal cells, show more elongated cell shapes and less cortical contractility. Cell contractility needs a short mechanical impulse to induce acto-myosin contraction of the cell cortex, even below initial cell elongation. We will focus on how these findings correlate to different migratory and jamming behavior in healthy and mesenchymal cell clusters.

BP 10.34 *(72)* Mon 17:30 Poster C

Dynamic patterns of the plant growth regulator auxin — •João Ramos and Karen Alim — Max Planck Institute for Dynamics and Self-Organization

Auxin is a phytohormone whose patterns are responsible for plant morphogenesis and triggering cell fate decisions. Patterns of auxin concentration and flow change dynamically throughout plant development with the help of membrane bound efflux (PIN) and influx carriers (AUX/LAX). Nevertheless, the mechanisms behind auxin transport are still not fully understood, in particular, current models fall short on explaining fountain-like auxin flow patterns during lateral root formation. Recently, observations show that PIN localisation is influenced by mechanical stress/strain, which coupled with the auxin-induced local decrease of cell wall stiffness, has the potential to unlock our understanding of auxin transport phenomena. Moreover, experimental efforts in observing morphodynamics and auxin carriers during lateral formation were recently boosted with the advent of light sheet microscopy, in effect turning lateral root formation into a new prime model system for auxin transport. Here, we study a vertex model for cell wall mechanics, coupled with a compartment model of auxin transport from a cell to its immediate neighbours both passively and carrier mediated. More specifically, the effect of cell wall stress on PIN cycling, auxin-induced wall softening and AUX/LAX expression positive feedback on auxin levels, are taken into account. This model will later be coupled to a tissue growth model, in order to study how auxin patterns change dynamically during lateral root formation.

BP 10.35 *(119)* Mon 17:30 Poster C

Inferring the rules of single cell behavior from video recordings of collective tumor cell systems — •Claus Metzner, Julian Übelacker, Nico Wunderling, Christoph Mark, Franziska Hoersch, Christina Hillig, and Ben Fabry — Biophysics Group, Friedrich-Alexander Universität, Erlangen, Germany

Collective effects in multicellular systems emerge from the behavior of the individual cells and their mutual interactions. Identifying the rules of this cell behavior is difficult, due to their stochastic nature. Moreover, different microscopic rules can be consistent with the same macroscopic effects. We therefore present a machine learning method that extracts a stochastic model of single cell behavior from video recordings of multicellular systems. The method is based on a Maximum Likelihood approach that analyzes the motion of individual cells relative to their immediate neighbors. In particular, we extract the average speed and directional persistence of individual cells, as well as a pair-wise, distance-dependent interaction potential between nearby cells. First, we demonstrate the feasibility of the method by extracting the rules from simulated data with known model parameters. Next, we apply the method to multicellular systems consisting of a single cell type (MDA-MB-230, or HT1080), seeded on a flat cell culture dish. Finally, we investigate mixed systems of immune cells (Natural Killer (NK) cells, T-cells) and tumor cells (K562 lymphoma and MeWo melanoma cell lines) in a collagen gel and extract the maximum distance from which the immune cells can detect their targets.

BP 10.36 *(133)* Mon 17:30 Poster C

3D collective migration in cancer spheroids and during invasion — •Swetha Raghuraman and Timo Betz — Institute of Cell Biology, ZMBE, University of Münster, Von-Esmarch-Straße 56,48149 Münster

Cancer cells move collectively in order to migrate and overcome space constrictions and geometric obstacles. This movement is characterized by cell-cell adhesion differences, the extracellular matrix or cell-substrate interactions, as well as intercellular cross-talks during invasion, morphogenesis and wound healing. The mechanisms and the physics behind coordinated behavior of cells have been studied recently at the 2D level, and in-vivo tissue homeostasis. However, due to the challenges involved in reproducing and imaging tumor spheroids, collective motion of 3D cancer invasion remains a complex task. With the use of Light Sheet Microscopy, we have been able to record cancer spheroids with fluorescently marked nuclei over several days at sub-cellular resolution. 3D particle tracking of several thousand cells allows well defined velocity correlations and density fluctuation measurements within the spheroid, and at the cell invading a collagen matrix. By combining these parameters we will test the hypothesis whether cancer cell migration in 3D is physically similar to active jamming, as recently suggested in 2D situations.

BP 10.37 *(141)* Mon 17:30 Poster C

Light-Switchable Adhesion of Soil-Dwelling Microalgae — •Christian Titus Kreis[1], Christine Linne[1], Marine Le Blay[1], Alice Gragnier[1], Marcin Michal Makowski[1], Maike Lorenz[2], and Oliver Bäumchen[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, D-37077 Göttingen, Germany — [2]SAG Culture Collection of Algae, Nikolausberger Weg 18, D-37073 Göttingen, Germany

Freshwater microalgae live in heterogeneous, aqueous habitats, such as soil, aquatic sediments, puddles, and lakes. Besides having fundamental ecological functions and enormous technological potential in photobioreactors, microalgae form biofilms on surfaces in wet environments, which may affect the functionality of any anthropogenic structures. Despite the relevance of controlling microalgal adhesion, the biological mechanisms and intermolecular forces that govern microalgal adhesion to surfaces are poorly understood. We discovered in micropipette-based *in vivo* force spectroscopy that the adhesion of the unicellular microalgae *Chlamydomonas reinhardtii* to surfaces can be reversibly switched on and off by tailoring the light conditions [1]. Here, we present results on the underlying molecular mechanism of light-switchable flagella-mediated adhesion. Additionally, we performed experiments with other unicellular microalgae indicating that actively controlled flagella adhesiveness might be a more generic trait of soil-dwelling microalgae.

[1] Kreis et al., *Nature Physics*, 2017, doi:10.1038/nphys4258.

BP 10.38 *(149)* Mon 17:30 Poster C

Dynamics of actin stress fiber patterns in laterally confined cells — •Andreas Müller and Tilo Pompe — Universität Leipzig, Institute of Biochemistry, Johannisalle 21-23, 04103 Leipzig, Germany

Cell shape and function are inseparably linked. Cell shape can be regulated intracellularly by structural proteins or extracellularly by adaption to the surroundings. In this way, the extracellular geometry can be used to manipulate cell function.

We use glass substrates and soft polyacrylamide hydrogels that are micro-structured with stripe-like patterns to study the adaptation of cells to adhesion geometry. Isolated HUVECS are studied for several hours in order to correlate the their morphology, the reorganization of their actin cytoskeletons, and the dynamics of cell traction forces in response to lateral constraint. Current work focusses on live-cell imaging to reveal stress fiber dynamics and concurrent traction forces. We found that aligned stress fibers in polarized cellssmove inward, perpendicular to their orientation and the direction of main traction forces. In addition, the directionality and magnitude of traction forc-es are

strongly correlated to cell shape and actin cytoskeleton pattern with an overall dependence on the degree of confinement.

Overall, our setup allows us to quantitatively analyze in a time-resolved manner the cell's morphological and mechanical adaption to spatial confinement in correlation to the actin cytoskeletal components as the main contributors to the force homeostasis. By that, we aim to contribute to elucidate the mechanisms behind the mutual relationship between cell shape and function.

BP 10.39 *(151)* Mon 17:30 Poster C

Bacterial adhesion on nanostructured silicon surfaces — •Friederike Nolle[1], Johannes Mischo[1], Christian Spengler[1], Nicolas Thewes[1], Markus Bischoff[2], and Karin Jacobs[1] — [1]Department of Experimental Physics, Saarland University, Saarbruecken — [2]Institute for Medical Microbiology and Hygiene, Saarland University, Homburg/Saar

To prevent the inflammation of a medical implant, its material specifications are of crucial importance. An ideal surface would hinder bacterial biofilm formation and/or kill adhering pathogens without harming surrounding somatic cells. Surface modifications of single attributes have to be controlled and possible changes in adhesion of bacteria to these surfaces have to be observed. This study focuses on the nanoroughness of silicon surfaces, obtained by wet chemical etching, and its influence on bacterial adhesion (*Staphylococcus aureus*). The adhesion of bacteria is mediated by biopolymers, the properties of which we are able to characterize by AFM force spectroscopy, where the probe is a single bacterium. With our setup an insight into the adhesion force of *Staphylococcus aureus* was gained and also changes of the bacterial viability on the rough surfaces compared to smooth silicon surfaces were examined. In addition, the impact of hydrophobicity of rough silicon surfaces on adhesion was considered by silanizing the hydrophilic silicon.

BP 10.40 *(158)* Mon 17:30 Poster C

Phase field modeling of moving cells - shedding light on the motility onset — Cody Reeves[1,2], Benjamin Winkler[3], Igor Aranson[2,4], and •Falko Ziebert[5,3] — [1]Engineering Sciences and Applied Mathematics, Northwestern University, Evanston, USA — [2]Materials Science Division, Argonne National Laboratory, USA — [3]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany — [4]Department of Biomedical Engineering, Pennsylvania State University, University Park, USA — [5]Institute for Theoretical Physics, Ruprecht-Karls-University Heidelberg, Germany

Substrate-based crawling motility of eukaryotic cells is essential for many biological functions, both in developing and mature organisms. Although a comprehensive understanding remains elusive, progress has been achieved recently in its modelling on the whole-cell level. We survey the recent advances made by employing the phase field approach, a powerful method to implement moving, deformable boundaries. The developed approach in addition is modular in the sense that, depending on the problem at hand, different model components (e.g. adhesion dynamics, substrate deformation and membrane feedback) can be included or disregarded without changing the formalism. We exemplify the approach by showing that our framework captures the spontaneous rotational states prior to the cell motility onset and cell polarization, recently found for keratocytes by two groups (S. Lou et al. JCB 2015; F. Raynaud et al. Nature Phys. 2016), and interpret them as nonlinear shape deformation waves.

BP 10.41 *(170)* Mon 17:30 Poster C

3D-environments shape T-cell motility and cell-cell contacts during HIV-1 infection — Andrea Imle[1], •Nikolas Schnellbächer[2,3], Peter Kumberger[3], Jana Fehr[3], Paola Carillo-Bustamante[3], Frederik Graw[3], Ulrich Schwarz[2,3], and Oliver Fackler[1] — [1]Department of Infectious Diseases, Integrative Virology, University Hospital Heidelberg — [2]Institute for Theoretical Physics, Heidelberg University — [3]BioQuant, Heidelberg University

The spread of HIV-1 can progress either through cell-free infection or through direct cell-cell contacts between immune cells. The latter mode is assumed to be more efficient, but it remains elusive which strategy is favored under different conditions and how tissue structure might change the contribution of each mode of infection to viral spread. To address this problem, we study HIV-1 infection dynamics of primary T-lymphocytes in tissue-like 3D environments (collagen matrices of different densities). Based on single cell tracking data, we developed a quantitative analysis to study how different 3D environments influence cell migration and shape the kinetics of cell-cell contacts. This information is then used to parameterize a Cellular Potts Model (CPM). Applying this CPM in combination with population dynamics models to the infection dynamics data, we infer kinetic parameters of HIV-1 spread under different environmental conditions. Together, our work provides mechanistic and quantitative insight to understand how 3D environments shape HIV-1 spread.

BP 10.42 *(202)* Mon 17:30 Poster C

Tissue competition: The role of cross adhesion — •Tobias Büscher and Jens Elgeti — Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

Cells grow and divide, which implies a change in volume. In physical terms, the conjugate force to a change in volume is a pressure. Thus, in order to grow, cells must exert mechanical pressure on the neighbouring tissue. In turn, mechanical stress influences growth. Indeed, experiments on the growth of a cancer cell line display a reduction in proliferation due to mechanical pressure [1,2,3]. This effect leads to a mechanical contribution when tissues compete for space. The tissue with higher homeostatic pressure, i.e. the pressure at which cell division and death balance, overwhelms the weaker one [4,5]. We expand these works to include different adhesion properties. We find that the cross adhesion between the two tissues plays a crucial role in the dynamics of the competition. Besides one overwhelming the other, we observe a variety of states in which the two tissues coexist, ranging from spherical inclusions to a bi-continous structure. Interestingly, cancer cells typically express less adhesion proteins.

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[2] Delanrue *et al*, 2013, *PRL***110**, 138103
[3] Podewitz *et al*, 2016, *EPL* **109**, 58005
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[5] Podewitz *et al*, 2016 *New J. Physics* **18**, 083020

BP 10.43 *(211)* Mon 17:30 Poster C

Role of mechanics in morphogenesis control — •Jason Khadka, Jean-Daniel Julien, and Karen Alim — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

A major question in developmental biology is to understand how reproducible shapes arises from the collective behaviour of individual cells. What is the role of feedback of mechanical forces on cell growth? In plants, cell shapes are controlled by individual cell wall stiffness, which itself is controlled by tissue-wide mechanical stresses via the dynamics of cortical microtubules. The prime model to investigate the impact of this mechanical feedback on cell growth is the tip of a plant shoot termed shoot apical meristem. This stem-cell niche is the source of all above-ground plant organs, where mechanics is well defined by its near dome-like structure. We built a quasi-three dimensional vertex model for plant tissue growth. Using the model, we investigate the role of mechanics for robust tissue shape formation by studying morphological changes of shoot shape that arise from limiting cellular ability to read mechanical signal. Further, we employ our model to analyse the importance of cell division in maintenance of shoot shape by investigating tissue morphologies with different underlying cell division patterns.

BP 10.44 *(237)* Mon 17:30 Poster C

Visualization of intracellular calcium levels in *Dictyostelium discoideum* with a genetically encoded reporter — •Manuel Frey, Sven Flemming, Serena Cucinotta, and Carsten Beta — Biological Physics, Universität Potsdam

Ca^{2+} is an important second messenger in eukaryotic cells and is crucial for several signaling pathways related to cellular functions such as chemotaxis and cell motility. In order to visualize Ca^{2+} in the social amoeba *Dictyostelium discoideum*, we expressed a genetically encoded GFP based Ca^{2+} reporter at the plasma membrane. This enabled us to monitor spatiotemporal changes in the intracellular Ca^{2+} levels. As expected, we could detect global increases in calcium levels after chemotactic stimulation with cyclic AMP. Mechanical stimulation of cells with a micropipette led to a local calcium response. Furthermore, we could detect short, focal increases of Ca^{2+} at the basal plasma membrane, which coincided with the appearance of F-actin foci at the same location. In cells exposed to continuous shear flow, we observed periodic oscillations of the intracellular Ca^{2+} levels. Interestingly, once excited these oscillations continued for several minutes even after the shear flow was stopped. In contrast, application of a short pulse of shear flow induced only single responses. Our results show that local-

ized increases in Ca^{2+} can be visualized with our new reporter in live cell imaging experiments and revealed interesting oscillatory behavior under shear flow. Currently, we work on the co-expression of other reporters, which will provide more information on the biological function of this behavior and the related signaling pathways.

BP 10.45 *(240)* Mon 17:30 Poster C

Evolution of simple multicellular life cycles in a dynamic environment — •Yuriy Pichugin and Hye Jin Park — Max Planck Institute for Evolutionary Biology, August-Thienemann-Str. 2 24306 Plön

Reproduction is a defining feature of living systems. To reproduce multicellular organism must fragment into smaller parts. To investigate evolutionarily optimal strategies of fragmentation under the dynamic environment, we use the model in which groups arise from the division of cells that do not separate but stay together until the moment of group fragmentation. The environmental conditions change in our model by alternating between two seasons, and different group sizes have a different birth rate of cells depending on the season. We outline which fragmentation strategies are evolutionarily optimal at given environmental conditions.

BP 10.46 *(245)* Mon 17:30 Poster C

Sorting of malaria-infected red blood cells based on adhesion in shear flow — •Anil Kumar Dasanna and Ulrich Schwarz — BioQuant & Institute of Theoretical Physics, Heidelberg University, Heidelberg

Malaria is an infectious disease caused by the unicellular parasite Plasmodium falciparum. Once inside the human body, the parasite hides from the immune system inside the red blood cells, where it multiplies over a period of 48 hours, before it ruptures the host cell and infects new red blood cells. Infected red blood cells can be cleared by the spleen based on their altered mechanics. In order to avoid this, the parasite induces an adhesive system on the surface of the red blood cells, which is built up progressively over the 48 hours of the intracellular stage. Recently white blood cells have been shown to be sorted out using ligand patterns arranged with a small inclination angle with the shear flow direction. Using adhesive dynamics simulations for round cells, we show that this method can be also extended to sort out different stages of malaria-infected red blood cells. We predict an optimal range for key parameters, such as inclination angle and shear rate. Round shapes are only appropriate for the late stage of the infection and in order to understand sorting in the earlier stages, we also have implemented a deformable red blood cell model.

BP 10.47 *(263)* Mon 17:30 Poster C

Amoeboid cells as a candidate for drug delivery — •Valentino Lepro, Oliver Nagel, Setareh Sharifi, and Carsten Beta — Institut für Physik und Astronomie, Universität Potsdam

The increasing interest towards new frontiers of drug delivery and micro-actuators raises the need to develop systems able to transport micron-sized objects in a directed fashion. A promising strategy that recently emerged is to exploit living cells as smart, steerable, and biochemically powered carriers. Inspired by amoeboid cells such as leukocytes migrating in our bodies, this project explores the potential of chemotactic eukaryotic cells as micro-carriers, using Dictyostelium discoideum as a model organism. Such chemotactically guided transport by amoeboid cells proved to be robust and reliable. However, due to the complex and not fully understood nature of amoeboid motion and cell-substrate interaction, the details of this process are not well understood and it remains difficult to regulate. Here, we present a more quantitative analysis indicating that cells loaded with a microparticle tend to displace more efficiently than unloaded ones, resulting in a particle-size dependent diffusion coefficient of loaded cells. Moreover, isolated cell-particle pairs may behaved like non-linear oscillators suggesting that the cell-particle interaction acts as a stimulus that enhances cell motility. In particular, the different adhesion geometries induced by the additional confinement could favor cytoskeleton polarization, which in turn promotes motility. Furthermore, we used gelatin gels as a simplistic model of a 3D tissue structure, to mimic a more natural environment for cell-based microtransport.

BP 10.48 *(265)* Mon 17:30 Poster C

Morphology to encode information — •Mirna Kramar and Karen Alim — Max Planck Institute for Dynamics and Self-Organizaton, Göttingen

The challenges of living in a complex environment require organisms to develop reliable sensory and information processing mechanisms. For an organism that explores its environment by foraging, remembering sources of food or harm is essential for survival. We study *Physarum polycephalum* as a model organism at the verge between simple and complex life. The body of *P. polycephalum* is a network of cytoplasm-filled tubes lacking any organizing centre. This unicellular, multinucleate organism relies on shuttle streaming of its cytoplasm caused by peristaltic contractions of the actomyosin lining the tubes. As a response to stimuli, *P. polycephalum* reorganises its network to exploit a food source or avoid harm. The mechanism by which *P. polycephalum* memorises information about stimuli is not yet explained. Potentially there are three interrelated ways of information encoding, acting on different timescales: the peristaltic contractions (short term), the morphology of the network (intermediate) and the deposition of extracellular slime (long term memory). In particular, we here focus on the mechanism of information encoding in the network morphology, achieved by reinforcing of important connections and pruning of unimportant ones. To study this kind of memory, we use time series of images of the foraging organism, as well as simulations of network dynamics.

BP 10.49 *(315)* Mon 17:30 Poster C

Cellular Potts Models for Neural Tissue Simulations — •Jakob Rosenbauer and Alexander Schug — Forschungszentrum Jülich, 52428 Jülich, Germany

Experimental capability in biology has been leaping forward in the last decades. Methods such as light-sheet microscopy have given more and more insights into the dynamics of tissue. Computational models are of rising importance for biological questions. The cellular Potts model (cpm) is a computational model derived from the Potts model. The development of tissue can be modelled with single cell resolution, up to a very high number of cells. A parallel version was developed, facilitating large three dimensional simulations of tissue dynamics on large cluster networks, which can be applied to a large variety of biological questions. Through a high scalability this model allows for modelling of much larger specimen than possible to date. The patterning of the neural plate in zebrafish embryonal development was modelled using the parallel cpm. The tissue dynamics during epiboly were modelled by the cpm. In that developmental stage the neural plate starts its patterning into different regions via a signalling molecule. Different modes of transport of that molecule, diffusion and so called cytonemes, were compared.

BP 10.50 *(317)* Mon 17:30 Poster C

Does peristaltic pumping account for mass transport in *Physarum polycephalum*? — •Felix Bäuerle and Karen Alim — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Physarum polycephalum, the infamous "intelligent" slime mold, has proven time and time again that it can solve complex problems. For example, it is able to find the shortest path through a maze, connect food sources in an efficient fashion or choose a balanced diet. In all of these efforts the adaptation of the morphology to a changing environment is the key. In detail cytoplasmic flows transport cytosolic fluid from pruning regions to growing ones. At the same time a peristaltic wave of contractions spans the whole body plan. Can this traveling wave generate enough pressure to account for the relatively fast reorganisation speed in *P. polycephalum*? While the contractions are known to account for the shuttle streaming, no investigations have been done so far on the net flow. We are presenting calculations of flow stemming from the contraction patterns in stimulated plasmodia and relate these to the morphology reorganisation.

BP 10.51 *(332)* Mon 17:30 Poster C

Single cell migration and transitions to different substrates on micro patterns — •Christoph Schreiber, Felix J. Segerer, and Joachim O. Rädler — Faculty of Physics and Center for NanoScience, LMU München

When cells migrate in the body, for example during cancer metastasis, cells are facing different extra cellular matrix (ECM) proteins that can influence the cell migration behavior. To study the effects of different ECM proteins, standardized experimental conditions and suitable metrics to characterize cell motility are needed. We use micro-contact printed stripes or rings to get race tracks for cells with defined protein coatings. The tracks constrict cells to move only in 1D, which simplifies the analysis of the movement.

We find bimodal migration behavior with states of directional migration (run states) and reorientation (rest states).[1] We extract characteristic persistence times, which, in combination with the velocity of cells in the run state, provide a set of parameters quantifying cell motion. To be able to study transitions of single cells to different ECM proteins like fibronectin and collagen IV we developed a new patterning technique based on two stamping processes. Thus, transition rates and velocities on different protein coatings can be analyzed. Together this results in a fingerprint-like set of parameters characterizing cell migration that can be used to distinguish cell lines as well as to quantify the effects of motility affecting drugs.

[1] Schreiber et al. Sci. Rep. 6, 26858 (2016)

BP 10.52 *(344)* Mon 17:30 Poster C

Scanning Ion Conductance Microscopy on osteoblasts with regard to their adhesion on surfaces — •Christian Völkner[1], Regina Lange[1], MohammadReza Bahrami[1], Martina Grüning[2], Henrike Rebl[2], Ingo Barke[1], Barbara Nebe[2], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics, 18059 Rostock, Germany — [2]University Medical Center Rostock, Dept. of Cell Biology, 18057 Rostock, Germany

Our aim is to elucidate mechanisms of initial cell adhesion and migration of osteoblasts (MG63) on material surfaces. To this end we prepare substrates with different properties such as surface charges, polarisability, electric potential and electromagnetic field landscapes. Furthermore we implement an electro-stimulation chamber to apply fields in the quasistatic regime [1]. Our main approach is Scanning Ion Conductance Microscope (SICM), in which a nanopipette is used as a probe and the ion current serves as localized interaction signal. In contrast to other scanning probe methods like Atomic Force Microscopy it allows one to obtain the nanomorphology of the surface of living cells reducing forces between cell and nanoprobe and respective cell responses [2]. Especially, substructures of the migration fronts of adhering osteoblasts are being addressed.

[1] N. W. S. Kam, E. Jan, N. A. Kotov, Nano Lett. 9, 273 (2009)

[2] Y. E. Korchev, C. L. Bashford, M. Milovanovic, I. Vodyanoy, M. J. Lab, Biophys. J. 73, 653 (1997)

BP 10.53 *(351)* Mon 17:30 Poster C

Examining Anticipation in Physarum polycephalum — •Nico Schramma, Felix Bäuerle, and Karen Alim — Max Planck Institute for Dynamics and Self-Organisation, Göttingen, Germany

Memory and anticipation are complex mechanisms that have developed in higher species to predict and adapt to changing conditions. Even the unicellular slime mold *Physarum polycephalum* has been shown to anticipate periodic events. As a plasmodial vascular network, *P. polycephalum* changes its morphology in order to forage, and pumps cytoplasma through the organism using oscillatory contractions of tubes organized in a peristaltic wave. Saigusa et. al. showed that lateral restricted foraging *P. polycephalum* networks decrease their speed when stimulated periodically by unfavorable conditions. Interestingly, even after omission of the stimulus *P. polycephalum* still anticipates the withhold stimulus. However, the mechanism of this sophisticated behavior is not yet understood and cannot be extracted from their low resolution data. Here we show that periodic blue light stimulation of *P. polycephalum* networks entraines frequency modulations of tube contractions, which persist after the omission of further stimuli. Kymograph analysis of microscope pictures shows that the entrained frequency changes overall with a period similar to the periodic stimulation, with overall frequency minima coinciding with the blue light stimulus. Our analysis therefore suggests that the anticipation behaviour of *P. polycephalum* is a function of the entrainment of frequency modulations.

BP 10.54 *(355)* Mon 17:30 Poster C

Limitations of Murray's law in a dynamic network — •Noah Ziethen, Felix Bäuerle, Nico Schramma, and Karen Alim — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The morphology of biological networks is often regarded as the result of optimization under a given demand. Optimization for minimal dissipation under cost for the maintenance of a tubular network leads to a relation between the radii of tubes meeting at a network node, denoted Murray's law. So far, the theoretical prediction of Murray's law has been found to agree surprisingly well with what seems to be any kind of vascular networks ranging from plants and animals. Contrary to the uni-directional flows in vascular networks the slime mould Physarum polycephalum exhibits oscillatory shuttle flow, providing an excellent test case to investigate the limitations and underpinnings of Murray's law.

Here, we image and analyze the dynamic network morphology of P. polycephalum over time. Quantification of Murray's law does not yield accordance with the theoretical predictions. A widely spread distribution of branching ratios was observed in which the mean value did not agree with Murray's law. Nevertheless, a decreasing trend of the branching ratio was observed. The time evolution of the decrease correlated with the phenomenon of pruning. The relation between the local branching ratio and the different regions of the slime mould showed a slightly different distributions in branching ratios for pruning and non-pruning regions.

BP 10.55 *(375)* Mon 17:30 Poster C

Organ-on-a-chip meets traction force microscopy: *In situ* characterization of forces in 3D μ-tissues — •Stefanie Fuchs, Oliver Schneider, Christopher Probst, and Peter Loskill — Department of Cell and Tissue Engineering, Fraunhofer Institute for Interfacial Engineering and Biotechnology IGB, Stuttgart, Germany

Organ-on-a-Chip (OoC) systems are microfluidic devices which enable the cultivation of 3D tissues in a precisely controllable, physiological microenvironment. In combination with human induced pluripotent stem cells these systems have the potential to revolutionize the drug development process. Therefore, it is essential to accurately characterize the integrated tissues. An important characteristic of many tissues is the force exerted by the cells. This information is useful to characterize for instance the growth of cells and the contraction state of (cardiac) muscle cells. Traction force microscopy (TFM) is a commonly used tool to spatially resolve these forces.

Here, we present a TFM system directly embeddable into OoC systems, which consists of an elastic layer with integrated fluorescent nanobeads on the surface. Based on the elastic modulus of the substrate, the force on the surface can be derived from the bead displacement. We highlight that our system directly integrates a gauging mechanism for the determination of the substrate's mechanical properties, allowing the accurate determination of forces by considering each individual sample composition. The presented system enables precise *in situ* measurements of forces exerted by different tissue types in an OoC with a simple fluorescence microscope.

BP 10.56 *(393)* Mon 17:30 Poster C

Fluid and Jammed Behaviour in Cell Spheroids — •Steffen Grosser, Linda Oswald, Jürgen Lippoldt, and Josef A. Käs — Peter-Debye-Institut für Physik weicher Materie, Universität Leipzig

Cell Spheroids are many-particle "droplets" of soft matter with a constant volume fraction of one, which however can display fluid or "jammed"/glassy behaviour, as we can show with bulk rheology and single-cell tracking. Full three-dimensional digital segmentation of spheroids into single cell volumes reveal that for epithelial vs. cancerous spheroids (MCF-10A vs MDA-MB-436), this change in fluidity is reflected in the cell arrangements (cell shape). This could affect histopathology, where malignancy and dedifferentiation are detected via cell shape changes.

BP 10.57 *(411)* Mon 17:30 Poster C

The influence of Rac1 on motility into 3D extracellular matrices andmechanical properties — •Tom Kunschmann, Stefanie Puder, and Claudia Tanja Mierke — Biological Physics Division, Peter Debye Institute for Soft Matter Physics, University of Leipzig, Germany

The formation of membrane ruffles and lamellipodia promotes the motility of adherent cells. In 2D cell motility assays, these protrusions are important for sensing of the microenvironment and initiation of substrate adhesions. The influence of structures such as lamellipodia or invadopodia for providing cellular mechanical properties and 3D motility of cells is still not yet clear. Hence, we showed that Rac1 affects cellular mechanical properties and facilitates the invasion in 3D microenvironments. We analyzed whether fibroblast cell lines genetically deficient for Rac1 possess altered mechanical properties such as cellular deformability and altered motility into 3D ECM. Thus, we analyzed Rac1 wild type and knockout cells for alterations in cellular deformability using an optical cell stretcher. We found that Rac1 knockout cell lines were pronouncedly more deformable compared to Rac1 wild type cells. The increased mechanical deformability of Rac1 knockout cells is suggested to be responsible for their reduced motility in dense 3D ECM. Thus, we investigated whether increased deformabil-

ity of Rac1 knockout cells suppresses cellular motility into 3D collagen fiber matrices. Rac1 wild type cells displayed increased motility in 3D compared to Rac1 knockout cells. These results were validated by using Rac1 Inhibitor EHT1864 which revealed similar results.

BP 10.58 *(413)* Mon 17:30 Poster C

Parameter-free high-resolution traction force microscopy — •Yunfei Huang, Gerhard Gompper, and Benedikt Sabass — Institute of Complex Systems 2, Forschungszentrum Juelich , 52425 Juelich, Germany

In Traction Force Microscopy, elastic displacements caused by mechanical interaction of cells with their environment are employed to calculate cellular traction forces. Calculation of traction from displacement is a linear problem. However, as a result of insufficient measurement density and a long-range interaction kernel, the calculated traction values strongly depend on the chosen method for solving the problem. Here, we systematically test the performance of state-of-the-art methods from sparse learning, computer vision, and Bayesian inference for traction force microscopy. Classical approaches include L2- and L1-regularization or spatial filters that depend on an ad-hoc choice of parameters. We also study three further parameter-dependent approaches, namely Elastic Net (EN) regularization, Proximal Gradient Lasso (PGL), and Proximal Gradient Elastic Net (PGEN). Next, we pioneer the use of parameter-free methods such as Bayesian Compressive Sensing (BCS), Bayesian Lasso (BL), and Bayesian Elastic Net (BEN). We introduced novel computational methods for traction force microscopy that eliminate the need for user-defined filter-parameters and also exhibit excellent performance with regard to resolution and accuracy. These methods can enable an objective detection and quantitative measurement of forces at minute cellular adhesion sites.

BP 10.59 *(195)* Mon 17:30 Poster C

Interkinetic nuclear migration as a stochastic process in the zebrafish retina — Afnan Azizi[1], •Anne Herrmann[2], Salvador J. R. P. Buse[1], Yinan Wan[3], Philipp J. Keller[3], Raymond E. Goldstein[2], and William A. Harris[1] — [1]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, United Kingdom — [2]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge, United Kingdom — [3]Howard Hughes Medical Institute, Janelia Research Campus, Ashburn, VA, USA

Interkinetic nuclear migration (IKNM), a movement of nuclei between the apical and basal surfaces of proliferating cells in developing epithelia, was first observed more than 80 years ago. Since, IKNM has been studied in multiple organisms but despite these efforts many questions about the role and mechanism of this process remain unsolved. In earlier studies, only single or sparsely labelled nuclei in an otherwise unlabelled tissue were imaged. Here, we present data from light sheet microscopy on wholly labelled retinas, where the movement of all nuclei in a tissue section can be followed with high temporal resolution. This approach enables us to study the movements of individual nuclei as well as their collective behaviour in a systematic fashion. Our data, in combination with mathematical models, support the hypothesis of IKNM as a stochastic process. These results present IKNM as a possible precursor for the observed stochasticity in progenitor differentiation and have important implications for understanding the organisation of developing vertebrate tissues.

BP 10.60 *(209)* Mon 17:30 Poster C

Neuronal model for startling coupled with a collective behavior model — •Andrej Warkentin[1] and Pawel Romanczuk[1,2] — [1]Bernstein Center for Computational Neuroscience, Humboldt Universität zu Berlin — [2]Institute for Theoretical Biology, Department of Biology, Humboldt Universität zu Berlin

Many aspects of fish school behavior can be explained qualitatively by self-propelled agent models with social interaction forces that are based on either metric or topological neighborhoods. Recently, startling of fish has been analyzed in its dependence of the network structure [1] but a neurophysiological model and its influence on the collective behavior is missing. Here, we coupled a model for collective behavior with a neuronal model that receives looming visual stimulus input to initiate a startle response, inspired by the neurobiologically well-studied Mauthner cell system. First, we analyzed the basic properties of the startle behavior of a single fish as a reaction to one or multiple looming stimuli. On the group level, we looked at startling frequency and cascades as well as group cohesion, polarization and mobility depending on neuronal and collective behavior parameters via simulations of the combined model. Our results indicate that the startling frequency strongly depends on the dynamics of the group structure, e.g. when the group approaches a boundary of the arena. In summary, we took first steps towards a biologically plausible model for startle response initiation in the context of collective motion.

[1] Rosenthal, S. B., Twomey, C. R., Hartnett, A. T., Wu, H. S., and Couzin, I. D. (2015). PNAS, 112:4690-4695

BP 10.61 *(248)* Mon 17:30 Poster C

Decision-Making across the Lifespan: Neurocognitive Models of Ageing and Dementia — •Gunther Klobe — Department of Clinical Neurosciences, University of Cambridge, UK

In the study of healthy ageing and neurodegenerative diseases, there are marked variations between individuals in terms of behaviour and decision-making. I examine these individual differences, using neurally inspired models of decision-making based on the accumulation of evidence for each possible response in simple perceptual reaction time tasks.

By analysing behavioural data using such models (Linear Ballistic Accumulator, Drift-Diffusion Model), one gains insight into individual differences that are not apparent from a simple comparison of mean reaction times and error rates because the latter approach ignores crucial information hidden in the cross-trial distribution of reaction times within a single subject.

My initial work examines the effects of ageing on decision-making processes using behavioural data from a large cross-sectional study, known as CamCAN (Cambridge Centre for Ageing and Neuroscience). In due course I will perform a similar analysis on data from clinical studies with dementia patients.

In both populations the decision-making model parameters can then be correlated with existing structural brain imaging data and thus become interpretable in terms of neural architecture and physiology, hopefully improving our understanding of the links between brain structure and task performance.

BP 11: Bioimaging and Biopspectroscopy I

Time: Tuesday 9:30–13:00 Location: H 1028

Invited Talk BP 11.1 *(10)* Tue 9:30 H 1028

Cryo-Electron Tomography: Method Development and Application on Cell-Cell Junctions and Nuclear Exploration — •Achilleas Frangakis — BMLS, Goethe University, Frankfurt

Cryo-electron microscopy is the major technique used in my laboratory and my talk will focus on two applications: The first involves the understanding of the macromolecular supra-organisation in the nucleus. Within cryo-electron tomograms we could visualize the complete ribosome biogenesis in a frozen hydrated state, from which the structure of the elongating RNA Polymerase I was solved at 25 Å resolution. Subsequent cryo-EM single particle analysis of the isolated RNA Polymerase I led to a structure at 3.8 Å resolution that unravelled how the RNA Polymerase I is allosterically controlled.

The second involves the analysis and the structure of cell-cell junctions that are of major importance for tissue homeostasis and are heavily involved in disease and signaling. We studied the adherens junctions and the slit diaphragm of the kidney but also the interaction of Mycoplasmas to the host cells.

Ultimately my talk should highlight our efforts towards visualizing interactions of macromolecular machineries within the unperturbed cellular context.

BP 11.2 *(311)* Tue 10:00 H 1028

Microstructural analysis of the walls of termite nests using X-ray micro-tomography — •Kamaljit Singh[1], Bagus P. Muljadi[2], Ali Q. Raeini[1], Veerle Vandeginste[2], Martin J. Blunt[1], Christian Jost[3], Guy Theraulaz[3], and Pierre Degond[1]

— [1]Imperial College London, UK — [2]The University of Nottingham, UK — [3]Centre de Recherches sur la Cognition Animale, CNRS, Toulouse, France

Termite nests have long been investigated for thermoregulation and ventilation by self-sustaining CO2 exchange to the outer atmosphere. Although the outer walls of termite nests are believed to be porous, and have been hypothesized as a source of gas exchange, the morphological features of the walls, and their role in controlling ventilation and heat conduction are unknown. We have investigated the microstructure of the outer and inner walls of the Trinervitermes geminatus termite nests (from Senegal and Guinea) in three dimensions using high-resolution X-ray micro-tomography. In the Senegal nest, we observe inter-connected network of larger and smaller pores. By contrast, the walls of the Guinea nest contain only the inter-connected larger pores. The smaller pores do not form, due to larger fraction of clay in the nest. From the 3D flow field simulations, we show that the presence of larger inter-connected pores in both nest materials enhances the permeability and CO2 diffusion across the outer walls. Moreover, the network of larger pores help in draining the water from the nest walls after rainy periods, therefore, re-establishing the ventilation of the nest as well as providing structural stability to the nest.

BP 11.3 *(287)* Tue 10:15 H 1028

High resolution imaging of the drug delivery into stratum corneum of human skin probed with scanning near-field optical microscopy — •P. Patoka[1], G. Ulrich[1,2], K. Yamamoto[1], A. Klossek[1], F. Rancan[3], A. Vogt[3], U. Blume-Peytavi[3], P. Schrade[4], S. Bachmann[4], G. Ulm[2], B. Kästner[2], and E. Rühl[1] — [1]Physical Chemistry, Freie Universität Berlin, Takustr. 3, 14195 Berlin — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 12587 Berlin — [3]Klinisches Forschungszentrum für Haut- und Haarforschung, Charité Universitätsmedizin, 10117 Berlin — [4]Abteilung für Elektronenmikroskopie at CVK, 13353 Berlin

Understanding the mechanism of topical drug delivery into human skin requires the use of multiple techniques. Among those techniques label free methods are of special interest, avoiding drug-labels or skin-label interactions. Scanning near-field optical microscopy can be used to obtain detailed information on the correlation of the local drug distribution with highly resolved topographical information. Recent results from optical near-field microscopy imaging, investigating the penetration of the anti-inflammatory drug dexamethasone in human skin, are reported.

After resonant excitation of dexamethasone by a quantum cascade laser, operating in the mid-infrared regime, the penetration of dexamethasone in the stratum corneum is visualized. Imaging with high spatial resolution of <10 nm gives access to detailed information of the local drug distribution within the lipid matrix of the stratum corneum and its substructures. By using this technique also the presence of natural corticosteroids within the stratum corneum and ceramides is revealed. These measurements can be correlated with recent results obtained from X-ray microscopy and high resolution electron micrographs allowing us to reach an improved understanding of the drug penetration in human skin using label-free spectromicroscopy.

BP 11.4 *(361)* Tue 10:30 H 1028

Observing the Plasmonic Photothermal Effect on Individual BaF3-Cells using Targeted Gold Nanostructures — •Phillip Witthöft, Lisa Prisner, and Alf Mews — Universität Hamburg, Institut für Physikalische Chemie, Hamburg, Deutschland

The exploitation of the plasmonic photothermal effect of gold structures such as gold nanorods for photothermal therapy in cancerous tissue is of great interest for the scientific community. While a wide array of specific and non-specific applications has been developed in the past, further understanding of this process and the parameters involved at the cellular level is of utmost importance for the development of these systems. In our project, we investigate the photothermal effect of gold nanorods in detail on the single cell level. We have developed a method to irradiate only an individual cell with the desired wavelength to induce a plasmonic photothermal effect and successfully observe the reaction of one individual cell to the temperature rise in real time by plotting the color saturation of the cell over time in the presence of trypan blue. We use a targeted delivery system facilitated by the interaction of the Interleukin-6 receptor with the Interleukin-6 specific aptamer AIR-3A and compare the efficiency for plasmonic photothermal therapy of these targeted nanostructures to the efficiency of non-targeted PEG-coated nanostructures. We were able to observe that cells incubated with targeted nanostructures already show their maximum color saturation after half of the time compared to non-targeted nanostructures. Based on our observations we discuss the mechanism and specificity of the photothermal effect on the single cell level.

BP 11.5 *(280)* Tue 10:45 H 1028

NV based modular sensor platform for intracellular environmental sensing — Jan Vavra[1,4], Ivan Rehor[2], •Torsten Rendler[3], Mona Jani[4], Jan Bednar[6,7], Michael M. Baksh[5], Andrea Zappe[3], Joerg Wrachtrup[3], M. G. Finn[5], and Petr Cigler[4] — [1]Department of Chemistry, University of Oslo, Norway — [2]Debye Institute for Nanomaterials Science, University of Utrecht, Netherlands — [3]3th Physical Institut, University of Stuttgart, Germany — [4]Academy of Sciences, Institute of Organic Chemistry and Biochemistry, Czech Republic — [5]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, United States — [6]CNRS, University Grenoble Alpes, France — [7]Fac Med 1, Charles University Prague, Czech Republic

Monitoring intracellular concentration of chemical moietis is important for biomedical applications. We utilize the so called nitrogen vacancy color center (NV) in nanodiamonds (NDs) as a sensor working under physiological conditions. NVs itself are photostable and allow to sense for example magnetic fields or temperature in their direct vicinity. NDs have been shown to be of low toxicity and therefore form the perfect host for intracellular sensing. To enable chemical sensing we developed a hybrid sensor platform. A polymer is crafted to the ND surface hosting Gd(III) complexes that alter the NV spin lattice relaxation time T_1. By triggering the release of Gd(III) by a chemical species, the change in T_1 can be used to measure for example pH. In the current work we concentrate on the development and description of a new sensor by coating fluorescent nanodiamonds with a supported lipid bilayer.

15 min. break

BP 11.6 *(268)* Tue 11:15 H 1028

Wide-Field Nuclear Magnetic Resonance Imaging using Nitrogen-Vacancy Centers in Diamond — Florestan Ziem, •Marwa Garsi, Helmut Fedder, and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart

Electron and nuclear magnetic resonance are essential tools in the life and material sciences. Significant advances in high resolution, high sensitivity sensing at sub-cellular length scales have been shown using nitrogen-vacancy (NV) centers in diamond, promising label-free imaging and single molecule analysis. E.g. by controlling and detecting the electronic state of individual NV centers, single molecule detection [1] and nanoscale NMR with resolution of chemical shift [2] have been demonstrated. Here, we show our recent progress towards transferring these techniques to wide-field imaging using ensembles of NV centers and multiplexed quantum state detection on a CCD camera. One of our key achievements is the homogenous manipulation of all NV centers over a large area. For this, we use optimal control algorithms to shape the driving microwave pulses to accomplish parallel orchestration of NV centers in a field of view of 60 x 60 μm^2. By performing nuclear magnetic wide-field imaging on solid state thin films on the diamond surface, we demonstrate an optical resolution of ∼300 nm and B-field sensitivity of 100 nT $\mu m^{3/2}$ $Hz^{-1/2}$. Our results pave the way towards rapid magnetic resonance imaging with sub diffraction limited optical resolution, with the ultimate goal to understand fundamental processes at the level of single cells and organelles. [1] Lovchinsky et al, Science 351, 836 (2016). [2] Aslam et al, Science 357, 67 (2017).

BP 11.7 *(321)* Tue 11:30 H 1028

CellMOUSE: A novel high throughput real-time measurement method for suspended cells and particles — •Tobias Neckernuss, Daniel Geiger, Jonas Pfeil, Markus Sporer, Stefan Reich, and Othmar Marti — Institute of Experimental Physics, Ulm University

The optical measurement of cells has proven to be a viable tool in biology and in clinical applications. It is used to distinguish different cell types as well as healthy, mutated and dead cells based on parameters like size, shape and morphology. Common methods, based on video microscopy or light scattering, are either limited in throughput, analysis speed or information content.

We present a new optical measurement device, the so called CellMOUSE, that is able to measure suspended cells and particles in real-

time with very high throughput of more than 500 cells per second. Measurement quantities like speed, size, morphology and shape of the cell are obtained immediately after passing the detector. In contrast to other techniques, CellMOUSE measures and evaluates each cell individually and the result is not based on the statistics of an ensemble. This is, for instance, important for cell sorting applications. Furthermore, the measurement does not require buffering so that continuous screening of cell properties over an unlimited time span is possible.

BP 11.8 *(59)* Tue 11:45 H 1028

Theoretical simulation of biomarkers for *in vivo* MRI of extracellular pH — •Simone Köcher[1,3], Stephan Düwel[1,2], Christian Hundshammer[1,2], Franz Schilling[2], Steffen J. Glaser[1], Josef Granwehr[3], and Christoph Scheurer[1] — [1]Department of Chemistry, Technische Universität München, Garching, Germany — [2]Department of Nuclear Medicine, Klinikum rechts der Isar, Technische Universität München, Garching, Germany — [3]IEK-9 - Fundamental Electrochemistry, Forschungszentrum Jülich, Jülich, Germany

Up to now, there are no techniques available to routinely measure extracellular pH in the clinic. Pathological deviations from the systemic pH are often caused by cancer, inflammation, infection, and other diseases. Hyperpolarized [1,5-$^{13}C_2$]zymonic acid (ZA) was recently introduced as a novel MRI biomarker for dissolution dynamic polarization (DNP) measurements of extracellular pH with good resolution. Systematic, time-consuming, experimental screening for promising biomarker molecules can be facilitated by theoretical *ab initio* calculations of chemical shifts and pK_a values. We introduce a theoretical screening approach for pH-sensitive biomarkers and point out the important technical aspects. For ZA, the calculations show good accuracy in the prediction of the pH-dependent ^{13}C chemical shift sufficient for a theoretical pre-screening of potential biomarker molecules.

BP 11.9 *(105)* Tue 12:00 H 1028

Imaging in Biologically-Relevant Environments with AFM Using Stiff qPlus Sensors — •Korbinian Pürckhauer[1], Alfred J. Weymouth[1], Katharina Pfeffer[1], Lars Kullmann[1], Estefania Mulvihill[2], Michael P. Krahn[3], Daniel J. Müller[2], and Franz J. Giessibl[1] — [1]University of Regensburg, Regensburg, Germany — [2]ETH Zürich, Basel, Switzerland — [3]University Hospital of Münster, Münster, Germany

High-resolution imaging of soft biological samples with atomic force microscopy (AFM) is challenging because they need to be imaged with very low forces to prevent deformation. Typically, AFM of those samples is performed with soft silicon cantilevers ($k \approx 0.1 - 10\,\mathrm{N/m}$) and optical detection in a liquid environment.

In this work we demonstrate the advantages of using stiffer sensors ($k \approx 1\,\mathrm{kN/m}$) which were used to obtain unprecedented spacial resolution of molecules in vacuum at low temperatures [1]. In liquid environments, the high stiffness of the qPlus sensor allows us to use small amplitudes in a non-contact mode and obtain high quality factors [2]. The samples are immersed in aqueous solution in a liquid cell and we use qPlus sensors with long tips, only submerging the tip apex.

Atomic resolution of muscovite mica was achieved in various solutions. To prove that we can non-destructively image soft biological samples with stiff sensors, we show images of lipid membranes and finally molecular resolution images of a lipid bilayer.[3]

[1] Gross et al., Science 325, 1110 (2009). [2] Ichii et al., Jpn. J. Appl. Phys. 51, 08KB08 (2012). [3] Pürckhauer et al., submitted.

BP 11.10 *(225)* Tue 12:15 H 1028

Simulation of FRET Dyes Allows Direct Comparison Against Experimental Data — •Ines Reinartz[1], Claude Sinner[1], and Alexander Schug[1,2] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]John von Neumann Institute for Computing, Forschungszentrum Jülich, Jülich, Germany

Single molecule Förster Resonance Energy Transfer (smFRET) experiments provide valuable insight into protein dynamics. Akin to a molecular ruler, different protein conformations can be observed by measuring the energy transfer depending on the distance between selected residues labeled with dyes. Besides this distance, the energy transfer is also dependent on the mutual orientation of the dyes. Both can be gained from atomistic simulations.

We develop a coarse-grained simulation technique with few parameters while maintaining full protein flexibility and including all heavy atoms. The computational efficiency of these simulation protocols allows for simulating large systems and heterogeneous ensembles as found in, e.g., protein folding.

The FRET efficiency histograms we gain from our simulations are directly comparable to experimental measurements. With access to distances and orientations from atomically resolved trajectories, we want to improve the planning and interpretation of smFRET measurements. As an example, we compare distributions from 2-color and 3-color FRET experiments and simulations for ClyA in monomer and protomer conformation, as well as folded and unfolded ensembles of different systems.

BP 11.11 *(365)* Tue 12:30 H 1028

Optical Mapping of Contracting Hearts — •Johannes Schröder-Schetelig[1], Jan Christoph[1,2], and Stefan Luther[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]German Center for Cardiovascular Research (DZHK e.V.), Göttingen, Germany

Optical mapping of isolated, intact hearts or myocardial cell cultures using fluorescent dyes has become a very well established tool in cardiac research. However, the method as such can be very sensitive to movement of the sample, resulting in severe motion artifacts in the recorded optical signals. In order to prevent this, in the past either the contraction had to be suppressed or more sophisticated strategies like ratiometric imaging had to be applied.

Here, we present a new method, which combines marker-free 2D video tracking techniques with panoramic optical mapping of freely beating and contracting Langendorff-perfused hearts using multiple calibrated cameras. We find that it is possible to accurately track and reconstruct the 3D deformation of the cardiac surface. The tracking is achieved without the need for additional landmarks or special patterned lighting schemes. By projecting the fluorescence videos directly onto the deforming mesh geometry, motion artifacts become significantly reduced. This opens up a new way, where the contraction of a heart is not considered a disturbing limitation any longer, but is now a property which can be measured and studied.

BP 11.12 *(360)* Tue 12:45 H 1028

Synchronization-based Reconstruction of Cardiac Electrical Wave Dynamics from Mechanical Deformation using High-speed 4D Ultrasound — •Jan Christoph, Jan Lebert, Ulrich Parlitz, and Stefan Luther — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Heart rhythm disorders such as ventricular or atrial fibrillation are determined by turbulent electrical vortex wave activity, which occupies the heart muscle and causes irregular contractions and inefficient beating of the heart. Both cardiologists and basic scientists are highly interested in obtaining visualizations of this highly dynamic and complex wave structure and its 3D spatio-temporal organization throughout the heart muscle, to be able to develop strategies for its efficient and reliable termination during ablation or defibrillation therapies. In recent work, we have shown that high-resolution 4D ultrasound can be used to image vortex-like mechanical structures in the fibrillating heart and that it is possible to reconstruct an electromechanical vortex filament structure that characterizes the spatio-temporal organization of ventricular fibrillation within the heart wall. Here, we show that in addition to imaging the mechanical activity, it is possible to reconstruct the electrical wave dynamics, which caused the deformations of the tissue, and which remains invisible in the imaging experiments, numerically. Using a synchronization-based approach, we demonstrate that even complex electrical vortex wave patterns, such as spiral waves or spiral wave chaos, can be reconstructed in elastic excitable media from the analysis of the deformation mechanics.

BP 12: Computational Biophysics I

Time: Tuesday 9:30–13:00 Location: H 1058

BP 12.1 *(314)* Tue 9:30 H 1058

Langevin modeling of targeted molecular dynamics: a novel approach to calculate equilibrium free energies from non-equilibrium simulations — •Steffen Wolf and Gerhard Stock — Bimolecular Dynamics, Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

We present an approach to calculate free energy surfaces based on non-equilibrium biased molecular dynamics simulations. Based on a comparison of Jarzynskis equality and the Langevin equation we derive an expression for non-equilibrium friction factors $\Gamma_{\mathrm{NEQ}}(x)$. Force fluctuations $\delta f(t)$ of a simulated trajectory ensemble were derived from targeted molecular dynamics simulations as constraint forces using a holonomic constraint $\Phi(t) = (x(t) - x_0(t) - v_c t)^2 = 0$ with a constant constraint velocity v_c. Using a NaCl/water test system, we show that a surprisingly high accuracy in the prediction of the equilibrium free energy profile can be achieved with a relatively small number of $N = 30$ simulations at comparatively high constraint velocities of >10 nm/ns. Non-equilibrium friction profiles however need at least $N = 500$ simulations to converge. Comparison with equilibrium simulations shows a general agreement between non-equilibrium and equilibrium-derived friction factors for $v_c \to 0$. The non-equilibrium factors however contain intrinsic constraint velocity dependence, and outperform equilibrium factor-based corrections. Our approach allows for the calculation of near-continuous $\Gamma_{\mathrm{NEQ}}(x)$ profiles directly from non-equilibrium trajectories, and thus for the on-the-fly correction of non-equilibrium simulations to obtain equilibrium free energy profiles.

BP 12.2 *(39)* Tue 9:45 H 1058

Refolding dynamics of molecular constructs after a force quench — •Ken Schäfer and Gregor Diezemann — Institut fuer Physikalische Chemie, Johannes Gutenberg-Universität Mainz, Duesbergweg 10-14, D-55128 Mainz, Germany

In typical force-probe molecular dynamics simulations (FP-MD) one end of a molecular complex is fixed in space and another end is pulled away with a constant velocity. This allows to gather detailed atomistic information about the mechanical unfolding of the complex and the corresponding free energy landscape.

The folding process can be studied by first mechanically unfolding the system and afterwards releasing the external force either completely or to a finite value. This method allows to study the mechanical folding pathway in a systematic way as a function of the quench force. In FP-MD simulations this is of particular interest because it allows to consider forces much smaller than typically used in the standard protocol with a time-dependent force.[1]

We apply the method to study the refolding transition in a calixarene catenane system investigated earlier[2] and extract the kinetic rates for the transition that are analyzed using stochastic models.

[1] C. Hyeon, G. Morrison, D. Thirumalai, PNAS, 2009, 106, 48.
[2] T. Schlesier et al., 2011 J. Phys. Chem. B, 115, 6445.

BP 12.3 *(255)* Tue 10:00 H 1058

G-PCCA - a generalized Markov state modeling approach for both equilibrium and non-equilibrium systems — •Bernhard Reuter[1], Konstantin Fackeldey[2,3], Susanna Röblitz[2], Marcus Weber[2], and Martin E. Garcia[1] — [1]Theoretical Physics II, University of Kassel, Germany — [2]Zuse Institute Berlin (ZIB), Germany — [3]Institute of Mathematics, Technical University Berlin, Germany

Markov state models (MSMs) have received an ongoing increase in popularity in recent years as they enable the conflation of data from simulations of different length and the identification and analysis of the relevant metastabilities and kinetics of molecular systems. However, so far methods and tools for building MSMs, like PyEMMA and MSMBuilder, are restricted to equilibrium systems fulfilling the detailed balance condition. This constitutes a severe constraint, since molecular systems out of equilibrium, e.g. disturbed by an external force, have attracted increasing interest. To overcome this limitation we have developed and implemented - in Python and MATLAB - a generalization of the widely used robust Perron cluster cluster analysis (PCCA+) method, termed generalized PCCA (G-PCCA). This method, based on the utilization of Schur vectors instead of eigenvectors, can handle both data from equilibrium and non-equilibrium simulations. G-PCCA is able to identify dominant structures in a more general sense, not limited to the detection of metastable states, unraveling cyclic processes. This is exemplified by application of G-PCCA on non-equilibrium molecular dynamics (NEMD) data of the Amyloid-beta peptide, periodically driven by an oscillating electric field.

BP 12.4 *(173)* Tue 10:15 H 1058

Structural-kinetic relationships determine consistent interpretations of coarse-grained peptide kinetics — •Joseph Rudzinski and Tristan Bereau — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz

Coarse-grained molecular simulation models have provided tremendous insight into the complex behavior of protein systems, but lack a straightforward connection to the true dynamical properties of the system. This lack of consistent dynamics severely limits coarse-grained models from providing accurate interpretations for kinetic experiments. In this work, we perform a detailed investigation into the kinetic properties of secondary structure formation generated by molecular simulation models. Our strategy is to systematically vary force-field parameters of a simple, native-biased coarse-grained model to identify relationships between the emergent structural, kinetic, and thermodynamics properties. We utilize Markov state models to efficiently and systematically assess the system's kinetic properties. Our investigation reveals robust structural-kinetic relationships that can be exploited to guarantee consistent kinetics through the reproduction of particular structural properties. These remarkable relationships are determined by the physics of the model, which shapes the free-energy landscape and restricts the attainable kinetic properties. Our results suggest an approach for constructing kinetically-accurate models that extends the capabilities and scope of current coarse-grained peptide models.

Invited Talk BP 12.5 *(13)* Tue 10:30 H 1058

Microtubule assembly governed by tubulin allosteric gain in flexibility and lattice induced fit — •Maxim Igaev and Helmut Grubmüller — Max Planck Institute for Biophysical Chemistry, Theoretical and Computational Biophysics Department, Göttingen, Germany

15 min. break

BP 12.6 *(162)* Tue 11:15 H 1058

Specific RNA-cation interactions: Individual binding site affinities from molecular dynamics simulation — •Sergio Cruz-León and Nadine Schwierz — Department of Theoretical Biophysics, Max Planck Institute for Biophysics, Max-von-Laue-Str. 3, 60438 Frankfurt, Germany

Metal cation-RNA interactions are essential for RNA folding and function. In this research, cation-mediated specific interactions between common RNA structural motifs and a set of biologically relevant metal cations including Li^+, Na^+, K^+, Cs^+, Mg^{2+}, Ca^{2+}, Sr^{2+} and Ba^{2+} are studied with all atom molecular dynamics simulations. Combining advanced sampling techniques and recent force fields for metal cations developed in our group, we investigate ion binding to individual binding sites on RNA by calculating ion binding affinities and kinetic rate coefficients. The calculated binding affinities agree well with available experimental data. Specifically bound cations and ions that diffusively surround the RNA affect the end-to-end distance of double stranded RNA and RNA-RNA interactions consistently with reported experimental findings. This detailed understanding of the metal cation-RNA interactions and its driving forces may provide a starting point to explore the exciting possibility to control structure formation and biological functions which have applications in nanotechnology and RNA based tools medicine.

BP 12.7 *(69)* Tue 11:30 H 1058

On the nature of cytosine pairing in DNA structures — Miriam Kohagen and •Jens Smiatek — Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany

Besides protonated cytosine pairs, recent experimental results indicate that non-Watson-Crick DNA structures can also be stabilized by intercalated metal cations. Whereas Au+, Cu+ and Ag+ can be regarded as stabilizing agents, alkali metal ions like Na+, Li+ and K+

are known as destabilizers. In this article, we rationalize the experimentally observed behavior with the help of density functional theory calculations. Our results demonstrate the dominance of covalent electrostatic bonds, meaning that a significant amount of electron density has to be located on the cations in order to stabilize cytosine pairs. Further findings imply that mixed higher electron orbitals, in addition to a pronounced electronegativity of the cations, are of fundamental importance for the binding mechanism. The outcomes of our calculations establish a consistent theoretical framework to understand the experimentally observed behavior, which is also important to achieve a more detailed understanding of nucleobase pairing in general.

BP 12.8 *(182)* Tue 11:45 H 1058

Loop formation of polyglutamines in the PRIME20 model — •Arne Böker and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg, 06099 Halle

Much effort has recently been put into understanding amyloid formation in polypeptides. The amyloid state is an aggregated structure of polypeptides and usually differs from the native state. Amyloid formation can have various effects, beneficial as well as damaging, including diseases such as Huntington's chorea, which is associated with an aggregated state of extended polyglutamine (polyQ) sequences. Loop structures or even β turns of single polyQ molecules may act as templates for aggregation, which motivates experimental investigation by energy transfer methods as well as our simulations.

We perform thermodynamic simulations of single polyQ chains represented by the intermediate-resolution PRIME20 model[1] using the SAMC[2] variation of Wang-Landau Monte Carlo sampling which provides insight into different statistical ensembles at the expense of dynamic information. Our results for the end-to-end distance distribution at physiological conditions agrees reasonably well with experimental findings. In this temperature range, the single-chain morphology for the chain lengths we studied is not yet dominated by hairpin structures which are formed at lower temperatures.

[1]M. Cheon, I. Chang, C. K. Hall, PROTEINS **78**(2010):2950

[2]B. Werlich, T. Shakirov, M. P. Taylor, W. Paul, Comp. Phys. Comm. **186**(2015):65

BP 12.9 *(101)* Tue 12:00 H 1058

Pro32 isomerisation effects on β2-microglobulin: a Metadynamics investigation — •Maria Celeste Maschio[1], Federico Comitani[2], Carla Molteni[3], and Stefano Corni[4] — [1]Dept. FIM, University of Modena and Reggio Emilia, Italy — [2]Dept. Chemistry, University College London, UK — [3]Dept. Physics, King's College London, UK — [4]Dept. Chemistry, University of Padova, Italy

β2-microglobulin (β2-m) is the protein responsible for the Dialysis Related Amyloidosis disease. The isomerisation of a specific proline, Pro32, is a debated amyloidosis triggering factor, inducing the β2-m aggregation. In this work, we investigated the structural rearrangements observed in the protein upon isomerisation of Pro32. Metadynamics simulations of the β2-m wild type (WT), the D76N amyloidogenical mutant and the W60G aggregation-resistant mutant were run to shed light on the structural and dynamical changes upon isomerisation and to identify the effects of mutations on the relative free energies of the cis and the trans isomers.

[1] Stoppini M et al, J Biol Chem, 290(16), 2015 [2] Melis C et al, J Phys Chem B, 113(35), 2009 [3] Laio A et al, PNAS, 20(99), 2002

BP 12.10 *(205)* Tue 12:15 H 1058

Metadynamics Simulations of the Fibrinogen Protomer — •Timo Schäfer[1,2], Lorenz Ripka[1], Friederike Schmid[1], and Giovanni Settanni[1,3] — [1]Johannes Gutenberg-University Mainz — [2]Graduate School Materials Science in Mainz — [3]Max Planck Graduate Center with the Johannes Gutenberg-University Mainz

Fibrinogen is a dimeric multi-chain serum protein that polymerizes into fibrin when activated by thrombin as part of the coagulation cascade. Fibrinolysis, the cleavage of fibrin by the enzyme plasmin, controls the dissolution of blood clots. While the major factors contributing to fibrin formation and dissolution have been identified, the atomistic details of these mechanisms are largely unknown.

Here, the connection between structure and function of fibrinogen is studied using classical atomistic molecular dynamics simulations coupled to metadynamics, a technique that allows for a thorough exploration of the important degrees of freedom of the system. Based on our previous characterization of a hinge along the coiled-coil region of the fibrinogen protomer, we used metadynamics to explore the major degrees of freedom related to this hinge, represented by the two largest principal components of motion. The simulations reveal the presence of two specifically distinct modes of bending, characterized by a different loss of secondary structure and exposure of plasmin cleavage sites. The bending modes occur in plane to the available models of double-stranded fibrin protofibrils. We show how they could be integrated into available models of fibrin protofibril formation and play a role in fibrinolysis

BP 12.11 *(61)* Tue 12:30 H 1058

Integration of SAXS Data into Biomolecular Simulations — •Marie Weiel, Ines Reinartz, and Alexander Schug — Karlsruhe Institute of Technology, Karlsruhe, Germany

Structural analyses in biophysics aim at revealing the interrelation between a macromolecule's dynamic structure and its biological function. Small-angle X-ray scattering (SAXS) is a useful experimental approach to this and complementary to common high-resolution techniques such as X-ray crystallography and NMR spectroscopy. In order to effectively interpret scattering intensities in terms of structural models, we include the limited information from SAXS into molecular dynamics (MD) simulations using computationally efficient native structure-based models (SBMs). A particular initial structure is defined as the global minimum in a smooth single-basin energy funnel dominated by native interactions. To incorporate information from SAXS, a bias term is added to the potential so as to energetically favour conformations reproducing the original target intensity. Dynamically fitting an initial structure to the scattering curve within MD, we obtain physical atomistic conformations according to the experimental input data. In this vein, SAXS data may be reasonably interpreted whilst simultaneously retaining chemical knowledge and sampling power of molecular force fields. Giving fast and reliable structure predictions for transiently populated conformations, we hope to make a significant contribution to unraveling the relation between macromolecular structure and function.

BP 12.12 *(266)* Tue 12:45 H 1058

Terminal Electron-Proton Transfer Dynamics coupled to Quinone reduction in Respiratory Complex I — •Ana Patricia Gamiz-Hernandez[1], Alexander Jussupow[1], Mikael P. Johansson[2], and Ville R. I. Kaila[1] — [1]Department of Chemistry, Technical University of Munich, Lichtenbergstr. 4, D-85747, Garching, Germany — [2]Department of Chemistry, University of Helsinki, P. O. Box 55, FI-00014 Helsinki, Finland

Complex I (NADH:ubiquinone oxidoreductase) contains 8-9 iron sulfur clusters (ISC) in its hydrophilic domain responsible of transferring two electrons from NADH/FMN couple to the quinone binding site, thus initiating the signal that triggers proton pump across its membrane. Although the exact coupling for this long-range proton-electron transfer process remains unclear, emerging data indicates that the initial quinone (Q) reduction to quinol (QH2) process plays a central role in activating the proton pumping machinery. In order to probe the energetics, dynamics, and molecular mechanism for the proton-coupled electron transfer (PCET) process linked to Q reduction, we employ here multi-scale quantum and classical molecular simulations, to model the relevant electronic states from Q to QH2 that may play a role in the activation of proton pump. We find that conformational changes in the hydrogen-bonded Q-binding modes regulate the rate of eT from the terminal N2 iron-sulfur center. Our combined data reveal how the dynamics of complex I-bound Q modulates the rate of terminal electron transfer, and how conserved residues in the Q-chamber contribute to the overall PCET process.

BP 13: Evolutionary Game Theory (joint session SOE/DY/BP)

Time: Tuesday 12:30–13:15 Location: MA 001

See SOE 11 for details of this session.

BP 14: Microswimmers DY I (joint session DY/BP/CPP)

Time: Tuesday 14:00–15:45 Location: BH-N 243

See DY 32 for details of this session.

BP 15: Postersession III

Topics: Membranes and Vesicles (15.1–15.18), Bioimaging (15.19–15.44), Biospectroscopy (15.45–15.51), Computational Biophysics (15.52–15.73), Statistical Physics of Biological Systems (15.75–15.84), Microswimmers (15.85–15.91), Active Matter (15.92–15.99), Statistical Physics-Based Methods in Molecular Evolution (15.100–15.101), Physics of Microbial Systems (15.102)

Time: Tuesday 14:00–16:00 Location: Poster B

BP 15.1 *(66)* Tue 14:00 Poster B

Microcapsule suspension characterisation and manipulation — •Pierre-Yves Gires — Universität Bayreuth Experimentalphysik I Universitätsstraße 30 95447 Bayreuth

Microcapsules, as submillimetric droplets embedded within a membrane, are present both in natural and artificial suspensions (e.g. cells and drug vectors in blood circulation, microalgae in algaculture). Improvements in both their characterisation and manipulation can lead for instance to better drug vectorisation or bioenergy harvesting. Three separate studies are presented, illustrating how the coupling of microfluidic tools with theoretical analysis, including if necessary numerical simulations, allows progress in this field. First, at the cell scale, the monitoring of capsule deformations in a microfluidic channel permits to characterise the membrane viscoelastic properties of cross-linked albumin microcapsules [1]. Then, a comparison between measured and simulated hydrodynamic interactions brings further insight into the origin of hydrodynamic diffusion of vesicles suspensions [2]. Last, the coupling of a thin plate subwavelength resonance with bubble secondary acoustic amplification allows to design a promising acoustofluidic device, for both locally concentrating and depleting microcapsule suspensions [3].

[1] Gires et al. "Pairwise hydrodynamic interactions and diffusion in a vesicle suspension." Physics of Fluids 26.1 (2014): 013304. [2] Gires et al. "Transient behavior and relaxation of microcapsules with a cross-linked human serum albumin membrane." Journal of the mechanical behavior of biomedical materials 58 (2016): 2-10. [3] to be published

BP 15.2 *(85)* Tue 14:00 Poster B

The Role of Lipids in Membrane Docking and Pore Formation of Pneumolysin — •Martin Vögele[1], Ramachandra Bhaskara[1], Katharina van Pee[2], Özkan Yildiz[2], Werner Kühlbrandt[2], and Gerhard Hummer[1,3] — [1]Department of Theoretical Biophysics, Max Planck Institute of Biophysics — [2]Department of Structural Biology, Max Planck Institute of Biophysics — [3]Institute for Biophysics, Goethe University, Frankfurt am Main

Streptococcous pneumoniae employs pneumolysin (PLY) to infect its human host. The specificity of PLY to cholesterol-rich membranes targets this virulence factor to mammalian cells. PLY is released in a water-soluble monomeric form. Subsequent docking and oligomerization of PLY result in the formation of membrane-embedded ring-like structures that induce cytolytic pores. Recent structural studies have resolved the structure of PLY rings in pore and pre-pore conformations on membranes. However, the detailed mechanism of pore formation and the role of lipids remain unclear.

Using large-scale coarse-grained molecular dynamics simulations, we study (1) the docking of PLY to membranes and (2) the subsequent formation of cytolytic pores. In simulations of large rings, we investigate the behavior of lipids during pore formation. We also perform all-atom molecular dynamics simulations of monomeric PLY in solution and of various membrane-docked states to understand conformational changes. These simulations, along with structural modeling, shed light on the mechanism of PLY-induced formation of membrane pores.

BP 15.3 *(86)* Tue 14:00 Poster B

Structural changes of lung surfactant Langmuir films in contact with compressed fluorocarbon gases — •Susanne Dogan, Michael Paulus, Julia Nase, Steffen Bieder, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

Current lung surfactant (LS) replacements consist of purified preparations of bovine LS (Survanta) or porcine LS (Curosurf), which are not devoid of potential viral contamination and inherent immunological risks. Fluorocarbon gases (FCs) have been investigated for various biological applications. The results suggest that FCs may be useful in pulmonary disease therapy. Thus, substituting the current LS replacements by FCs might be reasonable. However, FCs are potentially harmful to membranes and thus [1, 2] the aim of this study is the determination of structural changes in Langmuir films in contact with FCs. The effect of the external gaseous phase of octafluoropropan and decafluorobutan on DPPC, the primary component of lung surfactant or the surfactants Curosur and Survanta was studied. Knowledge on the structural organisation and reorganisation of these amphiphilic molecules under gaseous pressure is essential for the understanding of the basic biological principles, which are present in medicine [3, 4]. X-ray reflectivity is the ideal to study different properties of a layer system at interfaces, such as layer thickness, roughness, and electron density with sub-Angström in-situ. [1] Giebel, F. et al. J. Appl. Phys., 2014 [2] Giebel, F. et al. Eng. Asp, 2016 [3] Amann, A. et al. Int. J. Mass Spectrom, 2004, [4] Zasadzinski, Curr. Opin. Col. In. Sci., 2001

BP 15.4 *(90)* Tue 14:00 Poster B

Elasticity Measurements of Chloroplast Membranes — •Maike Jung and Friederike Schmid — Johannes Gutenberg-Universität Mainz, Mainz, Germany

Biological cells, which are the building blocks of all living organisms, and their intracellular components are all separated by plasma membranes. Those membranes are not only an important selective barrier between different parts of the cell but also serve as a platform for biological and chemical reactions. A detailed understanding of membranes is therefore essential for gaining a comprehensive insight into all living organisms. One important property that describes these plasma membranes is their elasticity, which is dependent on the lipid composition and the proteins incorporated into the membrane. We present experimental measurements of the elasticity for the outer and inner membrane of chloroplasts.

BP 15.5 *(106)* Tue 14:00 Poster B

The interaction of viral fusion peptides with model lipid membranes — •Göran Surmeier, Michael Paulus, Susanne Dogan, Yury Forov, Mirko Elbers, Paul Salmen, Metin Tolan, and Julia Nase — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

Viral fusion peptides (FP) are hydrophobic sequences of viral envelope proteins located in the ectodomain. Due to their position exposed to the external aqueous medium, FPs play an important role in the interaction of the viral envelope with target membranes. When a virus enters a host cell, the insertion of the FP into the target membrane leads to destabilization, thus catalysing the membrane fusion reaction. We investigated their influence on model membranes by studying the pressure dependent behavior of monoolein/water mixtures in presence and absence of the FPs of hemagglutinin 2, tick-borne encephalitis virus and vesicular stomatitis virus at a hydrophilic silicon dioxide surface using X-ray reflectivity (XRR) measurements. Previous studies demonstrated that various phase transitions between hexagonal, cubic and lamellar phases occur in monoolein/water mixtures and that the phase boundaries shift as soon as a FP is added. By applying the XRR technique, we were able to resolve the vertical membrane structure. Furthermore, we observed a modified phase behavior in the near-surface area by comparing the XRR data to additionally captured volume sensitive small angle X-ray scattering measurements. Experiments were performed at beamlines ID31 at the ESRF (Grenoble,

France) and BL9 at DELTA (Dortmund, Germany).

BP 15.6 *(175)* Tue 14:00 Poster B

A theoretical model of surfactant systems in computer simulations — •Simon Raschke and Andreas Heuer — Westfälische Wilhelms-Universität Münster, Institut für physikalische Chemie, Corrensstraße 28/30, 48149 Münster, Germany

The formation of self assembled structures such as micelles has been intensively studied and is well understood. The property of a system to develop micelles depends on the concentration of surfactant molecules and is typically indicated by the critical micelle concentration (cmc). Recent studies[1] use a lattice approach in order to determine cmc and show that the correct modelling and analysis of cluster formations is not trivial to achieve this. We developed a minimalistic and highly efficient model of the amphiphilic molecules in continuous space which were simulated using Monte Carlo and Molecular Dynamics simulations in the canonical (NVT) ensemble. The inaccessible volume of micelles needs to be taken into account for a theoretical characterization, and was calculated using Delaunay-triangulation and the powercrust algorithm. Particle densities and micellization rates are investigated and an order parameter is introduced, so that a precise predication on cmc can be made. We discuss that this model is fully appropriate to study frame-guided assembly processes, as reported by Dong et al. [2].

[1] A. P. Santos and A. Z. Panagiotopoulos, The Journal of Chemical Physics 144, 044709 (2016).

[2] Y. Dong, Y. Sun, L. Wang, D. Wang, T. Zhou, Z. Yang, Z. Chen, Q. Wang, Q. Fan, and D. Liu, Angewandte Chemie International Edition 53, 2607 (2014).

BP 15.7 *(183)* Tue 14:00 Poster B

Temperature Induced Structural Evolution of DMPC-Saponin-Mixtures: From Bicellar to Vesicular Structures — •Carina Dargel[1], Aurel Radulescu[2], and Thomas Hellweg[2] — [1]Bielefeld University, Germany — [2]Jülich Center for Neutron Science, outstation at FRM II, Garching, Germany

Vesicles composed of the phospholipid 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine are often used as model system to mimic cell membranes. The system allows to study effects of additives under different conditions, e.g. composition and temperature. Saponins are plant derived surfactants which occur among others in nuts and garlic and exhibit an amphiphilic structure built of a hydrophobic steroidic or triterpenic backbone with a varying number of hydrophilic sugar chains. For the saponin aescin an incorporation into the lipid bilayer was proven for low aescin amounts in a study with unilamellar vesicles. At low temperature and at aescin amounts higher than about 10 mol % the vesicles get solubilized into much smaller bicellar structures. By increasing temperature the bicelles convert into uni- and multilamellar vesicles due to removal of the saponin from the aggregates. These aggregates decompose again when lowering the temperature to about 23 °C, the main phase transition temperature of the phospholipid DMPC.

In this study the self-assembled structures are investigated in dependence on the aescin amount as well as the temperature mainly by dynamic light scattering and small angle neutron scattering to resolve the correlation between the lipids phase transition and the reconversion of the bicellar structures.

BP 15.8 *(228)* Tue 14:00 Poster B

Surface micelles in lipid monolayers in the LE phase — •Florian Gellert, Renko Kensbock, Heiko Ahrens, and Christiane A. Helm — Inst. f. Physics, Greifswald University, Germany

We investigate lipid and cardiolipin monolayers at the water-air interface with isotherms and real-time Brewster angle microscopy (BAM). These monolayers are in the LE phase; either they do not have an LC phase or the surface pressure is below the LE/LC phase transiton. Nevertheless, dependent on the ion concentration in the subphase the formation of domains is observed with BAM. On monolayer compression the domains increase mainly in number, not in size. The observation of surface micelles is correlated with the isotherm and the area compressibility modulus. Surface micelles of mobile lipids at a fluid interface can be used as a simple model of self-regulation of lipid membranes.

BP 15.9 *(261)* Tue 14:00 Poster B

Effect of Membrane Mediated Forces on Protein Organization — •Henning Stumpf[1] and Ana-Sunčana Smith[1,2] — [1]PULS Group, EAM, Institute for Theoretical Physics I, Friedrich-Alexander University Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Institute Ruđer Bošković, Zagreb, Croatia

Assembly of macromolecular complexes on membranes is a crucial step in many biological processes. For example, in cell adhesion, binding proteins need to be recruited to the site of contact. Recently, it has been suggested that membrane mediated interactions, through local changes in membrane composition, deformation and fluctuations, may induce long range attraction between proteins. To investigate these interactions we study membrane promoted aggregation of proteins that are modelled as harmonic springs, displacing the membrane and restricting membrane fluctuations. We calculate the forces between proteins in a mean field model and find a rich asymptotic behaviour depending on the membrane tension and bending stiffness. We use the second virial coefficient to determine under which conditions these interactions will lead to a change in local protein density. Furthermore, we study the effect of the aggregation on the transport coefficients of a protein. We find that in the relevant range of parameters, membrane mediated forces may have significant impact on protein diffusion.

BP 15.10 *(341)* Tue 14:00 Poster B

Lipid nucleic acid nanoparticles (LNPs) for delivery of single-stranded antisense oligonucleotides and targeted gene silencing — •Nicola Kerschbaumer, Rafal Krzyszton, and Joachim Rädler — Department of Physics, Ludwig-Maximilians-Universität (LMU) Munich, Geschwister-Scholl-Platz 1, 80539 Munich, Germany

Antisense oligonucleotides for gene silencing present a promising therapeutic strategy. Transfer of antisense oligonucleotides across cell membranes is limited and the development of an efficient and safe encapsulation of such antisense oligonucleotides for specific delivery becomes increasingly desirable. In previous work mononucleic acid lipid particles (mNALPs) were shown to form nanoparticles which self-assemble in a microfluidic setup when placing the lipids DOTAP, DOPE, DOPC, and DSPE-PEG2000 in a solvent solution with the usage of water as a buffer. Here we show that the same assembly strategy using microfluidic chips forms antisense LNPs with high encapsulation efficiency. The particles have 30 - 40 nm in diameter for 15 and 21 base-antisense oligonucleotides and are stable in blood serum over a period of several days as characterized using fluorescence correlation spectroscopy. We demonstrate that the particles bind specifically to cells expressing folate receptors and analyze their capability to silence targeted gene expression. Our LNP carrier provides a reasonable and effective approach for targeted delivery of single-stranded oligonucleotides for gene silencing.

BP 15.11 *(343)* Tue 14:00 Poster B

Radio Frequency Detection of Single Particles in Micorfluidic Circuits — •Marcel Hoeft — Center for Hybrid Nanostructures, Hamburg, Deutschland

I will present a method which operates on a different principle than the more common coulter-counting electric-based detection. It is an impedance-based microfluidic circuit that makes use of radio frequency reflectometry to measure the translocation of single particles through a micropore, filled with electrolyte. The device is a coplanar waveguide which lies perpendicular to the direction of flow. As a comparison measurement the change of the ion current is measured during the translocation of named particles. The structure of the cpw is brought onto a coverslip by optical lithography. An ArF excimer laser is used to drill the pore into the coverslip at the sensing region. A focused ion beam is used to reshape the sensing region to ensure that the pore lies within the confinde electric field. An integrated circuit is used to match the device to the 50 ohm. The biggest advantage of this device compared to the other coulter-counting devices is the sampling rate of up to 1 GHz. With such a rate it would be possible to analyze the dynamic of single translocation events of e.g. molecules.

BP 15.12 *(356)* Tue 14:00 Poster B

Floating Lipid Bilayers at the Liquid/Liquid interface — •Ernesto Scoppola[1], Ignacio Rodriguez-Loureiro[1], Samantha Micciulla[1], Lucas Kuhrts[1], Richard Campbell[2], Oleg Konovalov[3], Giovanna Fragneto[2], and Emanuel Schneck[1] — [1]Max Planck Institut fur Kolloid und Grenzfkachenforschung, Potsdam, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]ESRF, Grenoble, France

Biological membranes are vital components of all living organisms. They form the boundaries between the various compartments of cells and constitute platforms for essential biochemical processes. Struc-

tural insight is often a prerequisite to understand the details of these processes. X-ray and neutron reflectometry enable the structural characterization of model biological membranes and of their interactions with a variety of biomolecules. However, when using these approaches, studies on molecules crossing the membrane or deeply penetrating into the bilayer chain region turned out to be difficult, because membrane mobility often suffered from the presence of the solid surface. Here we immobilize lipid membranes near functionalized liquid/liquid (L/L) interfaces. The latter are intrinsically soft, self-healing, defect-free, and enable the manipulation of the interface from both sides. Lipid bilayers were immobilized via vesicle fusion onto oil/water interfaces functionalized with charged lipids and structurally investigated using specular reflectometry. The interaction between the bilayer and the L/L interface was tuned by variation of the ionic strength, as evidenced by a bilayer displacement relative to the interface.

BP 15.13 *(392)* Tue 14:00 Poster B

Synergetic Effects of a Cationic Surfactant and Alcohol in Antibacterial Function — •Judith Thoma[1], Wasim Abuillan[2], Ippei Furikado[3], Shigeto Inoue[3], Thomas Gutsmann[4], Klaus Brandenburg[4], Oleg Konovalov[5], and Motomu Tanaka[1,6] — [1]Institute for Physical Chemistry, University of Heidelberg, Germany — [2]Department of Fundamental Engineering, University of Tokyo, Japan — [3]Analytical Science Research, Kao Corporation, Tokyo, Japan — [4]Research Center Borstel, Leibniz-Center for Medicine and Biosciences, Germany — [5]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [6]Institute for Integrated Cell-Material Science, Kyoto University, Japan

The outer membrane of Gram negative bacteria displays a dense layer of lipopolysaccharides (LPSs) that protects the bacteria against environmental changes. Previously, Kao Co. (Japan) demonstrated significant improvement in anti-bacterial activity of cationic surfactants in coexistence with benzyl alcohol (BA). Simultaneous measurements of X-ray reflectivity (XRR) and grazing incidence X-ray fluorescence (GIXF) at the interface between sanitary agents and model bacterial surfaces based on LPSs determined how the fine structures and ion density profiles in the proximity of the interface is altered by cationic surfactants and benzyl alcohol. Focus is put on the localization of Ca^{2+} ions, which were proved to play a vital role in rejecting cationic antibacterial peptides from LPS monolayers. A significant enhancement of interactions between cationic surfactants and LPSs could be demonstrated by the addition of BA even in the presence of Ca^{2+} ions.

BP 15.14 *(428)* Tue 14:00 Poster B

Influence of phospholipid membranes on Beta2GPI conformation — •Peter Nestler[1,2], Ina Buchholz[1,2], and Mihaela Delcea[1,2] — [1]University of Greifswald, Institute for Biochemistry, Felix-Hausdorff-Str. 4, 17487, D-Greifswald, Germany — [2]ZIK HIKE, Fleischmannstr. 42, 17489, D-Greifswald, Germany

Beta 2 glycoprotein I (Beta2GPI) is abundant in human plasma and known to be the main antigen involved in autoimmune antiphospholipid syndrome (APS). Beta2GPI exists in two main structural conformations: The open/active form which potentially leads to the formation of immunogenic antibody-protein complexes and the closed/passive form in which Beta2GPI has undergone folding and binding to itself. However, the exact physiological function of Beta2GPI has not been fully understood. Here we study the interaction of Beta2GPI with phospholipid model membranes. Supported lipid bilayers (SLB) of tetramyristoyl cardiolipin (TMCL) as well as mixtures of dimyristoyl phosphoglycerol (DMPG) and dimyristoyl phosphocholine (DMPC) are prepared using Langmuir-Blodgett transfer. A novel approach using atomic force microscopy (AFM) imaging data allows to quantitatively determine the conformation of flatly adsorbed Beta2GPI in presence and absence of SLB, respectively. First findings promise to elucidate the role of phospholipids in Beta2GPI activation.

BP 15.15 *(439)* Tue 14:00 Poster B

Dynamic Optical Displacement Spectroscopy to Explore Ultrafast Bio-Membrane Dynamics — •Cornelia Monzel[1,2,5], Daniel Schmidt[3,4], Ana-Suncana Smith[3], Udo Seifert[4], Kheya Sengupta[2], and Rudolf Merkel[1] — [1]Forschungszentrum Jülich, Institute of Complex Systems 7, 52428 Jülich — [2]Université Aix-Marseille, CNRS UMR 7325 (CINaM), 13288 Marseille — [3]FAU Erlangen, EAM, 91052 Erlangen — [4]Universität Stuttgart, II. Institut für Theoretische Physik, 70550 Stuttgart — [5]present address: University of Düsseldorf, Department of Physics, 40225 Düsseldorf

The cell membrane not only forms a mechanical barrier, but is also involved in processes such as cell shape regulation, endo-/exocytosis, adhesion or membrane ruffling. To enable these physiological functions the membrane has to be soft and easily deformable, it exhibits active deformations and thermal fluctuations. Here we explore the nature of membrane fluctuations in model systems and cells with a novel method, called Dynamic Optical Displacement Spectroscopy (DODS). Based on a conventional Fluorescence Correlation Spectroscopy setup, this new approach combines the sensitivity of focal spot measurements (spatial detection limit of 20 nm) with a high dynamic range (10^{-5}-10 s). We validate DODS on giant unilamellar vesicles and derive fluctuation amplitude, membrane tension, and hydrodynamic damping with an extended membrane theory accounting for the experimental resolution. Moreover, we use DODS to quantify ATP-dependent membrane dynamics in red blood cells and effects of γ-interferon priming on the ruffling behavior of human macrophages.

BP 15.16 *(444)* Tue 14:00 Poster B

Study of elastic modulus of phospholipid bilayers — •MJ Retamal[1], R Catalan[2], M Cisternas[2], N Moraga[2], D Diaz[2], TP Corrales[3], M Busch[4], P Huber[4], M Soto-Arriaza[1], and UG Volkmann[2] — [1]Faculty of Chemistry and CIEN-UC, P. Univ Catolica de Chile, Santiago, Chile — [2]Institute of Physics and CIEN-UC, P. Univ Catolica de Chile, Santiago, Chile — [3]Department of Physics, UTF Sta Maria, Valparaiso, Chile — [4]TUHH, Hamburg, Germany

Study of artificial phospholipid membranes (PMs) on plane substrates has become relevant to contribute in the field of Bionanotechnology. In this work, we analyse the temperature dependence of Youngs modulus (YM) of several PMs (DPPC, DMPC and DSPC) performing Atomic Force Microscopy (AFM) and Surface Force Spectroscopy (SFS) measurements. Phospholipids were deposited in high vacuum on silicon substrates by physical vapour deposition (PVD). Using Raman Spectroscopy, we confirmed that the chemical structure of our phospholipids remains unchanged after PVD. AFM measurements in liquid confirm the self-assembly of the phospholipid bilayer. YM measurements obtained by SFS show the main transitions of the phospholipid bilayers. With this we have shown that PMs can be made by PVD in high vacuum, preserving their structure and mechanical properties after proper hydration. This study opens new pathways to assemble phospholipid mixtures by PVD. Acknowledgement: Postdoctoral grant FONDECYT 3160803 (MJR), FONDECYT grant #1141105 (UGV)and #1171047 (MSA), FONDECYT INICIACION grant #11160664 (TPC), CONICYT Fellowships (RC and MC) and CONICYT-PIA ACT 1409.

BP 15.17 *(446)* Tue 14:00 Poster B

Thin-film composite membrane characterization by positron annihilation lifetime spectroscopy — •Marcel Dickmann[1], Rhea Verbeke[2], Tönjes Koschine[3], Werner Egger[3], Ivo Vankelecom[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany — [2]Center for Surface Chemistry and Catalysis, Faculty of Bioscience Engineering Sciences, KU Leuven, Celestijnenlaan 200F, 3001 Leuven, Belgium — [3]Institut für Angewandte Physik und Messtechnik, Universität der Bundeswehr München, Werner-Heisenberg-Weg 39, 85579 Neubiberg, Germany

Thin-film composite membranes (TFC) are able to purify water via means of different pressure-drive processes such as nanofiltration (NF) and reverse osmosis (RO). Both mechanisms are strongly influenced by the pore size volume and concentration inside the selective layer. With the technique of positron annihilation lifetime spectroscopy (PALS) it is feasible to characterize these attributes. The pulsed low-energy positron system at the Munich research reactor FRM II provides a pulsed positron beam of variable energy, which offers the capability to investigate the free-volume distribution in materials as function of depth. We explain the measurement principle and present results for 3 different TFC membranes.

BP 15.18 *(447)* Tue 14:00 Poster B

End of Cooperativity: Chain Exchange Kinetics in Mixed Polymeric Micelles with Partially Crystalline Cores — •Nico König[1,2], Lutz Willner[1], Thomas Zinn[3], Vitaliy Pipich[4], and Reidar Lund[2] — [1]Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Forschungszentrum Jülich GmbH, Jülich, Germany — [2]Department of Chemistry, University of Oslo,

Oslo, Norway — [3]ESRF - The European Synchrotron, Grenoble, France — [4]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Garching, Germany

Here we present a kinetic study on the chain exchange in mixed polymeric micelles containing partially crystalline cores. We are interested in understanding how cooperative phenomena such as crystallization and melting affect the dynamics of self-assembled systems. As a model system we use n-alkyl-PEO with a molecular weight of roughly 5kg/mol. In water these molecules form star-like micelles with a strongly segregated alkane core that partially crystallizes. This creates an additional energy barrier that needs to be overcome during chain expulsion. We employ time-resolved small-angle neutron scattering (TR-SANS) to track the exchange kinetics. We investigated mixtures of C28-PEO and C22-PEO and determined the respective melting enthalpies using differential scanning calorimetry (DSC) which was quantitatively compared to the kinetic data obtained from TR-SANS. We found that the core crystallization occurs cooperatively while the intermicellar chain exchange processes of C28-PEO and C22-PEO are virtually decoupled.

BP 15.19 *(32)* Tue 14:00 Poster B

Segmentation of dark field images from scanning X-ray microdiffraction — •Chiara Cassini[1], Andrew Wittmeier[1], Manfred Burghammer[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, Georg-August-Universität Göttingen, Germany — [2]ESRF, Grenoble, France

Imaging nanostructures within cells presents several challenges: a high resolution method, capable of retrieving structural information at subcellular length scales, without the need for slicing the cells, is preferable. Optical imaging techniques and electron microscopy meet some, but not all of this requirements. Due to their small wavelength and high penetration depth, X-rays can access the nanometer range in intact cells. In particular, we focus on scanning micro-diffraction. Our samples are freeze-dried cells grown on SiN windows; each window contains several hundreds of cells. In the past, each cell scan took minutes to hours. However, we have recently employed a special fast scanning mode that allowed us to image an entire window within a single scan, in approximately 7 hours only. This approach ensures the collection of a statistically significant pool of data in a realistic timespan. However, the data analysis becomes more challenging: the selection of the different regions of interest to be analyzed is usually performed by hand on the dark field image of a single scan, but this is not feasible on images containing hundreds of cells. Thus, an automated alternative is required. A semi-automated segmentation strategy, based on Bradley's and Otsu's thresholding, is presented for the selection of background, cytoplasm and nuclei regions.

BP 15.20 *(45)* Tue 14:00 Poster B

Cyclic Olefin Copolymer as an X-ray Compatible Material for Microfluidic Devices — •Manuela Denz, Gerrit Brehm, and Sarah Köster — Georg-August-Universität Göttingen, Göttingen, Deutschland

Microfluidics is a well-established technique in biophysics, in particular in microscopy experiments. In recent years, microfluidic devices have also been combined with X-ray methods, taking advantage of the fact that with X-rays, smaller length scales can be probed than with visible light. For these applications, the choice of window material for the microfluidic chip is the key element. Therefore, a low background signal and high radiation resistance of the material are desired. Furthermore, reproducible and straightforward device fabrication is important for the establishment of such devices in the community. In this study, we present devices solely made out of cyclic olefin copolymer (COC). We fabricated the devices from two COC sheets with similar glass transition temperatures, so that no gluing or plasticization is necessary. In a comparative study with Kapton (polyimide) devices, a material widely used in relation with X-rays, we characterized the devices according to their suitability for our X-ray measurements and obtain data of equal quality. In a second step, we investigated the assembly process of weakly scattering vimentin intermediate filament proteins, which shows that the COC devices are very suitable for protein assembly studies and thereby open up a large variety of applications in biophysics.

BP 15.21 *(47)* Tue 14:00 Poster B

Lentiviral infection leads to blue fluorescent labeling of cancer cells — •Lorena Hentschel[1], Maja Strugacevac[1], Constanze Wiek[2], Julia Kristin[2], Marcel Glaas[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany — [2]Düsseldorf University Hospital, Department of Otorhinolaryngology, Moorenstraße 5, 40225 Düsseldorf

Previous studies in biophysics show that the behavior and properties of cells depend on their physiological environment, weather it is the coating or their coexistence with other cells. A simultaneous investigation of different cell types, such as in a human body, is indispensable. To do so, a specific labeling is necessary in order to distinguish one cell type from the other unambiguously.

Our group's research deals with the morphological differences between squamous cell carcinoma cells and non-tumor dysplastic oral keratinocytes of the head-neck area. Using a laser scanning fluorescence microscope, e.g., cell membrane and mitochondria can be investigated in detail. In order to label the carcinoma cells, a lentiviral vector is applied which results in translating a blue fluorescent protein. This method allows the research of two co-cultivated different cell types under the same experimental conditions and possible change of properties due to interaction.

As mitochondria play a huge role in the behavior of cancer cells, we focus on the investigation of their differences in the two observed cell types. Our latest results are presented in this contribution.

BP 15.22 *(51)* Tue 14:00 Poster B

Soft-landing of folded proteins by ES-IBD for imaging — •Sven Szilagyi[1], Hannah Ochner[1], Lukas Krumbein[1], Joseph Gault[2], Albert Konijnenberg[3], Esther Martin[3,4,5], Justin Benesch[2], Frank Sobott[3,4,5], Carol Robinson[2], Sabine Abb[1], Stephan Rauschenbach[1,2], and Klaus Kern[1,6] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — [2]Department of Chemistry, University of Oxford — [3]Department of Chemistry, University of Antwerp — [4]Astbury Centre, University of Leeds — [5]School of Molecular and Cellular Biology, University of Leeds — [6]École polytechnique fédérale de Lausanne, CH-1015 Lausanne

Native electrospray ionization has been shown to successfully bring proteins and protein complexes in their natively folded state into the gas phase, where further analysis by mass spectrometry and ion mobility spectrometry can be performed [1]. However, these methods are not sufficient for determining structural details at the level of imaging techniques such as TEM, AFM, STM or low energy electron holography (LEEH), which require a very clean sample preparation process. Here, we demonstrate the usage of electrospray ion beam deposition (ES-IBD) as a tool for sample preparation of folded proteins for single molecule microscopy [2]. We present examples of successfully deposited molecules imaged using the above techniques and explore the influence of different substrates and environmental conditions.

[1] Nat. Meth., 5(11), 2008, 927-933. [2] Annu. Rev. Anal. Chem. 2016, 9: 16.1-16.26

BP 15.23 *(52)* Tue 14:00 Poster B

Low Energy Electron Holography as a tool for imaging single proteins at high resolution — •Hannah Ochner[1], Sven Szilagyi[1], Wolfgang Stiepany[1], Peter Andler[1], Marko Memmler[1], Sabine Abb[1], Stephan Rauschenbach[1,2], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart — [2]Chemistry Research Laboratory Department of Chemistry, University of Oxford — [3]École polytechnique fédérale de Lausanne, CH-1015 Lausanne

Protein function is intimately linked to the protein's native 3D folding, hence determining these structures is of tremendous importance. Low Energy Electron Holography (LEEH) [1], pioneered by Fink and colleagues, is an elegant imaging method using coherent low energy electrons (50-200eV)[2] avoiding radiation damage and hence allowing for single molecules investigations [3]. Because holograms contain information regarding both amplitude and phase of the object wave field, a full 3D reconstruction can in principle be obtained by numerical reconstruction of experimentally acquired holograms. Thus, unlike in other structure determination methods such as Cryo-EM and XRD at FELs, averaging is not required. The poster gives an overview of the experimental technique and a new setup, along with the theoretical background and preliminary results.

[1] Phy. Rev. Lett, 1990, 65(10), 1204-1206.
[2] Phys. Scr., 1988, 38, 260
[3] PNAS 114, 1474-1479 (2017)

BP 15.24 *(56)* Tue 14:00 Poster B

Functionalizing AFM probes with fluorescent nanodiamonds

for multimodal spectroscopy approaches — •Frederike Erb[1], Thomas Reisser[1], Fedor Jelezko[2], and Kay-E. Gottschalk[1] — [1]Institute of Experimental Physics, Ulm University, Germany — [2]Intstiute of Quantum Optics, Ulm University, Germany

Fluorescent nanodiamonds (FNDs) offer various new imaging and metrology approaches, especially in the life sciences. Nanodiamonds containing nitrogen-vacancy centers (NV-centers) as fluorophores emit light in the near-infrared window of bioimaging. Their luminescence properties depend on the environment and thus FNDs can not only be used for bioimaging but also find an application as part of various biosensors. As they are biocompatible and non cytotoxic, they can be used for many experiments *in vivo*.

To offer an easy experimental procedure, it is considered practical to have an NV-center at the very tip of an AFM cantilever. [1,2] To build such a sensor, we want to attach an FND firmly to the cantilever. We present accomplishments and techniques on this task.

References:

[1] Hall, L. T. et al. (2010): Monitoring ion-channel function in real time through quantum decoherence. In: Proceedings of the National Academy of Sciences 107 (44), S. 18777-18782. DOI: 10.1073/pnas.1002562107.

[2] Zhou, Tony X. et al. (2017): Scanning diamond NV center probes compatible with conventional AFM technology. In: Appl. Phys. Lett. 111 (16), S. 163106. DOI: 10.1063/1.4995813.

BP 15.25 *(57)* Tue 14:00 Poster B

Distance sensing using Metal Induced Energy Transfer (MIET) — •Fabian Port and Kay-E. Gottschalk — Institute of Experimental Physics, Ulm University, Germany

In the last few decades the correlation between cell mechanics and different physiological or pathophysiological conditions, like stem cell differentiation [1] or cancer [2], has been a growing aspect of biophysical research. To understand the underlying mechano-chemical feedback cycles, it is important to understand the mechanical properties of cells under varying conditions. Cell mechanics is to a large extent determined by the cells' cytoskeleton. For a detailed analysis of the cytoskeletal structures, a method to measure small distances in cells is needed. A technique which meets this challenge is Metal Induced Energy Transfer (MIET) [3]. Here we show a first analysis of the distance between vimentin and the underlying surface in different cell lines and demonstrate the usefulness of MIET for analyzing cytoskeletal structures close to the basal membrane.

References:

[1] Suresh, S., Spatz, J., Mills, J. P., Micoulet, A., Dao, M., Lim, C. T.,and Seufferlein, T. (2005). Connections between single-cell biomechanics and human disease states: gastrointestinal cancer and malaria. Acta Biomaterialia, 1(1), 15-30.

[2] Sokolov, I. (2007). Atomic force microscopy in cancer cell research. Cancer Nanotechnology, 1-17.

[3] Chizhik, A. I., Enderlein, J. et al. (2014). Nature Photonics, 1-8. http://doi.org/10.1038/nphoton.2013.345

BP 15.26 *(62)* Tue 14:00 Poster B

X-ray Imaging of DNA Compaction During the Cell Cycle — •Andrew Wittmeier, Mareike Töpperwien, Clément Hémonnot, and Sarah Köster — Institute for X-ray Physics, Göttingen, Germany.

Imaging nanoscale structures within a cell presents several challenges. Visible light imaging techniques, such as phase contrast or fluorescence microscopy, can image living cells but they cannot access the nanoscale, with the exception of super-resolution techniques. Electron microscopy can access nanometer length scales but at the expense of detrimental sample preparation methods, e.g. staining and slicing the cell. To overcome these limitations, we combine complementary methods and employ imaging techniques involving X-rays: their high energies allow for high penetration depths without the need of disassembling the sample, and they can access the necessary length scales of nanostructures such as DNA. Although X-rays can be used to image living cells, the electron density contrast between the sample and aqueous environment is lower when compared to lyophilized cells. In order to follow the temporal evolution of the DNA compaction throughout the cell division process, we first record time-lapse phase contrast videos of the cells, thus ensuring their previous division history is known. After chemically fixing and lyophilizing the cells, measurements are taken of cells that are at different stages of the division process. The presented data includes analysis on the projected electron density, morphology, compactness, size and aggregation of the nuclear material, and was gathered by combining X-ray nano-diffraction, full-field holography and STED microscopy.

BP 15.27 *(67)* Tue 14:00 Poster B

An integrated platform for rapid semi-confocal imaging and spatially resolved fluctuation microscopy — •Adal Sabri, Andreas Veres, and Matthias Weiss — Experimental Physics I, University of Bayreuth

Fluorescence imaging is a key method when studying the secret life of cells. Due to the tradeoff between spatial and temporal resolution, rapid, high-quality data acquisition often comes at the cost of complex and technically challenging methods.

Here, we report on a simple line-illumination and slit-filtering approach for the rapid imaging of large specimen (up to 700μm edge length). The technique is about an order of magnitude faster than standard confocal microscopy approaches while maintaining a spatial resolution close to the diffraction limit.

In addition, swift switching to a second excitation/detection path within the same setup allows for performing two-point cross-correlation fluctuation spectroscopy measurements on sub-micron scales. The setup hence allows one to determine local transport coefficients as well as barriers to diffusion and flows in living cells.

Altogether, the setup provides a combination of rapid imaging and the analysis of dynamic intracellular events on subcellular scales.

BP 15.28 *(68)* Tue 14:00 Poster B

Assessing the Spatial Heterogeneity of Crowding in Living Cells — •Claudia Donth and Matthias Weiss — University of Bayreuth, Experimental Physics I

Although the interior of living cells consists of a plethora of unevenly distributed macromolecules and membrane-enclosed organelles covering several size ranges, cellular fluids are typically assumed to be homogeneously crowded solutions.

To explore the spatial heterogeneity of cellular fluids we used FRET, FLIM and confocal imaging as well as ratiometric confocal imaging in living cells. Based on the definition of the signal-to-noise ratio we defined the heterogeneity of an observable as the ratio of its standard deviation and its mean. By means of simulations we established the relation between the heterogeneity of crowding and the heterogeneity of emitted fluorescence intensity, allowing us to determine the local spatial heterogeneity of cellular crowding from imaging data.

Using different fluorescence markers we analyzed the spatial heterogeneity of macromolecular crowding states as well as that of the local ATP:ADP ratio. In addition to our measurements in interphase and metaphase cells we did time-lapse measurements in cells subjected to osmotic and oxidative stress as well as cells undergoing apoptosis to gain insight into possible dynamic changes of the local heterogeneity of cellular fluids.

Our results suggest a considerable spatial heterogeneity of cellular fluids with marked differences between nucleoplasm and cytoplasm that even persist after nuclear envelope breakdown.

BP 15.29 *(71)* Tue 14:00 Poster B

A comparison of quantitative diffusion measurement techniques in a light sheet microscope — •Philipp Struntz and Matthias Weiss — University of Bayreuth, Experimental Physics I , Universitätsstraße 30, 95447 Bayreuth, Germany

Monitoring the diffusion of particles and macromolecules with high spatiotemporal resolution yields important clues about the secret life of biological specimen. Heterogeneous biological samples may feature spatially varying diffusion characteristics while demanding gentle imaging approaches with low phototoxicity to maintain the specimen's viability. Combining single plane illumination microscopy (SPIM) and fluorescence correlation spectroscopy (FCS) provides a versatile and gentle measurement technique for spatially parallelized diffusion measurements, even in fragile developmental model systems like Caenorhabditis elegans [1]. In order to compare SPIM-FCS to complementary techniques like Single Particle Tracking (SPT) and Differential Dynamic Microscopy (DDM), we have used in-vitro systems of fluorescently labeled particles in aequous solutions. While SPIM-FCS and SPT basically report on a particle's mean square displacement, DDM is a light scattering technique based on the analysis of power spectra of difference images. All three techniques were implemented on the same custom-made SPIM setup. As a result, we observed that each technique has certain strengths and weaknesses regarding sample properties and setup characteristics.

[1] P. Struntz & M. Weiss, J. Phys. D 49, 044002 (2016).

BP 15.30 *(74)* Tue 14:00 Poster B

Tracking network dynamics and topology of the endoplasmic reticulum — •Konstantin Speckner, Lorenz Stadler, and Matthias Weiss — University of Bayreuth, Experimental Physics 1

The endoplasmic reticulum (ER) is an interconnected membrane system that extends throughout the cytosol of eukaryotic cells and serves specialized domains for essential cellular tasks. While the rough ER with membrane attached ribosomes is the major site of protein synthesis, the tubular meshwork of the smooth ER carries out lipid metabolism. The shape of this membrane network is constantly subject to modifications that are induced by cytoskeletal transport processes.

To gain insights into the ER's dynamic morphogenesis and topology, confocal fluorescence microscopy was used for cells at different conditions. By combining elements of morphological image processing and concepts of single-particle tracking experiments the organelle's shape was skeletonized to planar graphs composed of ER edges and nodes. When examining distinctive characteristics of complex networks, features of spatial networks were found for the ER's shape. Also, the subdiffusive and anticorrelated movement of individual ER network nodes was analyzed. Quantifying the motion of ER branchpoints in the presence and absence of cytoskeletal elements highlighted the role of active fluctuations for the ER's dynamic morphogenesis in the crowded interior of living cells. With this information, the motion of proteins and specialized domains on the ER could be compared to the overall motion of the ER network.

BP 15.31 *(84)* Tue 14:00 Poster B

Growth dynamics of interphase nuclei during the early embryogenesis of *Caenorhabditis elegans* — •Rolf Fickentscher[1], Akatsuki Kimura[2], Tomoko Ozawa[2], and Matthias Weiss[1] — [1]Universität Bayreuth, Bayreuth, Germany — [2]National Insitute of Genetics, Mishima, Japan

The nuclear-cytoplasmic ratio, i.e. the volume ratio of a cell's nucleus and cytoplasm, is known to be crucial for proper development: It regulates the midblastula transition in certain species but it is also linked to a variety of pathophysiological processes. Yet, how nuclear size is regulated is poorly understood. Here, we have used the model organism *Caenorhabditis elegans* to investigate the dynamics of nuclear volumes during interphase in early blastomeres. We show that nuclei grow with an exponential scaling towards an asymptotic volume that correlates linearly with the total cell volume. This result suggests a limiting component to govern the asymptotic nuclear volumes. Yet, due to an inverse scaling of interphase duration and cell volume, these asymptotic volumes are frequently not reached in early blastomeres. Moreover, nuclear growth rates are independent of temperature but are anti-correlated with cell size, consistent with a diffusion-limited process governing the nuclear expansion. The variability between different embryos is exceptionally small, highlighting once more the superb reproducibility of the organism's embryogenesis.

BP 15.32 *(112)* Tue 14:00 Poster B

Photonic Force Microscopy (PFM) on cell cultures — •Lilian Weisser, Tobias Neckernuss, Othmar Marti, and Heinrich Hörber — Institute of Experimental Physics, Ulm University

In confocal microscopy a high spatial resolution is obtained by focusing a laser to diffraction limit. Only the focus volume of the laser illuminating the sample is observed. The sample, usually biological cells, is a 100μm thick glass sample chamber. This chamber is located between a 100x oil immersion objective and condenser. In such a setup the laser focus allows also the manipulation of a nanoparticle using optical forces. An interference detection scheme using a quadrant photodiode enables position detection of nanoparticles in the focus with nanometer precision and time resolution of microseconds. Such a setup can be used to characterize interactions of nanoparticles with the environment. Until now this PFM was mainly used for mechanical characterization of the molecular motor Kinesin and so called membrane rafts in living cells. To do experiments directly in cell culture dishes with optically graded thin glass at the bottom, a 100x water immersion objective will be used as a condensor. The PFM can be employed for long time observations on living cells, which can be kept healthy in the dishes for the time of the measurement, even if it lasts for days.

BP 15.33 *(160)* Tue 14:00 Poster B

High-speed imaging of rotational diffusion of a gold nanorod on a supported lipid bilayer — •Mahdi Mazaheri[1] and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany. — [2]Department of Physics, Friedrich Alexander University (FAU) Erlangen-Nürnberg, Erlangen, Germany.

Many of the important functions of biomembranes depend on its fluidity because it determines the translational and rotational motion of lipids and membrane proteins. In this work, we use total internal reflection dark field microscopy (TIRDF Microscopy) to study the lateral and rotational diffusion of gold nanorods (GNR) linked to an artificial supported lipid bilayer.

Streptavidin-conjugated gold nanorods of length 71 nm and diameter of 25 nm were attached to headgroup-biotinylated DOPE lipids in DOPC supported lipid bilayers. GNRs were illuminated with laser light of well-known polarization and their scattered light was detected on a fast camera after separating various polarization components. By monitoring the time-dependent polarization of the detected signal, rotational and lateral diffusion of individual GNRs is imaged. Specifically, we can determine the angular orientation and center of mass position of the rod with microsecond temporal resolution. Using this approach, one can infer information on the physical properties and local dynamic behavior of the membrane such as local viscosity, short-range diffusion, and compositional heterogeneity.

BP 15.34 *(172)* Tue 14:00 Poster B

Quantitative phase imaging by focus series reconstruction on non-stained tissue — •Katharina Blessing[1,2], Alberto Eljarrat[2], Simone Gehrer[1], Christoph T. Koch[2], and Ana-Sunčana Smith[1] — [1]PULS-Group, Institiut für theoretische Physik I, Friedrich-Alexander-Universität, Erlangen — [2]AG Strukturforschung/Elektronenmikroskopie, Institut für Physik, Humboldt-Universität zu Berlin, Berlin

Many biological objects neither absorb nor scatter light, *i.e.* cells and tissue are widely invisible for conventional microscopy methods. However, most of their structural information is encoded in the phase. The field of quantitative phase imaging aims to make this information accessible.

Here we introduce a focal series reconstruction approach that only requires a standard optical microscope and computer. The reconstruction is done by a multi-focus transport of intensity equation (MFTIE) algorithm out of a focal series acquired around one in-focus shot. It reconstructs the TIE phase from multiple image pairs and refines it using a short iterative loop. Both steps take partial coherence effects into account in a flux-preserving manner. This algorithm provides amplitude and phase information separately. We tested the approach on human osteosarcoma cells. The applicability of the method to imaging epithelial tissue will be discussed with MDCK II cell colonies used as a model system.

BP 15.35 *(241)* Tue 14:00 Poster B

Design and Instrumentation of an Opto-digital Confocal Microscope — •Berk Zengin[1], Adnan Kurt[3], and Alper Kiraz[1,2] — [1]Department of Physics, Koc University, Istanbul, Turkey — [2]Department of Electrical and Electronics Engineering, Koc University, Istanbul, Turkey — [3]Teknofil Limited Company, Istanbul, Turkey

Confocal microscopy has become a vital technique for life sciences due to higher lateral and axial resolution it provides compared to standard epifluorescence microscopy. Improved axial resolution increases the sectioning capability, allowing for the observation of living specimens in three dimensions.

Despite these, accessibility to confocal microscopes did not escalate in proportion to its usage around the globe. Therefore, it was aimed to build an opto-digital confocal microscope, potentially leading to a product which will be affordable for researchers and organizations at a diverse scale.

In this work, we present a home-built confocal microscope setup using commercially available equipment. The design of the setup was realized using a 488 nm laser, an inverted microscope and optical/optomechanical parts. In addition, dual axis galvo scanner was controlled by using a custom built control electronics. Instrumentation was made using a National Instruments DAQ card and LabVIEW based software. For characterization purposes, calibration ruler and CD pattern were successfully imaged, followed by imaging of biological samples such as HeLa cells.

BP 15.36 *(322)* Tue 14:00 Poster B

High throughput optical measurement device for suspended cells and particles — •Daniel Geiger, Tobias Neckernuss, Jonas Pfeil, Markus Sporer, Stefan Reich, and Othmar Marti — Institute of Experimental Physics, Ulm University

We recently developed a novel device, called CellMOUSE that is capable of continuous, high throughput real-time measurement of suspended cells, bacteria and particles. Properties of the passing objects, like size, speed, shape and morphology can be determined for each object individually. The experimental data for all parameters is obtained with negligible delay to ease further processing of the passing objects. A throughput of more than 500 events per second can be achieved. Hence, measurements of large sample sizes are feasible. The focus in the development of CellMOUSE was on usability and fast processing of large amounts of data.

We present details of the working principle as well as the experimental setup of CellMOUSE.

BP 15.37 *(346)* Tue 14:00 Poster B

Acoustophoresis: A powerful application in microfluidics for focussing and sorting microparticles — •Toni Schildhauer[1], Thomas Henkel[2], and J. Michael Köhler[1] — [1]Technische Universität Ilmenau, FG. Physikalische Chemie/Mikroreaktionstechnik, Prof.-Schmidt-Str. 26, 98693 Ilmenau, Deutschland — [2]Leibniz Institut für Photonische Technologien IPHT Jena, AG. Mikrofluidik, Albert-Einstein-Str. 9, 07745 Jena, Deutschland

This work reports the implementation and testing of acoustophoresis into micro structured fluid channels for the purpose of focussing respectively sorting microparticles of different sizes and materials. To get valid images for e.g. flow cytometry cells need to be in the focal plane. Usually particles in microfluidic channels are distributed throughout its whole height, which is a multiple of the particles diameter as well as the range of the focal plane. Acoustophoresis was integrated into a microfluidic chip design of the IPHT Jena. Using micro algae and polystyrene particles in a size range of 10 um it was shown, that all particles can be moved into one plane under the influence of acoustophoretic forces and hence imaged sharply. Furthermore, two new microfluidic chips were designed for particle sorting application by acoustophoresis. With acoustophoresis, sorting by size is achievable up from 1 um upwards. With polystyrene particles in a diameter range from 3 to 25 um, the functioning of the sorting application was confirmed by microscopy imaging and DCS (differential centrifugal sedimentation spectroscopy).

BP 15.38 *(347)* Tue 14:00 Poster B

Monitoring activity of stem-cell derived cardiac pacemaker cells by scanning ion conductance microscopy — Lennart Gross[1], Julia Jeannine Jung[2], •Regina Lange[1], Christian Völkner[1], Sven Kraft[1], Ingo Barke[1], Christian Rimmbach[2], Gustav Steinhoff[2], Robert David[2], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics, 18059 Rostock, Germany — [2]University of Rostock, RTC, 18057 Rostock, Germany

Cell-based sensors and assays are typically used to aid drug design and to monitor water, medium, or air quality. A number of transduction mechanisms are employed, such as ion currents or luminescence. In our case we used scanning ion conductance microscopy (SICM) [1] to observe the live-cell morphology and dynamics of individual sinus nodal cardiomyocytes derived by forward programming from pluripotent stem cells [2]. The membrane displacements and surface morphology have been characterized by SICM in the native state on the pacing sinus nodal cells and while transiently inhibited pacing, respectively. Beating patterns in the range of a few Hertz and of a displacement of about 1 μm were observed. We noticed an influence of the distance between the nanopipette and the cell surface on the beating behavior. Characteristic features in the temporal spectra are analyzed with regard to the electro-mechanic pacing of the sinus nodal cells. An approach to discriminate possible participation of ion current variation directly from the cell is developed.

[1] C-C Chen et al., Annu Rev Anal Chem 5, 207 (2012)
[2] JJ Jung et al., Stem Cell Rep 2, 592 (2014)

BP 15.39 *(370)* Tue 14:00 Poster B

Motion artifact compensation in optical mapping studies with motion by combining marker-free tracking and ratiometric imaging — •Vineesh Kappadan[1], Johannes Schröder-Schetelig[1], Ulrich Parlitz[1], Stefan Luther[1,2], and Jan Christoph[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]German Center for Cardiovascular Research (DZHK e.V.), Göttingen, Germany

Fluorescence imaging or optical mapping provides highly detailed visualizations of cardiac electrophysiology in isolated, intact hearts. Recent developments in optical mapping have opened the path for being able to perform imaging with beating and moving hearts.

Here, we show that marker-free motion tracking and ratiometric imaging can be combined effectively to reduce motion artifacts when filming a beating Langendorff-perfused isolated rabbit heart. We also show that marker-free motion tracking with simultaneous imaging of action potential and calcium transient waves provides a novel tool for investigating the electromechanical dynamics of the heart.

We find that combining motion tracking and ratiometry can significantly enhance motion artifact reduction and allows the comparison and cross-validation of the two techniques with respect to each other.

BP 15.40 *(430)* Tue 14:00 Poster B

Qualitative detection, control and analysis of red blood cells (RBC) in a microfluidic channel by a commercially available 650 nm DVD laser pickup — •Max von Witzleben and Stefan Breuer — Institut für Angewandte Physik, Technische Universität Darmstadt, Schlossgartenstraße 7, 64289 Darmstadt, Germany

Commercially available DVD laser pickups are compact, robust and exhibit a good beam quality. They have been successfully employed in spatially controlling of cells by translating the laser beam inside a microfluidic channel by Kasurkurti et al. [1]. The full vertical control and contactless cell positioning however, was not possible due to constraints of the chosen experimental configuration. Here, we demonstrate experimentally that RBCs, placed in an appropriate solution can be fully controlled in 3 dimensions inside a tailored microfluidic channel. We experimentally access static and dynamic properties of RBCs based on a monolithic light detection configuration. [1] Kasukurti, A., Potcoava, M., Desai, S.A., Eggleton, C. and Marr, D. Optics Express, 19(11):10377-10386, 2011.

BP 15.41 *(431)* Tue 14:00 Poster B

Cost-efficient and compact Digital Inline Holographic Microscope (DIHM) enabling micrometer resolution for red blood cell analysis — •Stephan Amann[1], Max von Witzleben[1], Markus Susenburger[2], Zinan Liu[2], and Stefan Breuer[1] — [1]Institut für Angewandte Physik, Technische Universität Darmstadt, Schlossgartenstraße 7, 64289 Darmstadt, Germany — [2]iGEM, Schnittspahnstraße 4, 64287 Darmstadt, Germany

Light microscopes relying on digital inline holography principle and camera-based detection and retrieval of image information are the most compact and portable solution for imaging of cellular objects. DIHMs are currently emerging worldwide thanks to their cost-efficient semiconductor photonic light sources, rugged design, low number of optical and mechanical components and immediate 3D manufacturing potential. Here, we demonstrate experimentally a low-cost DIHM microscope that allow for imaging RBCs and cellular objects. The compact experimental setup enables to gain morphological information of red blood cells and can act as a portable imaging system for red blood cell quality control.

BP 15.42 *(432)* Tue 14:00 Poster B

Optical detection, control and analysis of plastic microspheres in a microfluidic channel by a semiconductor laser — •Max von Witzleben, Florian Bödicker, and Stefan Breuer — Institut für Angewandte Physik, Technische Universität Darmstadt, Schlossgartenstraße 7, 64289 Darmstadt, Germany

Micro-particles of sizes ranging from nanometres to micrometres and stemming from medications or cosmetic products contribute to the worldwide water pollution. They are hazardous as they readily enter the food chain of animals and humans. Hence, there is a strong need for micro-particle detection and filtering in fluids. Here, we present an all semiconductor photonic concept for detecting, relocating and dynamically studying plastic microspheres of sizes ranging from 3μm to 8μm. By optical control, interferometric detection and analysis, static and dynamic properties of micro-particles are experimentally accessed. A simple model allows to reproduce the experimental findings with good quantitative agreement.

BP 15.43 *(436)* Tue 14:00 Poster B

Detecting intracellular-changes below the optical resolution limit to investigate inflammation. — •Florian Schock[1,2,3,4], Jan Neumann[1,2,3], Anna Lena Leifke[2], Ulrich Pöschl[2], Kurt Lucas[2], and Christoph Cremer[1,2,3,4] — [1]Institute of Molecular Biology, University of Mainz, Mainz, Germany — [2]Max-Planck-Institut for Chemistry Mainz, Germany — [3]Institute of Pharmacy and Molecular Biotechnology, University of Heidelberg, Heidelberg, Germany — [4]Kirchhoff Institute for Physics, University of Heidelberg, Heidelberg,

Germany

As a result of the interdependency of form and function, microscopy of intracellular structure has become a standard tool to investigate biological processes and medical questions. Hence many projects of the last decades aimed to discover and improve (super-resolution-) light microscopy methods to visualize details far below the classical resolution limit. But it is also possible to use microscopy to identify structures and structural changes without the need to visualize these. Here we want to present and use such a method to investigate the effects of inflammation on mitochondria. Our simulations suggests the possibility to register changes clearly below the resolution limit by analysing wide-field images. We will present the results of an in-vitro study on fibroblasts and the comparison to our simulation. Additionally we will also report on super-resolution methods (SIM and SMLM) to image the mitochondria.

BP 15.44 *(443)* Tue 14:00 Poster B

Fast Correlative Optical Tweezers-Fluorescence Microscopy (CTFM) for the study of dynamic molecular processes — •Philipp Rauch, Jordi Cabanas-Danés, Rosalie Driessen, Gerrit Sitters, and Andrea Candelli — LUMICKS B.V. De Boelelaan 1085 1081 Amsterdam

Using optical tweezers in combination with confocal fluorescence microscopy in a controlled microfluidics environment, results in a robust and versatile methodology to study mechanisms occurring at all levels of the cellular metabolism, up to cell membrane interactions and beyond. Both the high temporal and spatial resolutions that correlative optical tweezers-fluorescence microscopy (CTFM) offers represent an asset to investigate processes with short lifetimes. Additionally, by being able to manipulate and exert tensions to selected molecules, we gain access to important structural features. To demonstrate the potential of this hybrid technique, we performed a series of experiments to study the folding/unfolding dynamics of an intracellular signaling protein, the packaging of DNA within a bacteriophage capsid and the dynamics of cytoskeletal filaments and related motor proteins. Our results show that the applications of this single molecule technology are not limited to the field of nucleic acids research and quickly advance to new venues.

BP 15.45 *(33)* Tue 14:00 Poster B

Mechanical properties of membranes under asymmetric buffer conditions — •Marzie Karimi, Jan Steinkühler, Debjit Roy, Reinhard Lipowsky Mitra, and Rumiana Dimova — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany

Biological membranes consist of molecular bilayers which are intrinsically asymmetric in nature. This asymmetry can be induced not only by leaflet composition and specific adsorption but also by differences in the cytosolic and periplasmic solutions containing macromolecules and ions. Membranes are surrounded by aqueous buffers inside and outside the cell exhibiting strong concentration asymmetry of e.g. sodium, potassium and chlorine ions. There has been a long quest to understand the effect of these ions on the physical and morphological properties of membranes. Ion-lipid interactions and, in particular, the effect of ion trans-membrane asymmetry are crucial not only for the membrane phase state [Kubsch et al. Biophys. J. 110:2581–2584, 2016] but also influence the mechanical properties of membranes. Here, we set to explore the changes in the mechanical properties of membranes exposed to asymmetric buffer conditions. As a model membrane, we employed giant unilamellar vesicles (GUVs) and first improved existing protocols for generating GUVs in physiologically relevant salt concentrations. To assess the membrane mechanical properties, we aspirate a GUV into a micropipette and by means of an attached bead manipulated via optical tweezers, we pull an outward tube to measure the spontaneous curvature and the bending rigidity of the bilayer. With increasing the aspiration pressure, the bead is displaced from the equilibrium position in the optical trap, which in return gives us the bending rigidity and spontaneous curvature of GUVs [Lipowsky, Faraday Discuss. 161:305-331, 2013]. We explore the effect of asymmetric distribution of salt and sugars across the membrane.

This work is part of the MaxSynBio consortium which is jointly funded by the Federal Ministry of Education and Research of Germany and the Max Planck Society.

BP 15.46 *(41)* Tue 14:00 Poster B

Photoinduced processes of free bilins in solution: fs TA absorption spectroscopy on phycocyanobilin and biliverdin IXα — •Maximilian Theiss[1], Tilman Lamparter[2], Maria Andrea Mroginski[3], and Rolf Diller[1] — [1]TU Kaiserslautern, D-67663 Kaiserslautern — [2]Karlsruhe Inst. of Techn., D-76131 Karlsruhe — [3]TU Berlin, D-10623 Berlin

Bilins are linear tetrapyrrols with rich photochemistry in solution (1,2), involving C-C single- and double-bond isomerization of one or several of the pyrrole methine bridges. When bound to proteins they serve as chromophore in plant-phytochromes, bacterial sensor proteins and in optogenetic systems (3). In the bound form protein-chromophor interaction restricts the potentially possible degrees of freedom (4). For a better understanding of the underlying mechanisms we study the primary photochemistry of the bilins phycocyanobilin (PCB) and biliverdin IXα (BV) in solution, employing fs transient absorption in the UV/Vis and mid-IR spectral region, complemented by quantum chemical calculations. In particular, both bilins show conformational changes, PCB additionally indicates alteration of protonation state via photoexcitation, which is consistent with previous studies (5).

(1) Falk. (2012) The chemistry of linear oligopyrroles and bile pigments (Vol. 1). SSBM
(2) Carreira-Blanco et al. (2016) PCCP. 18:7148-7155
(3) Gasser et al. (2014) PNAS. 111.24: 8803-8808.
(4) Singer et al. (2016) CPC. 17:1288-1297
(5) Dietzek et al. (2011) CPL. 515:163-169

BP 15.47 *(53)* Tue 14:00 Poster B

Adjustment of pulsed laser radiation for strob oscopic exp eriments — •Stefan Krüger[1], Tobias Löffler[1], Maja Strugacevac[1], Julia Kristin[2], Constanze Wiek[1], Jörg Schipper[2] und Mathias Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf — [2]Düsseldorf University Hospital, Department of Otorhinolaryngology, Mooren- strasse 5, 40225 Düsseldorf, Germany

This contribution aims to adjust the laser radiation of a fluorescence microscope depending on the oscillating movement of a piezoelectric actuator. Through this a stroboscopic effect can be achieved and the periodic movement of cell parts, depending on the phase of the acoustic stimulation, can be observed. The laser can be switched by TTL-signals, the piezoelectric actuator is controlled using sinus voltages with frequencies from 0,5 to 10 kHz. The piezo-control-signal is translated to TTL and the phase and signal-length is adjusted. By controlling the phase shift between the stimulating wave and the laser pulse we can select which phase of the cell movement we observe. The adjustment of the laser pulse length helps to regulate the output power and time resolution of output signal. The set up and a function test will be presented.

BP 15.48 *(93)* Tue 14:00 Poster B

Analysis of photoinduced processes of the cyanophage-encoded phycobiliprotein Lyase ΦCpeT:PEB using femtosecond transient absorption spectroscopy — •Christopher Carlein, Maximilian Theiss, Natascha Riedel, Nicole Frankenberg-Dinkel, and Rolf Diller — TU Kaiserslautern, 67663 Kaiserslautern, Germany

Phycobiliprotein lyases mediate the chromophore assembly of light harvesting phycobiliproteins in cyanobacteria (1). Interestingly, some cyanophages, viruses that infect cyanobacteria, also possess genes encoding phycobiliprotein lyases. It has been suggested that they might contribute to increasing photosynthetic efficiency in cyanobacteria during infection (2). The cyanophage P-HM1 encoded phycobiliprotein lyase ΦCpeT is forming a stable non-covalent complex with the linear tetrapyrrole phycoerythrobilin (2). To get a better understanding of how the phycobiliprotein lyases might facilitate the phycobiliprotein assembly we study the interaction of ΦCpeT with its chromophore PEB, employing fs transient absorption in the UV/Vis spectral region. This provides insights into the processes after photoexcitation in protein bound linear tetrapyrroles in contrast to their free form (3,4). Additionally, we use binding site mutants of ΦCpeT to study the conformation of PEB within the lyase.

(1) Overkamp et al. (2014) JBC. 289:26691-26707
(2) Gasper et al. (2017) JBC. 292:3089-3098
(3) Dietzek et al. (2011) CPL. 515:163-169
(4) Singer et al. (2016) CPC. 17:1288-1297

BP 15.49 *(200)* Tue 14:00 Poster B

Dielectrophoretic characterization of *E. coli* membrane integrity under influence of organic solvents — •Armin Grundmann[1], Marco Radukic[1], Harald Gröger[2], Dario

Anselmetti[1], and Martina Viefhues[1] — [1]Experimental Biophysics, Faculty of Physics, Bielefeld University, Bielefeld, Germany — [2]Organic Chemistry I, Faculty of Chemistry, Bielefeld University, Bielefeld, Germany

E. coli are of great importance for biotechnological applications as a whole cell biocatalyst. In combination with organic solvents, new possibilities arise, given that they do not harm the cells. To study the effects of solvents, we characterized the integrity of the *E. coli* cell membrane before and after incubation by determining its dielectrophoretic properties. For that purpose we applied an alternating electric field to a microfluidic channel featuring a region with insulating posts generating an inhomogeneous electrical field. The bacteria can be trapped at the posts if sufficient dielectrophoretic forces are applied. Using *E. coli* that express GFP, we were able to characterize the electric field dependent DEP behavior based on the fluorescence intensity. The resulting data were fitted with a logistic model and contain information on the integrity of the cell membranes. Comparing the DEP behavior of incubated *E. coli* with control measurements reveals the impact of the solvents on the cells.

BP 15.50 *(201)* Tue 14:00 Poster B

Label-free microfluidics using electrical impedance spectroscopy — •Armin Grundmann, Dario Anselmetti, and Martina Viefhues — Experimental Biophysics, Faculty of Physics, Bielefeld University, Bielefeld, Germany

Label-free detection of particles in microfluidic devices is an important step towards Lab-on-a-Chip devices, allowing for the analysis of unlabeled biomolecular samples. Using electrical impedance spectroscopy (EIS) we were able to detect both polystyrene beads and biological samples based on their (di)electrical properties. After successfully integrating this method into our microfluidics setup using a specially designed chip and holder system, we characterized it by simultaneously detecting impedance and fluorescence of fluorescent polystyrene beads. Thus, we investigated the dependencies of the detection on sample concentration, measurement signal frequency and external influences. To drive the samples during the measurements, hydrostatic pressure was applied, which also turned out to effect the signal. Using EIS we were then able to detect DNA and *E. coli* bacteria at various concentrations. While the detection of small sample concentrations has proven to be difficult, we obtained promising results for the detection of higher concentrations. Having found the optimal parameters and the minimal detectable sample concentration, we will be able to introduce EIS to microfluidic experiments for detection e.g. in separation applications.

BP 15.51 *(256)* Tue 14:00 Poster B

Efficient coupling between phycobilisomes, chlorophyll a and far red light induced chlorophyll f in the cyanobacterium Halomicronema hongdechloris — •Züleyha Yenice Campbell, Franz-Josef Schmitt, Mai Vi Bui, and Thomas Friedrich — TU Berlin, Institut für Chemie, Bioenergetik, Deutschland

The excitation energy transfer processes in the antenna system of the phototrophic cyanobacterium *Halomicronema hongdechloris* that contains Chlorophyll *a* and *f* in photosystem II with red light induced accumulation of Chl *f* was investigated. While H. hongdechloris has only very low amounts of Chl *f* in white-light culture conditions the ratio of Chl *f* to Chl *a* is reversibly changed up to 1:8 under illumination with far red light (720-730 nm). We performed UV-Vis absorption spectroscopy, time-integrated and time-resolved fluorescence spectroscopy and calculated decay associated spectra (DAS) indicating that highly efficient EET occurs from phycobilisomes to Chl *a* with time constants of about 100 ps in white light. Charge separation occurs with a typical apparent kinetics of 200-300 ps from Chl *a* as known from Chl *a* containing cyanobacteria like Synechocystis sp. PCC 6803. In H. hongdechloris, maximal Chl *f* concentration was observed after 3-4 days of growth under far red light (720-730 nm) and EET from PBS reached Chl *f* within 200 ps. However, fast charge separation was not observed from Chl *f*. Therefore, it is proposed, based on modeling of possible rate equation systems of EET that the charge separation occurs from Chl *a* and excitation energy is funneled from Chl *f* to Chl *a* via an energetic uphill transfer mechanism.

BP 15.52 *(26)* Tue 14:00 Poster B

Combination of Monte-Carlo simulations and experimental results to determine the microscopic energy depoit at DNA — •Marc Benjamin Hahn[1,2], Tihomir Solomun[2], and Heinz Sturm[2,3] — [1]Freie Universität Berlin — [2]Bundesanstalt für Materialforschung — [3]Technische Universität Berlin

The quantification of radiation induced damage to DNA in aqueous environment is of fundamental interest for dosimetry and its application in radiation-therapy and protection. We present a combined experimental and simulational approach to quantify and compare radiation induced damage to biomolecules in liquid environment for a wide range of primary radiation sources e. g. photons, electrons or ions and targets, such as DNA, proteins or cells.[1] To show its viability, we will apply this method to an experimentally challenging systems, the direct irradiation of plasmid DNA (pUC19) in water with electrons as primary particles. Here we combine Geant4 electron-scattering simulations with calculations concerning the diffusion and convection induced movement of the biomolecules, within a coarse-grained model of the irradiated liquid. Additionally a microscopic target model for the plasmid DNA based on the relation of lineal energy and radiation quality is used to calculate the effective target volume.

[1] Hahn *at al. Phys. Rev. E* **95** 052419 (2017)

BP 15.53 *(36)* Tue 14:00 Poster B

Developing a coarse-grained potential for double-stranded RNA from quantum-mechanical calculations — •Sergio Cruz-León[1,2], Álvaro Vázquez-Mayagoitia[3], Nadine Schwierz[2], and Maria Fyta[1] — [1]Institute for Computational Physics, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Department of Theoretical Biophysics, Max Planck Institute for Biophysics, Max-von-Laue-Str. 3, 60438 Frankfurt, Germany — [3]Argonne National Laboratory, 9700 S. Cass Avenue, Building 240, Argonne, Illinois, USA

A coarse-grained model for double-stranded (ds) RNA is derived based on quantum mechanical calculations. Our model extends a previous work developed for dsDNA by accounting for chemical and structural differences between dsDNA and dsRNA. Our coarse-grained model is a four bead representation where the total energy is derived from a bottom up approach using density functional theory calculations. The interactions within dsRNA are divided into four physical meaningful terms: hydrogen bonding, stacking, backbone, and electrostatic interactions. Our coarse-grained model is able to successfully reproduce the dsRNA structure. The model predicts a persistence length in good agreement with reported experimental data in a broad range of salt concentrations. Overall, our coarse-grained model has the potential to extent the relevant time and length scales in dynamic simulations of dsRNA.

BP 15.54 *(73)* Tue 14:00 Poster B

Exploiting ecology in drug pulse sequences in favour of population reduction — Marianne Bauer[1], •Isabella Graf[1], Vudtiwat Ngampruetikorn[2], Greg Stephens[2,3], and Erwin Frey[1] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Munich, Germany — [2]Biological Physics Theory Unit, Okinawa Institute of Science and Technology Graduate University, Onna, Okinawa, Japan — [3]Department of Physics & Astronomy, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands

A deterministic population dynamics model involving birth and death for a two-species system, comprising a wild-type and more resistant species competing via logistic growth, is subjected to two distinct stress environments designed to mimic those that would typically be induced by temporal variation in the concentration of a drug as it permeates through the population and is progressively degraded. Different treatment regimes, involving single or periodical doses, are evaluated in terms of the minimal population size (a measure of the extinction probability), and the population composition (a measure of the selection pressure). We show that there exist timescales over which the low-stress regime is as effective as the high-stress regime, due to the competition between the two species. Our results suggest that when the duration of the high-stress environment is restricted, a treatment with one or multiple shorter pulses can produce better outcomes than a single long treatment. If ecological competition is to be exploited for treatments, it is crucial to determine these timescales.

BP 15.55 *(79)* Tue 14:00 Poster B

De Novo Protein Structure Prediciton by Integration of Coevolutionary Data into Replica Exchange Simulations — •Arthur Voronin[1] and Alexander Schug[2] — [1]Physics Department, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]John von Neumann Institute for Computing, Jülich Supercomputer Centre, Jülich, Germany

Proteins perform important tasks in every living organism and are an essential part of life. Studying the structure of proteins helps to understand interactions in a biological system which can be applied to other fields, such as improving drug design. Despite incredible progress in experimental techniques, protein structure determination is arduous. Here, we suggest a complementary method of de novo protein structure prediction. Direct coupling analysis (DCA) quantifies coevolution of amino acid pairs in large sequence alignments, where high scoring pairs can be interpreted as spatially adjacent. Regular molecular dynamics (MD) simulations are computationally too costly to identify the native conformation in straightforward simulations. One reason is entrapment in one of the many local minima. By integrating DCA-derived contacts as constraints into MD simulations we smoothen the energy landscape and guide structure prediction. Additionally, any residual entrapment will be overcome by replica exchange. With this combination of techniques, it should be possible to predict the native structure de novo, i.e. without prior knowledge of structural elements, in a single simulation run. To study our methods performance we investigate small proteins using various numbers and quality of constraints.

BP 15.56 *(89)* Tue 14:00 Poster B

MaxEnt-Stress Graph Drawing in Protein Structure Determination — •Oskar Taubert[1] and Alexander Schug[2] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Jülich Supercomputing Centre, Jülich, Germany

Proteins perform a wide range of functions in living systems, such as transport, catalysis, or signaling. A protein's function and structure are closely related. There are different experimental as well as computational methods for resolving protein structures. NMR in particular supplies a list of atom pairs with associated distance intervals and confidence scores. This information has to be translated to 3D atomic coordinates, solving a distance geometry problem.

Since graphs are suited to model this type of pairwise relationships as edges and vertices, we use MaxEnt-Stress graph drawing as an efficient solution to map a list of atomic distance constraints onto a 3D-structural model (cf. Wegner et al., *ESA* 2017). More specifically, we take input errors and distance intervals into account. Input consists of the amino acid sequence, secondary structure, and long range contact information, as it is provided by experiments or co-evolutionary analysis. To test our algorithm, we conduct simulations on input data generated from known structures of biomolecules of different types. We find the reference structure is reproduced with high fidelity, even from noisy data, when supplying roughly three times the number of heavy atoms as graph edges.

BP 15.57 *(123)* Tue 14:00 Poster B

Modelling Chemotaxis of swarm search — •Zeinab Sadjadi and Heiko Rieger — Theoretical Physics, Saarland university, 66123 Saarbrücken, Germany

We study the effect of chemotaxis in swarming search strategy of T cells. We hypothesize that a swarm of T cells might coordinate its search by secreting chemokines on their trail which send a signal to other searchers and eventualy enhances the search efficiency. We model T cells movement as if they avoid searching areas that other T cells have scanned already and explore regions that have not been visited yet. This leads to a searcher-searcher interaction which we investigate on a 2D lattice.

BP 15.58 *(125)* Tue 14:00 Poster B

Evolution on multiple scales - merging evolution and dispersal on landscape scales — •Michaela Hamm and Barbara Drossel — Technische Universität Darmstadt, Germany

Life forms on earth are stunningly diverse. This rich variety of species evolved in time spans inaccessible to any experiment. Evolutionary food web models were developed in the last decades as tools to analyse food web emergence and persistence on long time scales. Those models are based only on a handful of mutation or adaptation rules, from which the food web structure arises naturally in a self-organized way. But ecosystems are never isolated but coupled by species dispersal, i.e., evolutionary dynamics is affected by spatial structure.

In order to obtain a model that retains essential features of older evolutionary models but allows for fast computation on many coupled habitats, we developed an new model merging the following features of models from the literature: 1) Species are characterized by traits based on body mass, following for example [1, 2]. 2) The biomass density of species is calculated self-consistently from the network of interactions by using the difference equation approach as in [3]. 3) New species are introduced into the system by varying the traits of existing species. 4) Species spread to adjacent habitats based on a stochastic migration process. The second feature, which replaces explicit population dynamics with a fast estimation of equilibrium biomasses, is crucial for scaling the model to many (i.e., several hundred) habitats. We present first results how our new model performs on a local scale. [1] Allhoff et al.(2015);[2] Rogge et al.(in prep);[3] Caldarelli et al.(1998).

BP 15.59 *(127)* Tue 14:00 Poster B

Hydrodynamic mobility functions near elastic interfaces — •Abdallah Daddi-Moussa-Ider[1], Maciej Lisicki[2], and Stephan Gekle[3] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, Düsseldorf 40225, Germany — [2]DAMTP, University of Cambridge, Wilberforce Rd, Cambridge CB3 0WA, United Kingdom — [3]Biofluid Simulation and Modeling, Fachbereich Physik, Universität Bayreuth, Universitätsstraße 30, Bayreuth 95440, Germany

Elastic confinements are an important component of many biological systems and dictate the transport properties of suspended particles in a viscous flow. Using a fully analytical theory, we study the Brownian motion of a spherical particle moving in close vicinity of a living cell whose membrane is endowed with a resistance towards shear and bending. The analytical calculations proceed through the computation of the frequency-dependent mobility functions and the application of the fluctuation-dissipation theorem. Elastic interfaces endow the system with memory effects that lead to a long-lasting anomalous subdiffusive regime of nearby particles. The analytical predictions are validated and complemented with boundary-integral simulations.

References:

A. Daddi-Moussa-Ider and S. Gekle. Phys. Rev. E 95, 013108 (2017)
A. Daddi-Moussa-Ider, M. Lisicki, S. Gekle. Phys. Rev. E 95, 053117 (2017)
A. Daddi-Moussa-Ider, M. Lisicki, S. Gekle. Phys. Fluids 29, 111901 (2017)

BP 15.60 *(181)* Tue 14:00 Poster B

Investigation of an evolutionary foodweb model on a large lattice of habitats — •Johannes Reinhard, Tobias Rogge, and Babara Drossel — TU Darmstadt, Germany

We examine an evolutionary food web model without population dynamics. Each species is characterized by a few traits based on its body mass, and the network context (predators, prey, competitors) determines species survival. This approach uses far less computing time than models with population dynamics and can therefore applied to several hundred placed on a square grid. In addition to speciation, migration, and context-dependent extinction, the model includes also a spontaneous extinction rate. When this rate is set to zero, the system reaches a frozen state where no new species can enter, and the formation of this frozen state depends crucially on migration. Furthermore we investigate which properties allow a species to spread over many patches: its body mass has to be close to the feasible body mass interval of the respective trophic level.

BP 15.61 *(186)* Tue 14:00 Poster B

DPD with Energy Conservation Simulation of Thermophoretic Particle — •Fatemeh A. Soleymani, Dmitry Fedosov, Marisol Ripoll, and Gerhard Gompper — Forschungszentrum Jülich, Jülich, Germany

The self-propelled particle converts environmental energy into the directed motion. Examples range from chemotactic cells and bacteria to artificial micro-swimmers which are widely studied due to their applications in drug delivery and micro/nanomachines in fluid. The main physical mechanism of propulsion is an inhomogeneous field e.g. a flexible magnetic filament under an applied magnetic field or a self-propelled particle in an inhomogeneous concentration (diffusiophoresis phenomenon) or temperature field (thermophoresis phenomenon). Janus particles are colloidal particles with the inhomogeneous surface feature which can form the field gradient. The Janus particle with a metallic cap absorbs more energy from an external source which can be the heat source (laser beam) or magnetic field. Energy absorption increases the temperature of one cap and the temperature gradient is imposed mainly at poles. We investigate the behavior of the thermophoretic Janus colloid in its temperature gradient by the dissipative particle dynamics method with energy conservation (DPDE). The simulation results show how local fluid-colloid interactions and the temperature gradient near the colloid*s surface control the swimming

velocity.

BP 15.62 *(206)* Tue 14:00 Poster B

Adsorption Simulations of Plasma Proteins on Silica Surfaces — •Timo Schäfer[1,2], Friederike Schmid[1], and Giovanni Settanni[1,3] — [1]Johannes Gutenberg-University Mainz — [2]Graduate School Materials Science in Mainz — [3]Max Planck Graduate Center with the Johannes Gutenberg-University Mainz

Nanoparticle based therapeutics are a topic of ongoing research, promising effective use as drug delivery systems that shield aggressive and/or fragile drugs while transporting them to a target location inside the body. One of the major challenges in their application is the formation of a layer of adsorbed plasma proteins as soon as the nanoparticle enters the blood stream. This so-called protein corona can significantly impair the nanoparticle's functionality such as active targeting or enhancement of blood circulation times. While the corona formation can be limited, existing techniques cannot completely prevent it, and molecular details of the underlying mechanism are largely unknown. Here, we study the early adsorption of plasma proteins onto the surface of a silica nanoparticle using classical atomistic molecular dynamics simulations. Using a sophisticated silica surface model, adsorption dynamics, interaction patterns and the impact of the adsorption on protein structure and functionality are analyzed.

BP 15.63 *(208)* Tue 14:00 Poster B

Subthreshold signal encoding in coupled FitzHugh-Nagumo neurons — •Maria Masoliver and Cristina Masoller — Department of Physics, DONLL, Universitat Politècnica de Catalunya

Despite intensive research, the mechanisms underlying how neurons encode external inputs remain poorly understood. Recent work has focused on the response of a single neuron to a weak, subthreshold periodic signal. By simulating the FitzHugh-Nagumo stochastic model and then using a symbolic method to analyze the firing activity of the neuron, preferred and infrequent spike patterns were detected, whose probabilities encode information about the signal [1]. We study how a second neuron, which does not perceive the subthreshold signal, affects the detection and the encoding of the signal, done by the first neuron. Through simulations of two coupled FitzHugh-Nagumo neurons we show that the coding mechanism is indeed robust, as the neuron that perceives the signal fires a spike train that has symbolic patterns whose probabilities depend on the features of the signal. Moreover, we show that the second neuron facilitates the detection of the signal, by lowering the firing threshold of the first neuron. This in turn decreases the internal noise level need to fire the spikes that encode the signal. We demonstrate that the probabilities of the symbolic patterns achieve maximum or minimum values when the period of the external signal is close to (or is half of) the mean firing period of the neuron.

[1] M. Masoliver, C. Masoller, Subthreshold signal encoding in coupled FitzHugh-Nagumo neurons, arXiv:1711.08309, 2017.

BP 15.64 *(220)* Tue 14:00 Poster B

Mean field coarse-grained modeling of Protein Folding in Complex Lasso structures — •Claudio Perego and Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz (Germany)

Complex Lassos have been recently identified as a significant class of entangled proteins. These motifs are charactierized by a covalent loop determined by a disulphide bridge. As the protein collapses into its native fold the covalent loop is threaded by part of the polypeptide chain, forming a non-trivial topology. The disulphide bridge can establish under oxidizing conditions, while it does not in reducing environment. It is therefore possible to exploit this feature as an on/off switch of the lasso motif, investigating how topological complexity can affect the folding and the biological activity of the protein. We here present a molecular dynamics study of the Complex Lasso protein folding. We employ a coarse-grained description of the polypeptide, that includes only local interactions, plus an attractive potential modeling the disulphide bridges. The simplicity of our model makes it possible to collect a larger statistics of folding with respect to ordinary structure-based models. Building on this advantage we introduce a genetic scheme for the tuning of the force-field in order to optimize the protein folding rate. This procedure allows us to retrieve insights of great interest for the understanding of complex lasso folding, such as the optimal folding pathways. By excluding the disulphide bridge potential we can also compare the behavior of our model in the oxidized and reduced states, assessing the impact of the complex lasso topology.

BP 15.65 *(275)* Tue 14:00 Poster B

The Alignment of the Malaria Parasite Before Invasion — •Sebastian Hillringhaus, Gerhard Gompper, and Dmitry A. Fedosov — Institute of Complex Systems, Forschungszentrum Jülich, Jülich, Germany

Malaria is caused by *Plasmodium* parasites that reproduce within red blood cells. Before the parasite can enter a red blood cell, it must align with its apex towards the membrane. During the brief alignment stage, major deformations of the red blood cell membrane are observed. While these deformations can be visually classified in experiments, the underlying mechanics and mechanisms are not yet understood. We investigate this behavior *in silico* with a red blood cell model formulated within the dissipative particle dynamics framework. Different deformation states are quantified with a number of observables such as binding energy. We investigate how different interactions between the parasite and the membrane influence the parasite alignment as well as how the position of the first contact between cell and parasite affects red blood cell deformation. One of our aims is to answer the question, whether the observed deformations are crucial to the parasite alignment or byproduct of alignment mechanisms.

BP 15.66 *(293)* Tue 14:00 Poster B

Numerische Untersuchung der Dielektrophorese zur Separation von Mikroalgen — •Fabian Gringel[1], Vinzenz Abt[2], Peter Neubauer[2] und Mario Birkholz[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder) — [2]TU Berlin, Fachgebiet Bioverfahrenstechnik, Institut für Biotechnologie, Ackerstr. 76, 13355 Berlin

Mikroalgen als alternative Produzenten für Biokraftstoffe, Lebensmittel und Pharmazeutika sind in den Fokus der Biotechnologie gerückt. Um die Kultivierung im großtechnischen Maßstab wirtschaftlich betreiben zu können, werden neue Mikroalgenstämme mit optimierter Lipidproduktion benötigt. Mittels Dielektrophorese können Mikroalgen in Mikrofluidik-Kanälen nach ihrem Lipidgehalt kontinuierlich separiert werden, ohne sie mit Fluoreszenz-Farbstoffen zu markieren oder im Verlauf der Separation zu beschädigen. Anwendungsmöglichkeiten ergeben sich dadurch sowohl in der Entwicklung neuer Stämme als auch integriert in großtechnische Anlagen.

Wir berichten von begleitender Simulationen mit Finite-Elemente-Methoden (FEM) bei der Planung eines Dielektrophorese-Kanals zur Separation von Algen der Art Crypthecodinium cohnii. Sind die dielektrischen Eigenschaften der Algen in ihren verschiedenen Wachstumsstadien bekannt, so gibt die Simulation Aufschluss über die Kombinationen der Parameter Flussrate, elektrische Spannung, Frequenz, Kanalabmessungen und Elektrodenkonfiguration, bei der eine Separation erfolgreich durchzuführen ist. Darüber hinaus erlaubt sie den qualitativen Vergleich unterschiedlicher Konfigurationen sowie eine Einschätzung des Einflusses fertigungstechnischer Toleranzen.

BP 15.67 *(349)* Tue 14:00 Poster B

Computational Simulation of Tissue Engineered Heart Repair — •Moritz Kalhöfer-Köchling[1], Yong Wang[1], Martin Uecker[2], Jens Frahm[3], Wolfram Zimmermann[2], and Eberhard Bodenschatz[1] — [1]MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]University Medical Center Göttingen, 37075 Göttingen, Germany — [3]MPI for Biophysical Chemistry, 37077 Göttingen, Germany

Myocardial infarction is the leading cause of death globally. Remuscularization of the heart using engineered heart muscle (EHM) tissues is a promising technique for damage repair, not only supporting scarred tissue passively, but also contracting in unison with the surrounding healthy tissue. Thereby, in the best of cases, it might reconstitute normal cardiac function. To date, the affect of EHM implants on the elastic properties and thus on the cardiac pump functions are not well understood. Computational simulation provides virtual medical diagnosis and prospective output of surgery. Employing the Holzapfel-Ogden constitutive law together with patient MRI and pressure data, we developed a heart model and strive to find corresponding EHM qualities for an optimal cure of the patient. This work was supported by the Max Planck Society and the German Center for Cardiovascular Research, and was conducted within the Physics to Medicine Initiative at Goettingen Campus between MPG and UMG.

BP 15.68 *(350)* Tue 14:00 Poster B

Computational Simulation of Tissue Engineered Heart Repair — •Moritz Kalhöfer-Köchling[1], Yong Wang[1], Martin Uecker[2], Jens Frahm[3], Wolfram Zimmermann[2], and Eberhard Bodenschatz[1] — [1]MPI for Dynamics and Self-Organization, 37077

Göttingen, Germany — [2]University Medical Center Göttingen, 37075 Göttingen, Germany — [3]MPI for Biophysical Chemistry, 37077 Göttingen, Germany

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BP 15.69 *(366)* Tue 14:00 Poster B

The effects of polar co-solutes on the hydration interaction between lipid bilayers — •Amanuel Wolde-Kidan[1], Quoc Dat Pham[2], Emanuel Schneck[3], Emma Sparr[2], and Roland Netz[1] — [1]Fachbereich Physik, Freie Universitaet Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Division of Physical Chemistry, Chemistry Department, Lund University, P.O. Box 124, 22100 Lund, Sweden — [3]Department of Biomaterials, Max-Planck Institute of Colloids and Interfaces, 17746 Postdam, Germany

The so-called hydration interaction between lipid bilayers has been studied intensively, but a fundamental explanation remains elusive until today. Using molecular dynamics simulations we analyse the effect of the addition of different polar co-solutes, namely TMAO, urea and sodium chloride, on the interaction between DMPC and POPC lipid bilayer stacks. From our simulations we can determine the water chemical potential, while gradually swelling our bilayer systems, to asses the strength of the hydration interaction. Results from the simulations have been confirmed by calorimetry experiments. We find that the hydration interaction in systems with polar co-solutes is a combination of the hydration interaction of the lipid bilayers in neat water and the interactions of the co-solutes within the water slab.

BP 15.70 *(378)* Tue 14:00 Poster B

Molecular Dynamics Simulation of SIM-SUMO complexes — •Alexander Kötter and Andreas Heuer — Institut für physikalische Chemie, Universität Münster

The small ubiquitin related modifier (SUMO) plays an important role in many cellular processes [1]. In these processes SUMO forms non covalent bonds to target proteins via interactions with the sumo interacting motif (SIM). Complexes may be formed by a single SUMO interaction with a SIM of the target protein, but also by oligomers of SUMO proteins each interacting with one SIM of the target protein. Atomistic molecular dynamics simulations of a complex formed by a single SUMO (monoSUMO) and a single SIM (monoSIM) show the transient nature of these complexes, irrespective of the type of the SIM or its orientation towards the SUMO. To investigate further the nature of these monoSUMO-monoSIM complexes we calculate their standard binding free energies. To do so we employ a sophisticated scheme [2], that involves calculating the contribution of several degrees of freedom orthogonal to the distance of SUMO and SIM in order to get an accurate estimate of the binding free energy. Furthermore we investigate the structure of complexes of a SUMO dimer (diSUMO) and a peptide chain containing two SIMs (diSIM). We find that the complexation of the diSUMO with the diSIM has limited influence on the dynamics of the diSUMO as characterized by its root mean squared displacement (rmsd). [1] Xu et al. Nat. Comm. 5, 4217 (2014) [2] Gumbart et al. JCTC 9, 794 (2012)

BP 15.71 *(399)* Tue 14:00 Poster B

Synchronization-based reconstruction of cardiac electrical wave dynamics from mechanical deformation — •Jan Lebert, Ulrich Parlitz, Stefan Luther, and Jan Christoph — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The understanding of the mechanisms of heart rhythm disorders such as ventricular fibrillation is severely limited by the inability to experimentally observe the electrical activity within the heart muscle. From a dynamical systems viewpoint, heart muscle tissue is a nonlinear, excitable, electromechanically coupled medium with a complicated anisotropic structure consisting of interconnected sheets of muscle fiber. Based on recent experimental observations of localized correlation between mechanical deformation of the heart and the electrical activity on its surface, we propose a novel approach for reconstructing cardiac wave dynamics. We utilize a technique called data assimilation to synchronize observations of the mechanical deformation with a computational model of excitable cardiac tissue coupled with an elastic mass-spring system for deformation modeling. Here, we demonstrate that our approach is able to reconstruct complex spatio-temporal cardiac electrical wave dynamics from simulation-generated surrogate observations of mechanical deformation. We show that the synchronization recovers the dynamics of the unobserved state variables from the excitable tissue model as well as the observed mechanical deformation.

BP 15.72 *(412)* Tue 14:00 Poster B

Optogenetic modeling of murine ventricular cardiomyocytes — •Sayedeh Hussaini[1,2], Claudia Richter[1,4], and Stefan Luther[1,2,3] — [1]RG Biomedical Physics, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [2]Institute for Nonlinear Dynamics-Georg-August Goettingen University, Goettingen, Germany — [3]University Medical Center Goettingen (UMG), Department of Pharmacology and Toxicology, Goettingen, Germany — [4]University Medical Center Goettingen (UMG), Department of Cardiology and Pneumology, Goettingen, Germany

Current arrhythmia treatments applying high energetic electrical shocks still present severe side effects such as tissue damage due to electroporation hence worsening the prognosis. Optogenetics is a new method that enables selective photo-optical stimulation of the heart. Therefore, computational modeling can be of specific interest to predict changes in cardiac action potentials. However, in silico studies have been mainly implemented concentrating on human specific parameters ignoring the fact that the majority of experimental research projects are done in animal models. Because of this discrepancy, we successfully implemented the light-activated ion channel Channelrhodopsin-2 in an ionic model of murine ventricular cardiomyocytes (Bondarenko model). Ongoing work includes extending this single cell model into two dimensions. Results of the computational study are used to optimize and validate current experiments on transgenic mouse hearts. All results will be discussed in comparison to conventional electrical stimulation.

BP 15.73 *(442)* Tue 14:00 Poster B

Adding curvature to the vertex model of the Drosophila imaginal wing development. — •Joris Paijmans — MPI-PKS, Dresden, Germany

Vertex models describing the mechanics of epithelial cell tissues, have been very successful explaining the effect of planar cell polarity, cell elongation and topological transitions in the tissue. The fruit fly Drosophila has proven to be an excellent model organism to study tissue mechanics. In particular, the development of the wing of the fly, consisting of a double layer of cells, has been studied in great detail. This double layer forms in the pupal stage after the eversion (turning inside out) of the single layer imaginal wing disc. To understand the onset of eversion we require a vertex model that account for the curvature in the tissue, which was not possible in our previous description. I show how to make the 2D vertex model bend and how to describe the effect of curvature on the cell organization in the tissue.

BP 15.74 *(60)* Tue 14:00 Poster B

Efficiency and sensory capacity of molecular sensors with thermal noise — •Andreas Ehrmann[1], David Hartich[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Germany — [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

For a molecular sensory system following an external stochastic signal, we examine the efficiency and sensory capacity [1]. Within the framework of stochastic thermodynamics of bipartite systems, the efficiency relates the rate with which the sensor learns about the signal to the free energy that is dissipated by the sensor. On the other hand, the sensory capacity is a purely information theoretic quantity that achieves its maximum value 1 if the instantaneous state of the sensor contains as much information about a signal as the whole time-series of the sensor. For a two state sensor estimating a fluctuating ligand concentration as signal, which is modeled by a Langevin equation, the maximal sensory capacity is shown to be achieved if the time scales

of signal and sensor are almost equal, and if the noise amplitude of the signal is small enough. We show that the addition of a dissipative second component to the sensor, which serves as a memory, increases the sensory capacity. We compare our results to an analytically solvable model, in which signal, sensor and memory are approximated with coupled linear Langevin equations [1].

[1] D. Hartich, A. C. Barato, and U. Seifert, Phys. Rev E 93, 022116 (2016)

BP 15.75 *(63)* Tue 14:00 Poster B

A new understanding of system in the molecular biology — •Norbert Sadler — Norbert Sadler

It can be shown that in an open thermo dynamic and self-sustaining molecular system through supply of arranged energy states as assimilation or the cellular metabolism the entropy of the biological System can be kept constant. The physiological processes in the living nature will be structured, simulated and understood through physical and mathematical methods.

Further Information: www.cosmology-harmonices-mundi.com

BP 15.76 *(95)* Tue 14:00 Poster B

Non-equilibrium dynamics in marginally stable biological networks — •Federico Gnesotto and Chase Broedersz — Arnold Sommerfeld Center for Theoretical Physics and Center for Nanoscience, Ludwig-Maximiians-Universität, D-80333 München

Biological networks such as the actin cytoskeleton of a cell are inherently out of equilibrium. ATP-driven molecular motors constantly exert local stochastic forces on the fibers of these networks, thereby driving these assemblies into a non-equilibrium steady state. How does the network architecture affect this non-equilibrium state? Recent studies have proposed that biological networks are weakly connected and may be poised near a mechanical stability (isostatic) threshold, where the system exhibits critical behavior. Here we investigate how this criticality affects the non-equilibrium dynamics of such marginal networks. To this end, we propose a minimal model of a diluted triangular lattice with tunable connectivity and local motor activity. This essential approach allows us to study how the proximity to a critical point affects the non-equilibrium properties of networks at different length scales.

BP 15.77 *(98)* Tue 14:00 Poster B

Population dynamics of bacterial persistence in spatially heterogeneous environments — •Pintu Patra[1] and Stefan Klumpp[2] — [1]Institut für Theoretische Physik, Universität Heidelberg, Heidelberg, Germany — [2]Institut für Nichtlineare Dynamik, Georg-August-Universität Göttingen, Göttingen, Germany

Stochastic switching in bacteria is known to be advantageous for population growth and survival in temporally fluctuating environments. However, its role in population expansion and survival in spatially heterogeneous environments is unclear. In this work, we study the expansion of a bacterial population consisting of cells that can stochastically switch between normal and persister state in environments with nutrient-rich areas and stressful areas, for example containing antibiotics. Our results show that the population expansion speed in the nutrient-rich environment depends on the fraction of persister cells at the leading edge of the population wave. Further, when such population wave is stalled by an antibiotic barrier, the fraction of persister increases at the interface between the environments which allows the population to penetrate further into the antibiotic region. Interestingly, the extent of the population wave in the antibiotic region shows a maximum with the variation in phenotype switching rates. We explain this maximum as an interplay of population dynamics at the interface separating the two environments and the switching of persister cells to the normal state in the antibiotic region. Our study shows that stochastic switching in bacterial population determines the spatial expansion speed in nutrient-rich areas and helps in crossing antibiotic barriers.

BP 15.78 *(155)* Tue 14:00 Poster B

Diffusion of nanoparticles perpendicular to hard walls and cell membranes — •Katharina Gräßel and Stephan Gekle — Biofluid Simulation and Modeling, Bayreuth, Germany

The diffusion of nanoscaled spherical particles perpendicular to cell membranes has been investigated by Ider et al. [1], who presented an analytical theory which includes the deformation of the elastic membrane due to the diffusing particles. However, the distance of the particle to the wall or the membrane was taken to remain constant, as a first approximation.

We investigate a system with non-constant spatially varying diffusion coefficient in front of hard walls. Therefore we use a different approach: following Wang [2] we set up a Fokker-Planck equation and then solve it numerically.

In the next step, we introduce a memory function to the Langevin equation to model diffusion in front of elastic membranes and again solve the corresponding Fokker-Planck equation numerically. This method reproduces the results of Ider et al. [1] for a constant diffusion coefficient and additionally allows the computation of the concentration profiles.

[1] Ider et al., Physical Review E 93, 2016
[2] Wang, Physical Review A 45.2, 1992

BP 15.79 *(190)* Tue 14:00 Poster B

Non-equilibrium scaling behavior in driven soft biological networks — •Grzegorz Gradziuk, Federica Mura, and Chase Broedersz — Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, D-80333 München, Germany

Recent experiments indicate non-equilibrium activity in a host of biological systems, including chromosomes, cell membranes, and the cytoplasm. Measuring and quantifying non-equilibrium dynamics in such systems is a major challenge in biophysics, due to their many-body nature and the limited number of variables accessible in an experiment. We investigate what information concerning the system's non-equilibrium state can be extracted from non-invasive tracking of a subset of degrees of freedom. To this end, we develop a general, yet simple stochastic model of soft elastic networks with a heterogeneous distribution of internal activities, representing enzymatic force generation. Using this model, we determine the scaling behavior of non-equilibrium dynamics using the phase space currents of tracer particles with different spatial separations in the system. Our results provide insight in to how internal driving by enzymatic activity generates non-equilibrium dynamics on different length scales in a variety of biological systems, including polymers, membranes and networks.

BP 15.80 *(210)* Tue 14:00 Poster B

Modelling the motility of Cytotoxic T Lymphocytes inside infected lymph nodes — •Zeinab Sadjadi[1,2], Michael Meyer-Hermann[2], and Stephan Halle[3] — [1]Theoretical Physics, Sarrland University, 66123 Saarbrücken, Germany — [2]Helmholtz Center for Infection Research, 38124 Braunschweig, Germany — [3]Hannover Medical School, 30625 Hannover, Germany

Cytotoxic T Lymphocytes detect and kill infected cells in lymph nodes. The underlying mechanisms of this process are however still unclear. The results of 2-photon microscopy experiments in vivo have shown different migration patterns and processivities of CTLs during search and killing processes[1]. We aim to understand the possible roles of chemotaxis, T cells cooperativity during killing, and fibroblastic reticular network on the dynamics and search strategy of CTLs inside a lymph node. We develop a persistent random walk model for the motion of CTLs during search and killing phases which enables us to study the role of key parameters on search efficiency and killing.

[1] Nature Reviews Immunology 16, 193-201 (2016)

BP 15.81 *(214)* Tue 14:00 Poster B

Trapping in and escape from branched structures of neuronal dendrites — •Robin Jose, Ludger Santen, and M. Reza Shaebani — Saarland University, Saarbrücken, Germany

We present a coarse-grained model for stochastic transport of non-interacting chemical signals inside neuronal dendrites and show how first-passage properties depend on the key structural factors affected by neurodegenerative diseases or aging: the extent of the tree, the topological bias induced by segmental decrease of dendrite diameter, and the trapping probabilities in biochemical cages and growth cones. We derive an exact expression for the distribution of first-passage times, which follows a universal exponential decay in the long-time limit. The asymptotic mean first-passage time exhibits a crossover from power-law to exponential scaling upon reducing the topological bias. The analytical predictions are in remarkable agreement with simulations. Our results evidence that structural irregularities can create local traps and heterogeneous patterns of signal transmission.

BP 15.82 *(243)* Tue 14:00 Poster B

Can one hear the length of an axon? — •Frederic Folz[1], Lukas Wettmann[1], Giovanna Morigi[1], and Karsten Kruse[2]

— [1]Department of Theoretical Physics, Saarland University — [2]Department of Biochemistry and Department of Theoretical Physics, University of Geneva

Axons are linear processes of nerve cells that can range from a few tens of micrometers up to meters in length. In addition to external cues, the length of an axon is also regulated by unknown internal mechanisms. Molecular motors have been suggested to generate oscillations with a length-dependent frequency that could be used to measure an axon's extension. Here, we present a model, describing a mechanism that uses such an oscillatory signal to regulate the axon length. We show that in addition to the frequency also the form of the oscillations contribute significantly to determining the steady state length. By disclosing the underlying working principle of the regulation mechanism, we are able to generalize its applicability to other biological systems.

BP 15.83 *(262)* Tue 14:00 Poster B

Statistical Mechanics of the Bacterial Chromosome — •Jacqueline Janssen, Joris Messelink, and Chase Broedersz — Arnold-Sommerfeld Center for Theoretical Physics, Theresienstraße 37, 80333 München

The bacterial DNA outsizes the cell by roughly a factor of a thousand. The DNA must not only be highly condensed to fit inside the cell, but this condensed DNA must also be organized inside the cell to facilitate functional processes of the chromosome. Thus, understanding the three-dimensional spatial organization of the bacterial chromosome is important to understanding how the core biological processes are regulated inside of the cell. Recent chromosome conformation capture experiments provide genome-wide data on chromosome folding. In particular, the Hi-C method provides contact frequency maps of the chromosome, revealing its highly organized structure. We are developing a maximum entropy approach to extract the statistics of the three-dimensional structure of the bacterial chromosome using such data. The aim of our method is to develop a coarse-grained model for the statistical mechanics of the folding of the whole bacterial chromosome.

BP 15.84 *(398)* Tue 14:00 Poster B

Generalized exponential models for mean population growth on a set of stochastic substrates — •Andrey Khalin[1], Eugene Postnikov[1], and Alexey Ryabov[2] — [1]Kursk State University, Kursk, Russia — [2]Carl von Ossietzky University Oldenburg, Oldenburg, Germany

We use approximate analytical models confirmed by numerical simulations to describe the average population growth on a resource heterogeneously distributed in space. It can serve, for instance, as a model for growth of zooplankton feeding in a highly heterogeneous environment. It is shown that the model for the growth of population averaged over a set of patches, where substrate distribution satisfies the generalized exponential Taylor's law is equivalent to the search of the cumulant generating function corresponding to the substrate distribution function. We have found and analysed a set of solutions corresponding to the Tweedie distribution and different functional responses as well as shown that finite samples of patches lead to the asymptotical Malthusian growth, the parameters of which are found analytically. The work is supported by the Ministry of Education and Science, project 3.9499.2017/8.9.

BP 15.85 *(152)* Tue 14:00 Poster B

Wobbling dynamics of E. coli cells in bulk and at walls — •Mahdiyeh Mousavi, Thomas Eisenstecken, Gerhard Gompper, and Roland G. Winkler — Institute of Complex Systems and Institute of Advanced Simulations, Forschungszentrum Juelich, Juelich, Germany

Wall entrapment of swimming bacteria like E. coli has been observed both experimentally and theoretically. However, the underlying mechanism of such a cell-wall interaction needs to be further addressed. In this study we identified three main stages of wall entrapment (approach, alignment, and surface swimming) by a mesoscale hydrodynamic simulation method, as was resolved experimentally. While the cell swims toward the surface, the time evolution of the cell angle with respect to the wall shows a fast oscillation (wobbling) around the alignment of the cell to the wall (pitch angle). In order to study the cell orientation, we consider different starting angles of the cell. We observe that the collision angle is linearly dependent on the start angle as is expected from the experiments. Moreover, once the cell reaches the wall, as it wobbles, it swims in a nose-down configuration with the bundle pointing away from the surface. The tangent of the pitch angle decreases exponentially with time after the collision, indicating that steric interactions play a major role in reorientation along with hydrodynamic interactions.

BP 15.86 *(196)* Tue 14:00 Poster B

From solitary swimmers to swarms and back: trypanosomes on their journey through the tsetse fly — •Timothy Krüger[1], Sarah Schuster[1], Philip Kollmannsberger[2], and Markus Engstler[1,2] — [1]Cell and Developmental Biology, Biocentre, University of Würzburg, Germany — [2]Centre for Computational and Theoretical Biology, University of Würzburg, Germany

The flagellate microswimmer Trypanosoma brucei exhibits a complex developmental cycle during a journey through the different microenvironments of the tsetse fly host. For the trypanosomes this involves crossing various barriers, confined surroundings, as well as swimming against flow and peristaltic movement. Concomitantly, they undergo radical morphological changes. The parasite's motility, which is directly dependent on morphology, is essential for its survival and successful development.

This work details cell morphology, motility, and collective behaviour of trypanosome developmental stages from the tsetse fly, using high spatiotemporal resolution microscopy. Using fluorescently labelled parasites, swimming patterns of solitary swimmers were analysed in vivo and in vitro, as well as collective motion at the single cell level in vivo. We show that trypanosomes are able to synchronise their flagellar beats and produce superordinate wave patterns at high cell concentrations, probably by hydrodynamic self-organisation inside the fly interstices. Additionally, by using light sheet fluorescence microscopy, we provide 3D-analyses of tissue geometry and topology with unprecedented resolution.

BP 15.87 *(198)* Tue 14:00 Poster B

Simultaneous cell tracking and visualization of flagellar dynamics of *Pseudomonas putida* — •Zahra Alirezaei-zanjani, Veronika Waljor, Marius Hintsche, and Carsten Beta — Universität Potsdam, Institut für Physik und Astronomie, Potsdam-Golm, Germany

The soil bacterium *Pseudomonas putida* propels itself with a polar bundle of helical flagella. It senses changes in its environment and exhibits response of the flagella mediated by a chemosensory system. Our earlier research showed that *P. putida* exhibits a motion pattern dominated by persistent runs that are interrupted by sharp reversal events (M. Theves, et al. Biophys. J. 2013). Recently, we showed that *P. putida* may exhibit three different flagellar bundle configurations during swimming: the bundle can push, pull, or wrap around the cell body (M. Hintsche et al. Sci. Rep. 2017, accepted). Here, we present a modified experimental setup that allows us to acquire a large amount of cell trajectories together with information on the bundle configuration for each run. We will use this setup to study the statistics of transitions between the different swimming modes with the ultimate goal to elucidate *P. putida*'s swimming strategy when navigating in the direction of a nutrition gradient.

BP 15.88 *(204)* Tue 14:00 Poster B

A bacterial swimmer with a polar bundle of flagella that can push, pull, and wrap around the cell body — •Marius Hintsche[1], Veronika Waljor[1], Robert Grossmann[2], Marco Kühn[3], Kai Thormann[3], Fernando Peruani[2], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Laboratoire J. A. Dieudonné, Université Côte d'Azur, Nice, France — [3]Institut für Mikrobiologie und Molekularbiologie, Justus-Liebig-Universität Giessen, Giessen, Germany

Bacteria swim in sequences of straight runs that are interrupted by turning events. They drive their swimming locomotion with the help of rotating helical flagella. Depending on the number of flagella and their arrangement across the cell body, different run-and-turn patterns can be observed. Here, we present fluorescence microscopy recordings showing that cells of the soil bacterium *Pseudomonas putida* that are decorated with a polar tuft of helical flagella, can alternate between two distinct swimming patterns. On the one hand, they can undergo a classical push-pull-push cycle that is well known from monopolarly flagellated bacteria but has not been reported for species with a polar bundle of multiple flagella. Alternatively, upon leaving the pulling mode, they can enter a third slow swimming phase, where they propel themselves with their helical bundle wrapped around the cell body. A theoretical estimate based on a random-walk model shows that the

spreading of a population of swimmers is strongly enhanced when cycling through a sequence of pushing, pulling, and wrapped flagellar configurations as compared to the simple push-pull-push pattern.

BP 15.89 *(333)* Tue 14:00 Poster B

Layer-by-layer assembled micro-motors for controlled drug release — Tao Huang[1], Larysa Baraban[1], and •Gianaurelio Cuniberti[1,2] — [1]Institute of Materials Science and Max Bergmann Center of Biomaterials Dresden, TU Dresden, Dresden, Germany — [2]Center for advancing electronics Dresden, cfaed, Dresden

Micro-motor is a micro-scale device, capable of autonomous motion in liquid environment and having potential to find multiple applications in biomedicine.1 Here we present the light-driven micro-motors fabricated using different techniques combined, i.e. controlled template-assisted layer-by-layer (LBL) molecular assembly and electrodeposition of metals. Layer-by-layer assembled multilayer provide excellent delivery capacities and can also respond to various stimuli for controllable encapsulation and release of drugs. Composite top layer of the particles, fabricated by LBL technique represents the ideal container for drug loading and controlled release. Diverse geometries of micro-motors, including rod-like and spherical will be designed, and decorated with the biocompatible outer layer. Finally, we plan to investigate the efficiency of the micromotors for the real-time drug release during in-vitro assays.

1.*J. A. Spudich, Science, 2011, 331, 1143-1144.

BP 15.90 *(352)* Tue 14:00 Poster B

How molecular motors generate the ciliary beat — •Veikko F. Geyer.[1,4], Pablo Sartori[2], Frank Jülicher[3], and Jonathon Howard[4] — [1]B CUBE , TU Dresden, Dresden, Germany — [2]Institute for Advanced Study, Princeton, New Jersey, USA — [3]MPI-PKS, Dresden, Germany — [4]Department of Molecular Biophysics, Yale University, New Haven, Connecticut, USA

Cilia and flagella are slender organelles of eukaryotic cells. They are ubiquitous in nature propeling mucus along the respiratory epithelium, generate chiral flows in Henson's node and propel micro-swimmers like sperm or alga. The cilium is a mechanical beat-pattern-generator composed of molecular motors and cytoskeletal filaments. Cells can regulate beat patters to accommodate specific functions. Examples are the conversion of pushing forces into pulling forces or the change of the chirality of flows. To understand how beat-patterns are generated on the molecular level, we record the waveforms of cilia of the green alga Chlamydomonas Reinhardtii using high-speed microscopy. We perform theoretical analysis of the beats and investigate how waveform changes relate to cell propulsion. We formulate mechanical models of the axoneme to address the question of (1) how molecular motors are controlled and (2) how force deforms the axonemal structure. Together, we investigate how the molecular properties of micro-motors and cytoskeletal filaments give rise to self-organized ciliary beating and to cell-propulsion and cilia-generated flows.

BP 15.91 *(381)* Tue 14:00 Poster B

Flow fields and motions of droplets driven by active filament-bound point forces — •Leon Rückert and Reiner Kree — Georg-August-Universität Göttingen, Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Active intracellular motion of cargo carrying motor proteins or active motion of biological or artificial microswimmers caged in droplets drive internal and external flow, which in principle may also lead to translational and rotational motion of the whole system.

Extending methods of previous work [1], we study the intra- and extracellular flow fields and the trajectories of droplets at low Reynolds numbers, which are generated by point forces inside the droplet. The point forces are assumed to actively move along rigid filamentary tracks. A special focus is put on force dipoles as models of myosin or kinesin motors.

We analytically calculate the flow fields, and the induced center of mass and angular velocity of the droplet for single point forces and dipoles, and discuss examples of motions, including stationary, periodic and random motion on simple geometries of filamentary tracks.

[1] R. Kree, P.S. Burada and A. Zippelius, J. Fluid. Mech. 821, 595-623 (2017)

BP 15.92 *(65)* Tue 14:00 Poster B

Surface-Near Electrostatic Forces in Si-Chips guiding Self-Organisation of Polyelectric- and Biomaterials — •Daniela Täuber[1], Susanne Pahlow[1,2,5], Karina Weber[1,2,5], Martin Müller[3], Ilona Skorupa[4], and Heidemarie Schmidt[1,4] — [1]Leibniz-Institut für Photonische Technologien, Albert-Einstein-Str. 9, D-07745 Jena — [2]InfectoGnostics Forschungscampus Jena e.V., Philosophenweg 7, D-07743 Jena — [3]Leibniz-Institut für Polymerforschung, PO: 120411, D-01005 Dresden — [4]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, D-01328 Dresden — [5]Friedrich-Schiller-Universität, Institut für Physikalische Chemie und Abbe Center of Photonics, Helmholzweg 4, D-07743 Jena, Germany

The specific characterisation of biomaterials frequently requires adhesion or binding of the biological species of interest to matching species (antibodies, single DNA strands), which thus need to be well-organized on a substrate. The state-of-art here often requires the silanization of the substrate for providing covalent bonds to which the control species can be fixed by linkers.

Self-organization of the control species to a planar substrate by electrostatic adhesion via near surface electrostatic forces[1] is a very promising alternative approach. Here we report on self-organization of polyelectrolytes and biological species on silicon substrates with an implanted near surface electrostatic pattern. The physical adsorption of polyelectrolytes and biological species on such substrates is stable directly from solution and does not require silanization/a drying step.

[1] C. Baumgart, M. Helm, H. Schmidt, PRB, 80, 085305 (2009)

BP 15.93 *(115)* Tue 14:00 Poster B

Computational modeling of active membranes in flows — •Christian Bächer and Stephan Gekle — Biofluid Simulation and Modeling, Bayreuth, Germany

Active stresses induced by ATP-mediated processes within the cell cortex, can cause strong membrane deformations, which are highly important in blood platelet formation. In the framework of Lattice-Boltzmann/Immersed boundary method we numerically combine active cell membranes [1] and external flows, which have been experimentally found to strongly accelerate platelet formation [2]. Using differential geometry, we calculate the stresses within the curved, active membrane and the resulting forces onto the surrounding fluid. Membrane properties and forces are discretized on a triangulated thin shell coupled to the fluid. Forces of active origin are combined with shear and bending elasticity using Skalak and Helfrich model to cover realistic cell membrane behavior. Following blood platelet formation, we focus on instabilities of cylindrical shaped membranes under influence of external shear forces.

[1] G. Salbreux, F. Jülicher, Phys. Rev. E 96(3), 2017
[2] M. Bender et al., Blood 125(5), 2015

BP 15.94 *(174)* Tue 14:00 Poster B

Creating Sensorial Delay to Simulate Phototaxis Using Thermophoresis Applied to Gold-coated Microswimmers — •Alexander Fischer[1], Giovanni Volpe[2], and Frank Cichos[1] — [1]Molecular Nanophotonics, Peter-Debye-Institute, Universität Leipzig — [2]Department of Physics, University of Gothenburg

Sperm cells of marine invertebrates move towards the egg using chemotaxis. This task is rather challenging due to the noisy movement of the individuals (agents). The complex behavior of the agents can be simulated by using some simple rules. The autonomous agent performs directed motion in a plane and the orientation is subject to noise. The speed of the agent slows down in those regions where it measures a higher concentration of messengers. Thus, the probability of presence of the agent is higher in regions with higher concentration. According to Volpe et al. [1], a change between segregation and aggregation of the agents in the high messenger concentration regions can be achieved by introducing a delayed response to the messenger concentration. We implement this model by using gold-coated microparticles diluted in water. Here we explore this behavior in a system of active particles that are controlled remotely by a feedback loop.

[1] M. Mijalkov, A. McDaniel, J. Wehr, G. Volpe, Phys. Rev. X, 6, 011008 (2016)

BP 15.95 *(185)* Tue 14:00 Poster B

Light-Induced Adsorption of Photoactive Microalgae on Interfaces — •Alexandros Fragkopoulos, Christian Kreis, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, D-37077 Göttingen, Germany

For many organisms, adhering to an interface is of paramount importance from large species, like mussels, to microbes, such as bacteria and microalgae. Microorganisms that naturally grow in porous environments, like soil, constantly interact with interfaces and may

form biofilms that, among else, protects their communities from external influences. Chlamydomonas, a unicellular biflagellated microalga, can adhere almost to any substrate, and we have shown in previous work that its flagella-mediated adhesion to surfaces can be switched on and off by controlling the light conditions. Here, we exploit this light-switchability to study the adsorption-desorption dynamics of a *C. reinhardtii* population on solid interfaces that reversibly transitions between the planktonic (freely swimming) and the surface-associated state. Our results reveal physical details of the dynamics and how it depends on the cell density, as well as biological details surrounding the light-switchable adhesion. Morphological analysis of the patterns formed by the adsorbed cells evolve over time, possibly indicating that flagella-mediated gliding, a motility mechanism allowing for adhered cells to move on interfaces, can lead to a more efficient cell packing.

BP 15.96 *(306)* Tue 14:00 Poster B

Probing the non-equilibrium dynamics of the centrosomes in early *Drosophila melanogaster* embryos using fluorescent carbon nanotubes — •Constantin D. C. Kohl[1], Zhiyi Lv[2], Jörg Grosshans[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität, 37077 Göttingen, Germany — [2]Institut für Entwicklungsbiochemie, Universitätsmedizin Göttingen, 37077 Göttingen, Germany

In this project, a novel imaging method using near-infrared-fluorescent, DNA-wrapped fluorescent carbon nanotubes (CNTs) is applied to capture and characterize the non-equilibrium centrosomal dynamics in syncytial *D. melanogaster* embryos. During synchronized mitosis, the nuclei arrange into a 2 D cortical layer during stage 9 to 13. We target CNTs to Kin-5 motor proteins which, in turn, co-localize with centrosomes attached to the nuclei during mitosis and interphase. Semiconducting CNTs are highly photostable, non-blinking and non-bleaching. Hence, CNTs are good probes for long-time tracking inside living organisms. To observe the near-infrared fluorescence of CNTs, we have built a setup enabling the simultaneous use of visible and infrared widefield fluorescence microscopy and imaging of GFP tagged histones, in conjunction with infrared spectroscopy. We apply several methods to solubilize the hydrophobic CNTs in watery solutions and use biochemical linking methods to specifically target CNTs in the embryos. We superimpose fluorescent CNT signals on GFP labeled nuclei and present the dynamics of functionalized CNTs in wild-type *D. melanogaster*.

BP 15.97 *(357)* Tue 14:00 Poster B

Collective Behaviour of Microalgae Beyond Phototaxis — •Johannes Frey, Alexandros Fragkopoulos, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-organization (MPIDS), Am Faßberg 17, D-37077 Göttingen

Chlamydomonas reinhardtii is a unicellular, eukaryotic microalga that has two flagella allowing the cell to propel itself in its surrounding fluid. This microalga is photoactive since, among else, it can perform photosynthesis and phototaxis. Here, we present the discovery of a light-sensitive collective behaviour within a population of planktonic *Chlamydomonas* cells. At low light intensities, we observe the cells to form inhomogeneous patterns within the confinement, while above a threshold the distribution of cells becomes homogenous. All experiments are performed under red light indicating that this phenomenon is not related to phototaxis. The swimming behaviour is fully reversible and time-resolved experiments show a dependence of its appearance on the geometry and size of the compartment as well as on the cell density. For circular chambers, we quantify the dynamics of the spatial distribution of cells as a function of the radius and height of the compartment and the cell density. The light intensity dependence and a color discrimination of the effect suggest, that the change in the cell motility is related to photosynthesis, but the exact biological mechanism remains to be explored.

BP 15.98 *(367)* Tue 14:00 Poster B

MT-bundling activity of the MKLp2 kinesin — •Amna Abdalla Mohammed Khalid[1], I-Mei Yu[2], Anne Houdusse[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen, Germany — [2]Institut Curie Paris, France

The Kinesin-6 MKLP2 motor is N-terminal Kinesin, with unique features. It plays critical roles in cell division. Scientists know little about MKLP2; however, few earlier findings suggested that MKlp2 is a good candidate for new cancer therapies. To gain insight into the motor regulation and mechanism, we are studying truncated MKLP2. Here, I present the studies of a dimeric truncated MKlp2, in vitro using fluorescence microscopy. Our data confirm that the dimeric truncated MKlp2 motors are active and they display strong bundling activity. An astonishing finding, we observed the formation of novel three-dimensional microtubule-MKLP2 construct(s) networks with unique properties.

BP 15.99 *(410)* Tue 14:00 Poster B

Flocking without velocity-alignment — •Fernando Peruani and Lucas Barberis — Université Côte d'Azur

The spontaneous emergence of collective motion patterns is usually associated with the presence of a velocity alignment mechanism that mediates the interactions among the moving individuals. Despite of this widespread view, we show that several flocking behaviors can emerge in the absence of velocity alignment and as a result of short-range, position-based, attractive forces that act inside a vision cone. We argue that for this class of active systems three distinct macroscopic collective behaviors can be observed: i) the coarsening of aggregates with no orientational order, ii) the emergence of static, elongated nematic bands, and iii) the formation of moving, locally polar structures, which we call worms. We derive hydrodynamic equations for active particles interacting via position-based interactions to demonstrate that they belong to a distinct class of active systems fundamentally different from other active systems, including velocity-alignment-based flocking systems.

BP 15.100 *(289)* Tue 14:00 Poster B

RNA structure prediction using evolutionary constraints — •Mehari Bayou Zerihun[1,2] and Alexander Schug[1,3] — [1]Steinbuch Centre for Computing, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Department of Physics, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [3]John von Neumann Institute for Computing, Jülich Supercomputer Centre, Forschungszentrum Jülich, 52428 Jülich, Germany

Non-coding RNAs are involved in regulatory functions in cells. Understanding their three-dimensional structure helps to understand their function as structure and function are closely related. However, the extremely flexible nature of these biomolecules makes the experimental determination of their structure very challenging. A complementary approach is computational structure prediction starting from the sequences. Sequences undergo mutations during the course of evolution. To maintain structure and function, these mutations must be complementary, resulting in residue coevolution. We use direct-coupling analysis (DCA) to extract coevolving residue pairs and integrated the resulting information with molecular modeling tools for RNA structure prediction. The accuracy of this structure prediction workflow is tested by comparing predicted structures with experimental ones for RNAs of a known three-dimensional structure.

BP 15.101 *(327)* Tue 14:00 Poster B

Comparison of Coevolutionary Protein Structure Prediction Methods — •Lars Franke[1] and Alexander Schug[2] — [1]Karlsruhe Institute of Technology (KIT) — [2]Jülich Supercomputing Centre (JSC)

Analyzing the structure of proteins is the key to understanding the biological mechanisms they are involved in. While the experimental structure determination of proteins is expensive, the corresponding genetic sequences are easy to obtain. Correlated mutations in the sequences within a protein family provide information about the protein's function and therefore its structure. These correlations can be translated into residue-residue interactions using Direct Coupling Analysis (DCA). We generate contact predictions for eight proteins with known structure with three different methods—mean field DCA, Pseudo Likelihood Maximization and Deep Neural Networks—and compare the results. This study can provide orientation in the world of protein structure prediction tools.

BP 15.102 *(400)* Tue 14:00 Poster B

Adhesion enhances bacterial diffusivity close to surfaces. — •Emiliano Perez Ipiña[1], Stefan Otte[1], Rodolphe Pontier-Bres[2], Dorota Czerucka[2], and Fernando Peruani[1] — [1]Université Côte d'Azur, Laboratoire J.A. Dieudonné, UMR 7351 CNRS, Parc Valrose, Nice F-06108, France — [2]Centre Scientifique de Monaco (CSM), 8 Quai Antoine 1er, Monaco 98000, Principality of Monaco

It is well known that peritrichous bacteria are able to explore the space by performing "run and tumble" motion when they are far from

surfaces. Moreover, bacteria regulate the frequency of tumbling to perform chemotaxis and redirect their motion towards favorable environments. However, close to a surface, hydrodynamics interactions become dominants and run and tumbling patterns are replaced by smooth circular trajectories. In this context, where bacteria are trapped in circles and tumbling is highly suppressed, it is not clear how they can be in control of their motion and by which mediums chemotaxis is performed. Here, through mathematical modeling and statistical analysis of recorded trajectories, we characterize the motility patterns of *Escherichia coli* close to surfaces in *in vitro* experiments. We report that by adhering to the surface, *E. coli* is able to break the circular trajectories and get in control of their diffusivity. Remarkably, we found that *E. coli* was tuned to maximize its diffusion coefficient. Our results shed light on the explore strategies followed by bacteria near surfaces and suggest adhesion as a possible chemotactic mechanism.

BP 16: Membranes and Vesicles I (joint session BP/CPP)

Time: Wednesday 9:30–13:00 Location: H 1028

BP 16.1 *(161)* Wed 9:30 H 1028

Actin polymerization driving localized membrane deformation — •Remy Kusters[1], Camille Simon[1], Jean-Francois Joanny[1,2], Cecile Sykes[1], and Pierre Sens[1] — [1]Institut Curie, Paris, France — [2]ESPCI, Paris, France

The actin cytoskeleton is able to exert both pushing and pulling forces on the cell membrane, mediating processes such as cellular motility, endocytosis and cytokinesis. In order to investigate the exclusive role of actin dynamics on membrane deformations, the actin dynamics is reconstituted on the outer surface of a deformable liposome. Depending on the elasticity of the membrane and the forces generated by the actin polymerization, both tubular extrusions (i.e. towards the actin cortex) and localized spike-like protrusions occur along the surface of the liposome. In this talk I present a theoretical model where uniform actin polymerization can drive localized membrane deformations and show how polymerization kinetics and membrane/cortex mechanics impact their size and stability.

BP 16.2 *(164)* Wed 9:45 H 1028

Modeling the flat-to-curved transition during clathrin-mediated endocytosis — •Felix Frey[1], Delia Bucher[2], Kem Sochacki[3], Justin Taraska[3], Steeve Boulant[2], and Ulrich Schwarz[1] — [1]Institute for Theoretical Physics, Heidelberg University — [2]Department of Infectious Diseases, Virology, University Hospital Heidelberg — [3]NIH, Bethesda, U.S.A.

Clathrin-mediated endocytosis (CME) is essential for the cellular uptake of nutrients and receptors. Although CME has been studied for decades, the exact sequence of molecular and structural events remains elusive. Two basic models have been suggested for the way CME proceeds. (1) In the constant curvature model, it is assumed that clathrin-coated pits grow with constant curvature, determined by the geometry of clathrin triskelia. (2) In the constant area model, it is assumed that clathrin triskelia first assemble into flat hexagonal arrays that later invaginate with a constant surface area. This second model implicitly assumes that during bending, some hexagons are converted into pentagons. Here, we integrate data sets from correlative electron and light microscopy and quantify the sequence of ultrastructural rearrangements of the clathrin coat during endocytosis in mammalian cells with the help of some simple mathematical growth laws. Our analysis shows that clathrin-coated structures initially grow flat but start to acquire curvature when 70% of the final clathrin content is reached. Hence, our analysis suggests that elements of both suggested models are present and that mechanical and cellular factors will decide about the relative weights of growth versus curvature formation.

BP 16.3 *(249)* Wed 10:00 H 1028

Formation and Stabilization of Pores in Bilayer Membranes by Peptide-like Amphiphilic Polymers — •Ankush Checkervarty[1,2], Marco Werner[1,3], and Jens Uwe Sommer[1,2] — [1]Leibniz-Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany — [2]Institute of Theoretical Physics, Technische Universitat Dresden, Germany — [3]Universitat Rovira i Virgili, Departament dEnginyeria Quimica, Av. Paisos Catalans 26, 43007 Tarragona, Spain

We study pore formation in models of lipid-bilayer membranes interacting with amphiphilic copolymers mimicking anti-microbial peptides using Monte Carlo simulations rationalized by a simple brush-model for the fluid membrane. In our study at least a weak tension on the membrane is required to observe pore-formation induced by the adsorption of flexible amphiphilic copolymers. The copolymers enhance the pore stability by decreasing the line tension due to weak adsorption along the rim of the pore. Pore formation is enhanced with increasing length of copolymers or stronger stretching of the membrane. Both solvent and copolymer permeability increase as the pore becomes stable. Pore-formation proceeds via a meta-stable pore-state according to adiscontinuous phase transition scenario which lead to finite pore-sizes at once. Our generic model of copolymer-induced pore-formation does not require high polymer concentration at the pores nor any self-organization of the copolymers to open the pore.

BP 16.4 *(259)* Wed 10:15 H 1028

Shapes of red blood cell doublets — •Masoud Hoore, Dmitry A. Fedosov, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems, Forschungszentrum Juelich GmbH

Red blood cell (RBC) aggregates play an important role in determining blood rheology. RBCs in solution interact attractively to form various shapes of RBC doublets. Here, the attractive interactions can be varied by changing the solution conditions. A systematic numerical study on RBC doublet formation is performed, which takes into account the shear elasticity of the RBC membrane due to the spectrin cytoskeleton, in addition to the bending rigidity. The results are obtained from molecular dynamics simulations of triangulated surfaces considering thermal effects. The phase space of the RBC doublet shapes in a wide range of adhesion strengths, reduced volumes, and shear elasticities is obtained. Experimental images of RBC doublets in different solutions show similar configurations. Furthermore, it is shown that rouleau formation is affected by the doublet structure. It is shown that the shear elasticity of the RBC membrane changes the doublet phases significantly.

BP 16.5 *(260)* Wed 10:30 H 1028

Conditions of Spontaneous Translocation of Individual Nanotube Porin Through a Phospolipid Bilayer — Yachong Guo[1,2], Marco Werner[2], Ralf Seemann[3], Vladimir Baulin[2], and •Jean-Baptiste Fleury[3] — [1]Nanjing University, Nanjing , China — [2]Universitat Rovira i Virgili, Tarragona, Spain — [3]Saarland Univsersity, Saarbruecken, Germany

Single ultra-short nanotubes can be inserted in cell membrane to be used as a membrane nanosensor or to form artificial ionic channels. Recent studies reported that ultra-short nanotubes can passively be inserted perpendicularly to the lipid bilayer core. After this insertion, it is commonly expected that these ultra-short nanotubes should stay trapped into the lipid bilayer core as its represents a potential well. In contrast to such expectations, we investigate the possible conditions that could lead a single nanotube to translocate spontaneously across a lipid bilayer. We demonstrate that membrane stretching and subnanometer nanotube, are essential to enable this type of translocation, while no translocations are occurring in lipid bilayers under low tension. The proof of this tension-dependent translocation event is obtained by observating directly a single nanotube quitting a highly stretched lipid bilayer. A quantitative analysis of the kinetic pathway associated to this translocation event is measured by using a specially designed microfluidic device combining optical fluorescence microscopy with simultaneous electrophysiological measurements.

BP 16.6 *(303)* Wed 10:45 H 1028

Membrane fluctuations of malaria-infected red blood cells — •Julia Jäger[1,2], Benjamin Fröhlich[3], Motomu Tanaka[3], Michael Lanzer[4], and Ulrich Schwarz[1,2] — [1]Institut für Theoretische Physik, Universität Heidelberg — [2]Bioquant, Universität Heidelberg — [3]Institut für Physikalische Chemie, Universität Heidelberg — [4]Parasitologie, UniversitätsKlinikum Heidelberg

Once inside the body, malaria parasites invade red blood cells in order to hide from the immune system and to digest hemoglobin. Over the course of 48 hours the parasite completely remodels the red blood cell, so that the cell becomes round and stiff and eventually breaks open. One way to monitor this remodeling process is the measurement of the cell membrane's flickering spectrum, which is a standard approach to extract the mechanical properties of cell membranes. In addition to the usual interface Hamiltonian for the membrane, we take into account the connections between the outer lipid bilayer and the spectrin network underlying the plasma membrane, which are known to become increasingly clustered over the course of the infection. We focus on the confinement parameter in the interface Hamiltonian and show how it scales with the number and strength of the connections. Finally, we compare our results with experiments.

15 min. break

Invited Talk BP 16.7 *(1)* Wed 11:15 H 1028

Computer simulation of collective phenomena that alter the topology of membranes — •Marcus Müller — Georg-August-Universität Göttingen, Institut für Theoretische Physik, Göttingen, Germany

Using computer simulation and self-consistent field theory of coarse-grained models for lipid membranes, we study the free-energy landscape of collective phenomena that alter the topology of lipid membranes. These basic processes - pore formation, fusion and fission - often involve time scales of tens of nanometers and milliseconds that are large for atomistic simulation. Frequently, they involve transition states with high curvatures that are difficult to describe by Helfrich-like models. Coarse- grained models can access the relevant time and length scales, allow for a systematic exploration of parameters like the lipid architecture or membrane tension, and they are well suited to study collective phenomena that alter the topology of membranes.

The talk will discuss different computational techniques - Wang-Landau sampling, field-theoretic umbrella sampling, and the string method - to investigate metastable intermediates (like the stalk in the course of membrane fusion) and transition states of pore formation, membrane fusion and fission. Using coarse-grained models, we explore the universal aspects of topology-altering processes in membranes and comment on the extent, to which coarse-grained model capture specific effects of protein-mediated processes.

BP 16.8 *(331)* Wed 11:45 H 1028

Formation of Coatless Membrane Vesicles — •Susanne Liese[1], Rossana Rojas[1], Eva Wenzel[2], Camilla Raiborg[2], Harald Stenmark[2], and Andreas Carlson[1] — [1]University of Oslo, Department of Mathematics — [2]Oslo University Hospital, Institute for Cancer Research

The formation of membrane vesicles is an important part of various processes in cell biology. Among others, cells use vesicle formation as an uptake mechanism for controlling their activity and to communicate with other cells through the cargo material that is encapsulated in the membrane vesicle. It all starts with a small initial deformation of the membrane, which subsequently grows and leads to the formation of a vesicle. This dynamic process is induced by membrane associated proteins, which generate forces within the membrane. Membrane compartments inside the cell, such as the endosome, form coatless vesicles but the force generating membrane proteins are not becoming a part of the vesicle. To understand this process, we develop an elastic membrane model to study the biophysical origin of coatless vesicle formation. Our results highlight how elastic membrane parameters and transmembrane proteins determine the shape of the deformed membrane and the equilibrium size distribution of vesicles.

BP 16.9 *(338)* Wed 12:00 H 1028

Outperforming nature: synthetic enzyme built from DNA flips lipids of biological membranes at record rates — •Alexander Ohmann[1], Chen-Yu Li[2], Christopher Maffeo[2], Kareem Al Nahas[1], Kevin N. Baumann[1], Kerstin Göpfrich[1], Jejoong Yoo[2], Ulrich F. Keyser[1], and Aleksei Aksimentiev[2] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]University of Illinois at Urbana-Champaign, Champaign, IL, USA

Mimicking enzyme function and increasing performance of naturally evolved proteins is one of the most challenging and intriguing aims of nanoscience. Here, we employ DNA nanotechnology to design a synthetic enzyme that substantially outperforms its biological archetypes. Consisting of only eight strands, our DNA nanostructure spontaneously inserts into biological membranes by forming a toroidal pore that connects the membrane's inner and outer leaflets. The membrane insertion catalyzes spontaneous transport of lipid molecules between the bilayer leaflets, rapidly equilibrating the lipid composition. Through a combination of microscopic simulations and single-molecule experiments we find the lipid transport rate catalyzed by the DNA nanostructure to exceed 10^7 molecules per second, which is three orders of magnitude higher than the rate of lipid transport catalyzed by biological enzymes. Furthermore, we show that our DNA-based enzyme can control the composition of human cell membranes, which opens new avenues for applications of membrane-interacting DNA systems in medicine.

BP 16.10 *(354)* Wed 12:15 H 1028

Membrane-mediated interactions between inclusions: the role of shape and background curvature — •Afshin Vahid[1], Andela Saric[2], and Timon Idema[1] — [1]TU Delft, Delft, the Netherlands — [2]University Collage London (UCL), London, United Kingdom

Lipid membranes are vital to cell function. Their combination of fluid and elastic properties allows cells to cope with an out of equilibrium environment. Consequently, membranes exhibit a large variety of shapes, ranging from simple spherical liposomes to complex tubular networks. These shapes are regulated by protein inclusions, that can act both as curvature sensors and curvature inducers. We model the interaction between such inclusions in curved lipid bilayers. We show that in contrast to flat membranes, the inclusions can attract each other and collectively form biologically relevant patterns. For example, we find that even identical inclusions can spontaneously form rings on closed membranes, and those rings again act as curvature sensors. We further demonstrate that the curvature sensing and curvature inducing property of proteins are two sides of the same coin, depending on protein density. In particular, proteins can constrict tubular membranes and facilitate their splitting. This feature was recently observed in mitochondria, and can prevent entanglement with tubes of the ER network also present in the cell.

BP 16.11 *(376)* Wed 12:30 H 1028

Membrane curvature and nanobuds generated by lipids with bulky head groups — Aparna Sreekumari, Reinhard Lipowsky, and •Rikhia Ghosh — Theory and Bio-systems, Max Planck Institute of Colloids and Interfaces Golm, D-14424 Potsdam, Germany

We study the mechanical and curvature-elastic properties of bilayer membranes with compositional asymmetry by molecular simulations. The compositional asymmetry is achieved by inserting lipids with a bulky head group into one leaflet (or monolayer) of the bilayer. As we increase the mole fraction ϕ_1 of the bulky-head lipids, we observe a remarkable evolution of the stress profile across the bilayer and a strong increase in the first moment of this profile. In order to extract the spontaneous curvature from this moment, we also determine the bending rigidity of the bilayer which is found to exhibit a non-monotonic dependence on ϕ_1. The latter behaviour reflects changes in the mean density of the lipid tails and head groups. The resulting spontaneous curvature is found to be quite large compared to other molecular mechanisms for bilayer asymmetry. The generated curvature leads to the formation of nanobuds, which provide new membrane compartments, in close analogy to cellular budding processes.

BP 16.12 *(445)* Wed 12:45 H 1028

Formation and phase transitions of vapour deposited phospholipid bilayers on porous silicon substrates — Nicolas Moraga[1], Marcelo Cisternas[1], Diego Diaz[1], Rodrigo Catalan[1], Maria J. Retamal[2], Tomas P. Corrales[3], Mark Busch[4], Patrick Huber[4], Marco Soto-Arriaza[2], and •Ulrich G. Volkmann[1] — [1]Institute of Physics and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [2]Faculty of Chemistry and CIEN-UC, P. Univ. Catolica de Chile, Santiago, Chile — [3]Department of Physics, UTFSM, Valparaiso, Chile — [4]TUHH, Hamburg, Germany

Study of phospholipid artificial membranes on solid substrates has become a relevant way to gain insight into the physical behaviour of cell membranes. In this work, porous silicon substrates (pSi) were made using a two-electrode cell to produce different pore diameters. Substrates were characterized with Field Emission Electron Microscopy. The phospholipid (DPPC) was deposited in high vacuum from the gas phase on the pSi. Film thickness was controlled using Very High Resolution Ellipsometry (VHRE). Samples were hydrated in air with ultrapure water to assemble the bilayer. Phase transitions were mea-

sured with VHRE and Stray Light Intensity during temperature cycles. AFM was used to study morphological changes of bilayers as a function of temperature. Our results open new ways to hydrate lipid bilayers using pSi with a specific pore diameter. Acknowledgements: Postdoctoral FONDECYT #3160803 (MJR), FONDECYT #1141105 (UGV) and #1171047 (MSA), FONDECYT INICIACION #11160664 (TPC), CONICYT Fellowships (RC, MC) and CONICYT-PIA ACT 1409.

BP 17: Cell Mechanics I

Time: Wednesday 9:30–13:00 Location: H 1058

BP 17.1 *(35)* Wed 9:30 H 1058

Mechanical and Electrical Characterization of Cardiac and Skeletal Muscle Microtissues — •Delf Kah, Ingo Thievessen, Marina Spörrer, Wolfgang H. Goldmann, and Ben Fabry — Department of Physics, Biophysics Group, Friedrich-Alexander-University Erlangen-Nuremberg, D-91052, Erlangen, Germany

In-vitro engineered muscle tissue grafts are of growing interest for different applications including regenerative therapy, replacement of infarcted cardiac sites, or as a drug testing platform. Critical for the successful development of suitable models for engineered muscle grafts is the maturation into an in-vivo-like, highly aligned, and contractile tissue. To achieve this, we developed a stretchable and electrically paceable system consisting of an array of 4x2x2 mm microwells with two elastic pillars that serve as force sensors. Tissues can be grown from several cell sources including neonatal cardiomyocytes form rats, mice, as well as C2C12 skeletal muscle cells. Mechanical stretching with a linear stepper motor, electrical pacing with carbon electrodes, and microscopic imaging of the tissue is synchronized by a microcontroller, allowing us to study isotonic, isometric, or eccentric contractions for various pacing protocols. Cardiac tissues show remarkably uniform contraction induced by electrical pacing, which allows for imaging with a time resolution of up to 1000 Hz through heterodyning. Accordingly, contractile performance can be evaluated with high temporal precision.

BP 17.2 *(187)* Wed 9:45 H 1058

Substrate stiffness affects sarcomere coherence in hESC-derived cardiomyocytes — •Daniel Härtter[1], Til Driehorst[1,2], Malte Tiburcy[2], Kengo Nishi[1], Wolfram-H. Zimmermann[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen — [2]Institut für Pharmakologie, Universitätsmedizin, Georg-August-Universität Göttingen

The mechanical micro-environment affects the behavior of cells. For instance, stiff infarcted heart tissue inhibits the global contraction of cardiomyocytes. However, direct insight into how the mechanical environment influences dynamics on the sarcomere level is missing. We tracked the motion of individual sarcomeres using endogeneous z-line labeling in CRISPR/Cas9 modified hESC-derived cardiomyocytes on micro-patterned substrates with various physiologically relevant stiffnesses (7 kPa to 60 kPa). Individual sarcomere contraction is impeded for increasing substrate stiffness. Furthermore, on soft substrates sarcomeres contract coherently, whereas with increasing stiffness the sarcomere contraction gets increasingly incoherent and heterogeneous.

These findings suggest that rigid mechanical surroundings force sarcomeres into competition. Using a mechanistic muscle model, we show that z-lines elastically cross-linked to the substrate and heterogeneous elements can account for many features we observe. Theories of collective molecular motors predict emerging phenomena such as dynamic instabilities, and these experiments can provide quantitative data to understand the microscopic basis of real cardiac muscle function.

BP 17.3 *(342)* Wed 10:00 H 1058

Functional analysis of larval chordotonal organ mechanics in Drosophila — •Chonglin Guan[1], Martin Göpfert[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen — [2]Abteilung Zelluläre Neurobiologie, Schwann - Schleiden-Forschungszentrum, Georg-August-Universität Göttingen

In Drosophila larvae and adults, chordotonal organs (ChOs) are ubiquitous mechanoreceptors, converting a diverse range of physical forces such as sound, vibration and stretch into biological responses. The mechanoelectrical transduction, operated by an active, force-generating process, has been linked to adaptation motors. The underlying force generator, however, is poorly known, and the functional dissection of ChO mechanics in vivo has been challenging. We combine electrophysiological analyses with mechanical stimulation, and correlate mechanical properties and active manipulation with neuronal activity. We find that myosin II motors power contraction of the cap cells of ChO and regulate mechanosensation. Our in vivo model reveals larval ChOs as complex, but accessible organs to study the molecular machinery involved in the regulation and encoding of mechanical forces by primary mechanoreceptor neurons.

BP 17.4 *(426)* Wed 10:15 H 1058

Magnetogenetic Manipulation of Cellular Functions — •Cornelia Monzel[1,3], Chiara Vicario[1], Domenik Lisse[2], Elie Balloul[1], Koceila Aizel[1], Mathieu Coppey[1], Jacob Piehler[2], and Maxime Dahan[1] — [1]Institut Curie, Laboratoire Physico-Chimie, CNRS UMR168, 75005 Paris — [2]University of Osnabrück, Department of Biology, 49076 Osnabrück, — [3]present address: University of Düsseldorf, Department of Physics, 40225 Düsseldorf

Many cell functions rely on the coordinated activity and spatial distribution of proteins on a subcellular scale. However, few tools are hitherto capable of probing and perturbing intracellular proteins on scales matching their natural spatio-temporal distribution. Here, we develop a novel magnetogenetic approach where intracellular proteins are specifically targeted by magnetic nanoparticles (MNPs) and manipulated with magnetic forces to remotely control individual cell functions. Among these functions are changes in organelle dynamics or the activation of a cell signaling pathway. We demonstrate that semisynthetic MNPs based on the natural iron storage protein ferritin are ideally suited for our magnetic manipulation approach. We explain the MNP design, different means of magnetic stimulation, and show the corresponding biological response.

Invited Talk BP 17.5 *(6)* Wed 10:30 H 1058

Tension build-up and membrane deformations in actin-membrane biomimetic systems — •Cécile Sykes — Institut Curie/CNRS/Paris Science et Lettres — 11, rue Pierre et Marie Curie, F-75231 Paris cedex 05

In order to unveil generic mechanisms of cell movements and shape changes, we design stripped-down experimental systems that reproduce cellular behaviours in simplified conditions, using liposome membranes on which cytoskeleton dynamics are reconstituted. Such stripped-down systems allow for a controlled study of the physical mechanisms that underlie cell movements and cell shape changes. Moreover, these experimental systems are used to address biological issues within a controlled, simplified environment. We have reconstituted the actin cortex of cells at the membrane of liposomes, and characterized their mechanical properties. We will show how these cortices contract in the presence of myosin motors, and how such experiments shed light of the mechanisms of cell shape changes. We have reconstituted membrane tubules and spikes pushed or pulled by actin polymerization, and which reproduce the formation of endocytic vesicles and filopodia. We will show how membrane and actin mechanical properties govern their formation.

30 min. break

BP 17.6 *(328)* Wed 11:30 H 1058

dynamic RT-DC: time-resolved mechanical single cell analysis at 100 cells / second — •Bob Fregin[1], Fabian Czerwinski[1], Konstanze Aurich[2], Doreen Biedenweg[1], and Oliver Otto[1] — [1]ZIK HIKE, Universität Greifswald, Greifswald, Germany — [2]Universitätsklinikum Greifswald, Greifswald, Germany

Real-Time Deformability Cytometry (RT-DC) is a label-free technique for single cell mechanical analysis with high throughput of up to 1,000 cells / second. By observing the shape of cells passing a narrow microfluidic channel their deformation and thus material properties can be quantified. As RT-DC is in the current implementation a single

shot technique, i.e. for every single cell only one image at the end of the channel is captured, exclusively time-independent parameters like the elastic modulus can be derived.

Here, we are introducing an extension of RT-DC towards dynamic single cell measurements with the possibility to capture elastic and viscous properties of single cells for up to 100 cells / second. Measurements are carried-out in real-time and allow for monitoring cellular shape-changes along the entire length of the microfluidic channel. By varying the experimental conditions we are capable to access a dynamic range in cell response exceeding one order of magnitude in time.

Dynamic RT-DC on a precursor myeloid cell line HL60 as well as primary cells reveals two characteristic timescales which can be attributed to the non-uniform stress distribution at the inlet compared to the steady-state situation inside the channel. This approach allows to extract model-independent material properties from RT-DC assays.

BP 17.7 *(169)* Wed 11:45 H 1058

Force Spectroscopy for the Investigation of Cellular Mechanotransduction — •Sandra Sindt, Steven Huth, and Christine Selhuber-Unkel — Christian-Albrechts-Universität zu Kiel, Institut für Materialwissenschaft, Biokompatible Nanomaterialien

Cells permanently explore the mechanical properties of their surroundings by applying forces. Even though some knowledge about mechanical interactions of cells have been obtained, the mechanisms are not completely understood yet. Here, we present a method based on a combination of Traction Force (TFM) and Atomic Force Microscopy (AFM) to gain deeper understanding of cellular mechanotransduction. During the detachment of a cell with a cantilever from a substrate with embedded fluorescent marker beads, the beads within the substrate are displaced. If the elastic properties of the substrate are known, the traction forces of the cell can be calculated from the displacements of the beads. In order to calculate traction forces, a precise and reliable mechanical characterization of substrates is important. The AFM is a well-established technique to measure the stiffness at the cellular scale, yet values of Young's moduli published by different authors vary significantly. Here, we present an improvement of the previously used method for measuring the stiffness of biological substrates based on indentation experiments using AFM. In this procedure, cantilevers are pressed against biocompatible soft polymer substrates using different forces and speeds. Both cantilever movements, towards and away from the substrate, are recorded and plotted as a force-distance curve. The Young's moduli are acquired from a Hertzian fit of the approach curve.

BP 17.8 *(284)* Wed 12:00 H 1058

Applications of new optical high speed cell characterization device CellMOUSE — •Daniel Geiger, Tobias Neckernuss, Jonas Pfeil, Ralf Schuster, and Othmar Marti — Institute of Experimental Physics, Ulm University

For various applications in science and medicine the identification of different cell parameters of suspended cells is essential. We developed a novel tool to assess important cellular parameters like size, shape and morphology in real time for more than 500 cells per second. This allows completely new experiments in various fields of basic research and clinical applications. After a brief introduction to the technique we present different applications of the so called CellMOUSE device. A validation for the measurement principle with well known samples will be shown. Furthermore, the determination of cellular parameters from suspended cells with superior throughput and accuracy will be presented. The samples range from simple NB4 cells to leukocytes and erythrocytes to bacteria and bacterial clusters. In addition we will present a simulation method for an easy comparison of our results with well established techniques.

BP 17.9 *(192)* Wed 12:15 H 1058

Simultaneous measurement of the Young's modulus and the Poisson ratio of thin elastic layers — •Wolfgang Gross and Holger Kress — Department of Physics, University of Bayreuth, Bayreuth, Germany

The mechanical interplay between cells and their environment has become a major point of interest during the last decades. To quantify the interactions between cells and soft matrices with techniques such as traction force microscopy, precise knowledge of the elastic parameters of thin substrate layers is necessary. However, only few methods are available to simultaneously measure the elastic modulus and the Poisson ratio of thin substrate layers.

Here we describe a novel technique to measure both parameters in a single experiment. As a model system, we chose polyacrylamide and poly-N-Isopropylacrylamide layers with a thickness of 1/10th of a millimeter and a stiffness in the range of mammalian tissue. We place millimeter-sized steel spheres with different radii on the substrates which indent the surface due to gravity and visualize the indentation cap marked with fluorescent microparticles with an inverted microscope. Using a previously published model which takes finite thickness effects into account, we demonstrate experimentally for the first time that the model allows the simultaneous determination of both the elastic modulus and the Poisson ratio with high accuracy. Since the technique comes without the need of special equipment aside from an inverted microscope, we envision it to become a standard tool for the characterization of thin substrate layers.

BP 17.10 *(345)* Wed 12:30 H 1058

Measurement and simulation of light scattering by deformed red blood cells (RBCs) in flow cytometry — •Jonas Gienger, Hermann Gross, Markus Bär, Volker Ost, and Jörg Neukammer — Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2–12, 10587 Berlin, Germany

Light scattering of single cells is widely applied for flow cytometric differentiation of cells. We developed a dedicated flow cytometer to simultaneously observe forward light scatter (FSC) of RBCs for orthogonal incident wave vectors $\vec{k}_1 \perp \vec{k}_2$. Bimodal distributions are observed in two-dimensional dot plots of FSC($\vec{k}_1$) vs. FSC($\vec{k}_2$) of typically 7.5×10^4 RBCs, which is a result of the RBCs' random orientation around the direction of flow, their distribution of size and optical properties.

Simulations of the light scattering by single RBCs were performed using the discrete dipole approximation (DDA). Using the axisymmetric equilibrium shape of healthy RBCs employed in most light scattering simulation studies to date, the experimentally observed bimodality cannot be reproduced. This is because this model does not account for the significant elongation due to hydrodynamic forces in the flow cytometer, involving extensional flow and Poiseuille flow at speeds of up to 5 m/s in channels of a few 100 μm width. Thus we propose a simple ad hoc model for elongated RBC shapes, which reproduces the bimodal 2D-distributions qualitatively. However, to quantitatively analyze the data and retrieve elastic parameters from such high-throughput optical measurements a detailed modeling of RBC deformation in the given flow conditions seems necessary.

BP 17.11 *(38)* Wed 12:45 H 1058

Treatment of cancer cells with acoustic waves — •Maja Strugacevac[1], Nina Bartels[1], Tobias Löffler[1], Constanze Wiek[2], Marcel Glaas[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Heinrich-Heine-Universität Düsseldorf, Institute of Applied Physics, Düsseldorf, Germany — [2]Düsseldorf University Hospital, Department of Otorhinolaryngology, Düsseldorf, Germany

Our group is developing new, alternative, cell-selective treatment strategies for squamous cell carcinoma of the head-neck area based on the different mechanical properties of oral keratinocytes and cancer cells. As a first step we compared their cytoskeleton and observed the differences in actin filaments and microtubules, both playing a significant role in cell elasticity. Oral keratinocytes are differently formed and seem to contain more fibers then cancer cells which could lead to the conclusion that there is a difference in cytoskeleton between this cell types.

In a second step we have irradiated different cell lines with acoustic waves exhibiting frequencies from 0.5 up to 10 kHz. Using different frequencies and input power we investigated the behavior of the cells exposed to the sound waves. Our latest results will be presented and discussed.

BP 18: Focus Session: Physics of Microbial Systems - organized by Tobias Bollenbach and Benedikt Sabass

Time: Wednesday 9:30–13:00 Location: H 2013

Invited Talk BP 18.1 *(22)* Wed 9:30 H 2013

Dynamics of cellular metabolism, size, and motility — •Sander Tans — AMOLF, Amsterdam, the Netherlands

We use time-lapse microscopy to measure the dynamics of individual cells, focusing on a number of different questions. I will present work on the relation between fluctuations in the expression of catabolically active enzymes and cellular growth, how cells control their size in the presence of external and internal perturbations, and a surprising observation of motility in epithelial cells that is triggered by viral infection.

BP 18.2 *(407)* Wed 10:00 H 2013

Salmonella **Typhimurium in the search of host cells** — Emiliano Perez Ipiña[1], Stefan Otte[1], Rodolphe Pontier-Bres[2], Dorota Czerucka[2], and •Fernando Peruani[1] — [1]Université Côte d'Azur, Laboratoire J.A. Dieudonné, UMR 7351 CNRS, Nice, France — [2]Centre Scientifique de Monaco (CSM), Principality of Monaco

Combining experiments and theory, we study how *Salmonella* Typhimurium (ST) search for human T84 colonic epithelial cells (HC), which, anchored on the bottom surface of a chamber, are invaded by ST. Our study reveals that near the surface ST do not display biased motion towards HC and the localization of HC involves a random search. We find that this random search has a well-defined average search time $\langle\tau\rangle$, which is determined by the details of the near-surface motion of ST and particularly by the diffusion coefficient D. We show that this random search can be well-described by a model, analytically tractable, of chiral active particles with active speed fluctuations and find that these fluctuations are of biological origin and account for up to 40% of D. Using simple arguments and simulations, we show that the number of ST that invade HC (NIB) is fully determined by $\langle\tau\rangle$, proving that D controls $\langle\tau\rangle$, and $\langle\tau\rangle$ determines NIB. Furthermore, our study reveals that within the same bacterial population (same genome), there exists a large range of inter-individual variability of the bacterial exploring capacity, with D ranging over four orders of magnitude. This finding together with the relation between D, $\langle\tau\rangle$, and NIB suggests that the individual infection capacity is highly heterogeneous within the same bacterial population.

BP 18.3 *(364)* Wed 10:15 H 2013

Sex or Simplicity: Phenotypic interference and the cost of complexity in asexual evolution — Torsten Held[1,2], •Daniel Klemmer[1,2], and Michael Lässig[1] — [1]Institut für Theoretische Physik, Universität zu Köln, Köln, Deutschland — [2]Equal contribution

The asexual evolution of microbes and viruses often generates clonal interference, a mode of competition between genetic clades within a population. We show that interference strongly constrains genetic and phenotypic complexity. Our analysis is based on a minimal biophysical model that represents each gene by a quantitative molecular phenotype, its fold stability. The model displays a generic mode of asexual evolution called phenotypic interference, which occurs over a wide range of evolutionary parameters appropriate for microbial populations. It generates a strong burden of complexity: The fitness cost of mutations increases faster than linearly with the number of genes. We show that recombination eliminates the superlinear cost through a first-order phase transition to a mode of sexual evolution. This implies a large fitness advantage of even facultative recombination and provides a biophysically grounded scenario for the evolution of sex. In a broader context, our analysis suggests that the systems biology of microbial organisms is strongly intertwined with their mode of evolution.

BP 18.4 *(422)* Wed 10:30 H 2013

Dormant, dead or alive: measuring steady state free energy levels in bacterial cells — •Leonardo Mancini and Teuta Pilizota — University of Edinburgh

Bacteria can survive a variety of external stresses by entering a state of suspended growth that is commonly referred to as dormancy. Such response has historically been considered a unequivocal low metabolism-low energy state and a vast array of stressors seem to be avoidable through dormancy. Antibiotics are among the most notable examples of such stressors and tolerant, dormant cells are known as persisters. However, recent experiments show that some persisters might survive antibiotic challenges through mechanisms that are, in contrast, energy consuming. The findings open the possibility of several different dormant steady states with distinct cellular free energy levels. To verify such a hypothesis, molecular sensors that can provide information on cellular energetics in vivo and at the single cell level are needed. To this end, we have successfully optimized the expression of a previously reported QUEEN ATP sensor and characterized in E. coli the newly proposed membrane voltage dye, Thioflavin T. Our results provided insights that can be generalized to other dyes, such as TMRM and DiSC3(5). Using the sensors, we present measurements of free energy levels during dormancy when this is induced by different conditions and signals, such as starvation, quorum sensing, and stress signalling molecules.

BP 18.5 *(28)* Wed 10:45 H 2013

Localized hypermutations govern competition dynamics through positioning in bacterial colonies — •Robert Zöllner, Enno Oldewurtel, Nadzeya Kouzel, and Berenike Maier — Department of Physics, University of Cologne, Zülpicher Str. 77, 50539 Köln, Germany

Cellular positioning towards the surface of bacterial colonies and biofilms can enhance dispersal, provide a selective advantage due to increased nutrient and space availability, or shield interior cells from external stresses. Little is known about the molecular mechanisms that govern bacterial positioning. Using the type IV pilus (T4P) of Neisseria gonorrhoeae, we tested the hypothesis that localized hypermutations govern positioning and thus enhance bacterial fitness in expanding gonococcal colonies. By independently tuning growth rate and T4P-mediated interaction forces, we show that the loss of T4P and the subsequent segregation to the front confers a strong selective advantage. Sequencing of the major pilin gene of the spatially segregated sub-populations and an investigation of the spatio-temporal population dynamics was carried out. Our findings indicate that localized hypermutations generate a standing variation of pilin sequences within the inoculation zone, while variants associated with a non-piliated phenotype segregate to the front of the growing colony. We conclude that tuning of attractive forces by mutations is a powerful mechanism for governing the population dynamics of bacterial colonies.

15 min. break

BP 18.6 *(126)* Wed 11:15 H 2013

Quantitative modeling of nutrient-limited growth of bacterial colonies in microfluidic cultivation — •Jens Elgeti — Theoretical Soft Matter and Biophysics, ICS-2, Forschungszentrum Jülich, Germany

Nutrient gradients and limitations play a pivotal role in the life of all microbes, both in their natural habitat as well as in artifical, microfluidic systems. Spatial concentration gradients of nutrients in densely packed cell configurations may locally affect the bacterial growth leading to heterogeneous micropopulations. A detailed understanding and quantitative modeling of cellular behaviour under nutrient limitations is thus highly desirable. We use microfluidic cultivations to investigate growth and microbial behaviour under well-controlled conditions. With a reaction-diffusion type model, parameters are extracted from steady-state experiments with a one-dimensional nutrient gradient. Subsequentially, we employ particle-based simulations with these parameters to predict the dynamical growth of a colony in two dimensions. Comparing the results of those simulations with microfluidic experiments yields excellent agreement. Our modeling approach lays the foundation for a better understanding of dynamic microbial growth processes, both in nature and in applied biotechnology.

BP 18.7 *(277)* Wed 11:30 H 2013

Sensitivity, dynamics and robustness of extracellular PhrA-signaling in Bacillus subtilis — Heiko Babel[1,2], •Pablo Naranjo[1,2], Stephanie Trauth[1,2], Victor Sourjik[1], and Ilka Bischofs[1,2] — [1]MPI for Terrestrial Microbiology, Marburg, Germany — [2]BioQuant, University of Heidelberg, Germany

Communication is an essential for the self-organization of bacterial populations. The underlying molecular networks that serve this task are surprisingly diverse. In order to understand how the different architectures affect signaling performance, new biophysical tools are required that allow us to quantitatively characterize the function of individual network components and signaling processes in the bacterial cell. A common form of signaling in Gram-positive bacteria is by means of signaling peptides that are produced by an active export-import circuit and are sensed intracellularly. Here, we developed the first FRET-reporter to quantitatively study PhrA-signaling in Bacillus subtilis. Using acceptor photo-bleaching experiments we studied the intra- and extracellular dynamics in response to peptide stimulation and developed a mathematical model that fits the data well. We find that the PhrA signaling circuit, although relying on a low affinity receptor, exhibits exquisite sensitivity to low extracellular signal levels. Our data furthermore suggests that oligopermeases - a component that is shared by all RNPP-signaling circuits in Gram-positive bacteria - play a central role in governing the sensitivity and dynamics of extracellular peptide signaling, while potentially also limiting the robustness of signaling in the presence of other peptides.

BP 18.8 *(290)* Wed 11:45 H 2013

Modelling of front instabilities in surfactant-driven biofilm spreading — •Sarah Trinschek[1,2], Karin John[2], Sigolène Lecuyer[2], and Uwe Thiele[1,3] — [1]Institut für Theoretische Physik, WWU, Münster, Germany — [2]Université Grenoble-Alpes, CNRS, Laboratoire Interdisciplinaire de Physique, Grenoble, France — [3]Center for Nonlinear Science (CeNoS), WWU, Münster, Germany

The spreading of bacterial colonies at solid air interfaces hinges on physical processes connected to the properties of the involved interfaces. The production of surfactant molecules by the bacteria is one strategy that allows the bacterial colony to efficiently expand over a substrate. These surfactant molecules affect the surface tension which results in an increased wettability as discussed in [1] as well as in outward-pointing Marangoni fluxes that promote spreading. These fluxes may cause an instability of the circular colony shape and the subsequent formation of fingers. In this work, we study the front instability of bacterial colonies at solid-air interfaces induced by surfactant production in the framework of a passive hydrodynamic thin-film model which is extended by bioactive terms. We show that the interplay between wettability and Marangoni fluxes determines the spreading dynamics and decides whether the colony can expand over the substrate. We observe four different types of spreading behaviour, namely, arrested and continuous spreading of circular colonies, slightly modulated front lines and the formation of pronounced fingers.

[1] S. Trinschek et al., PRL 119, 078003 (2017)

BP 18.9 *(191)* Wed 12:00 H 2013

Pili-mediated substrate motility of bacteria — •Wolfram Pönisch[1], Christoph A. Weber[1,2], and Vasily Zaburdaev[1] — [1]Max Planck Institut für Physik Komplexer Systeme, Dresden, Germany — [2]Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, USA

Most bacteria live in complex multicellular communities, known as biofilms, colonizing various surfaces. A wide range of bacteria use cell appendages, so called type IV pili, to bind to a substrate and generate pulling forces, enabling the cells to actively move. The attachment of bacteria to a surface and surface associated motility represent the first steps of biofilm formation.

For *Neisseria gonorrhoeae* (NG) bacteria, it was shown that its motility could be described as a persistent random walk with a characteristic length scale that exceeded the average pili length. Previously, it has been suggested that such behavior would require a mechanism of directional memory in pili attachments. Here, we develop a stochastic model demonstrating that the persistent motion arises naturally from the force-dependent detachment rate of pili and the geometric properties of the cell and its pili, but does not require any directional memory of the pili. We confirm this result with the help of a computational model of NG cells interacting with a substrate via its multiple individual pili. Furthermore, in agreement with experimental data, both model describes the dependence of cell motility on the total number of pili per cell.

BP 18.10 *(418)* Wed 12:15 H 2013

Regulation of cell volume and intracellular biomass density in bacteria, elucidated by single-cell measurements and perturbations — •Enno Oldewurtel and Sven van Teeffelen — Morphogenesis and Microbial Growth Lab, Institut Pasteur, Paris, France

All cells must control their volumes to maintain a high level of macromolecular crowding. In bacteria, cell volume is set by the peptidoglycan (PG) cell wall, which counteracts high internal Turgor pressure. A regulation of PG synthesis and cleavage is required to ensure a match of volume increase with the rate of biomass growth and to prevent cell lysis. We ask: a) How strictly is cell-wall expansion tied to biomass growth? b) Which cell-wall remodeling process is rate-limiting for cell-wall expansion? Using *Escherichia coli* we monitored cell mass and cell dimensions at the single-cell level and over time using quantitative phase microscopy. First, we find control of biomass density both during steady-state growth and during changes in growth rate, suggesting a close coupling of cell-wall expansion with mass growth. Second we show normal volume expansion even if PG synthesis is inhibited, up to the point of cell lysis. Furthermore, transient changes in the rate of PG cleavage lead to rapid changes in the surface expansion rate, pointing to a control of expansion by the rate of PG cleavage. However, despite rapid changes in surface expansion rate, the biomass density stays constant as cell width decreases to maintain a constant volume expansion rate. This width change is likely due to a change in pressure. This suggest cell volume regulation by cell-wall cleavage on intermediate time scales, and an involvement of Turgor pressure on short times.

BP 18.11 *(291)* Wed 12:30 H 2013

Phenotyping Individual Microbes by Mechanical Stress — •Fabian Czerwinski[1], Bob Fregin[1], Albert Siryaporn[2], and Oliver Otto[1] — [1]Center for Innovation Competence: Humoral Immune Reactions in Cardiovascular Diseases, University of Greifswald, Germany — [2]Department of Physics and Astronomy, University of California Irvine, USA

Microbes typically thrive and prosper in colonies and biofilms, whilst responding very sensitively to their environment. Often, smaller subpopulations take on special tasks that are important for the fate of the bunch. However, probing them individually with high throughput is challenging.

Microfluidics allow for a rapid phenotying of whole bacterial populations ideally capturing individual cells and, therefore, special states. By using the platform of real-time deformability cytometry (RT-DC), e.g., one can distinguish different vegetative states within even huge populations at throughputs beyond 10,000 cells per minute.

We used finite-element simulations to optimize the microfluidic geometries used in RT-DC for geometrical constraints, for flow conditions, and for cellular features. For bacteria, deformation of individual cells as a result of mechanical stress experienced during flow can serve as a distinctive gate.

BP 18.12 *(203)* Wed 12:45 H 2013

Mechanics of twitching migration of the bacterium P. aeruginosa — •Ahmet Nihat Simsek[1], Matthias D. Koch[2], Benedikt Sabass[1], Gerhard Gompper[1], Zemer Gitai[2], and Joshua W. Shaevitz[2] — [1]Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute of Advanced Simulation, Forschungszentrum Juelich, D-52425 Juelich, Germany — [2]Lewis-Sigler Institute for Integrative Genomics, Princeton University, NJ 08544

Pseudomonas aeruginosa is an ubiquitous pathogen responsible for severe and chronic infections. The bacterium employs retractable type-IV pili for migration and colonizes a broad variety of biotic and abiotic surfaces. How surface properties affect migration and colony formation of P. aeruginosa is a potentially important factor for bacterial surface contamination and infections alike. Here, we theoretically and experimentally study the effect of surface properties on the migration of P. aeruginosa. In our model, we assume a rod-like bacterium and treat each pilus, as well as the substrate as elastic springs. Pilus assembly and retraction are modeled as stochastic, force-dependent processes. To generate experimental data, we perform extensive image analysis to record the migration of different strains of P. aeruginosa on polyacrylamide substrates. Experimental data shows a non-linear dependence of migration speed and mean square displacement on substrate properties, which is in accordance with simulations. Finally, we present an analytical theory including the calculation of effective diffusion coefficients and aggregation probabilities of bacteria.

BP 19: Networks (joint session SOE/CPP/BP/DY)

Time: Wednesday 9:30–12:15 Location: MA 001

See SOE 13 for details of this session.

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

Time: Wednesday 10:00–13:30 Location: BH-N 333

See DY 45 for details of this session.

BP 21: Microswimmers (joint session BP/CPP/DY)

Time: Wednesday 15:00–17:30 Location: H 1028

Invited Talk BP 21.1 *(18)* Wed 15:00 H 1028

Emergent Dynamics of Active Particles — •Roland G. Winkler — Institute for Advanced Simulation, Forschungszemtrum Jülich, 52425 Jülich, Germany

The stationary-state structural and dynamical properties of microswimmers are governed by their shape and hydrodynamic interactions, but also the effective dimensionality of the system matters, i.e., three-dimensional bulk versus thin film. As a generic approach for microswimmers, we have developed a model for a spheroidal squirmer, with hydrodynamics implemented by the multiparticle collision dynamics approach [1,2]. We study the swimming behavior, cooperative motion, and motility-induced phase separation (MIPS) of such squirmers in a narrow slit. For two squirmers, surface hydrodynamic interactions strongly influences their cooperative motion [2]. Considering the phase behavior of many squirmers, hydrodynamic interactions suppress MIPS for spherical squirmers. In contrast, hydrodynamic interactions enhance MIPS for elongated squirmers. Moreover, the shape affects the rheological properties of squirmers in shear and Poiseuille flow.

[1] J. Elgeti, R. G. Winkler, G. Gompper, Rep. Prog. Phys. 78, 056601 (2015)

[2] M. Theers, E. Westphal, G. Gompper, R. G. Winkler, Soft Matter 12, 7372 (2016)

BP 21.2 *(91)* Wed 15:30 H 1028

Magnetic behavior and chemotaxis of magnetic bacteria — •Agnese Codutti[1], Damien Faivre[1], and Stefan Klumpp[2] — [1]Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany — [2]Georg-August-Universität Göttingen Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Chemotaxis is the bacterial ability to bias their motility toward a preferred concentration of attractants or repellents. This chemotactic ability can be used by magnetic bacteria, coupling it to a passive alignment to external magnetic fields. Magnetic bacteria include the naturally-occurring magnetotactic bacteria, and lab-produced biohybrids, in which for example E. coli can be coupled to external magnetic beads. Therefore, a model to understand the coupling between magnetic fields, active swimming, and chemotaxis is needed to predict the behavior of these systems. We perform simulations based on an Active Brownian Particle model, modified to include active swimming, active changes of directions, chemotaxis, and passive alignment with external magnetic fields. The model allows us to reproduce the capillary experiments, and to throw some light on the possible aerotaxis models shown by magnetotactic bacteria. As main results, we show how run and tumble motion hinders the chemotactic/aerotactic abilities of the bacteria when coupled with magnetic fields, while run and reverse motility benefits from the magnetic field, leading to faster chemotaxis. We explore different magnetic behaviors of magnetotactic bacteria, where cells are either simply aligned by the external field or alternatively using it as proxy of oxygen gradient.

BP 21.3 *(148)* Wed 15:45 H 1028

The bacterial soliton in a nutrient field – re-examined — •Andrzej Palugniok[2], Maximilian Seyrich[1], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Worcester College, University of Oxford, Walton Street, OX1 2HB Oxford, United Kingdom

The gut bacterium *E. coli* with its run-and-tumble walk is a well-studied model swimmer in the active-matter field. One of the various interesting collective phenomena is a bacterial soliton or a traveling concentration pulse of bacteria [1]. It develops when bacteria start to consume a nutrient in an initially uniform field, in which they also perform chemotaxis.

To describe such a situation, we start from a Smoluchowski equation of a run-and-tumble particle in a chemotactic field. A Markovian tumble rate is derived from the usual linear response theory. We perform a multipole expansion to derive equations for the bacterial density and the local polar order decribed by the bacterial polarization. On times longer than the typical relaxation time for the polarization, one recovers the Keller-Segel equation. Solving it together with the diffusion equation for the nutrient, we are able to reproduce the bacterial soliton. Thereby, we demonstrate that one does not need a second, signalling chemical field as introduced in Ref. [1] nor a singular chemotactic drift term as demanded in Ref. [2].

[1] J. Saragosti et al., PNAS **108**, 39 (2011).
[2] E.F. Keller and L.A. Segel, J. Theor. Biol., **30**, 2 (1971).

BP 21.4 *(150)* Wed 16:00 H 1028

Dynamic Propulsion Force Measurements of Chlamydomonas Microalgae using Micropipette Force Sensors — •Thomas Josef Böddeker, Christian Titus Kreis, Quentin Magdelaine, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Faßberg 17, D-37077 Göttingen, Germany

Although the swimming dynamics of microbes, such as bacteria and microalgae, have received a lot of attention in recent years, methods for direct propulsion force measurements are still limited. We present a new approach utilizing micropipettes as force sensors to study the propulsion forces and wall interactions of the unicellular, biflagellated microswimmer *Chlamydomonas*. Fourier signal analysis of the micropipette deflection reveals a clear signature of the energy output of the microswimmer and provides a handle to measure the frequency and energy associated to the flagella beating. Continuous measurements in a liquid cell allow us to characterize the propulsion of individual cells and to probe the extent of steric and hydrodynamic interactions between beating flagella and solid interfaces. For controlled environmental conditions, we quantify the difference in propulsion energy and beating frequency between swimming in bulk and in close proximity to solid interfaces.

BP 21.5 *(235)* Wed 16:15 H 1028

Applying an Extended Kalman Filter to extract bacteria statistics — •Oliver Köhn — Universität des Saarlandes

Bacteria tend to swim in liquids in absence of food facilitated by creation of flagella. The trajectories are determined by slightly curved lines (running states) and randomly interrupted by short intervals with strong direction changes (tumbling state)[1]. This behavior seems to be efficient in finding food in unknown environments. We assume an intrinsic randomness in the running states as well in the appearance of the tumbling intervals.[1] Furthermore in real experiments the extracted positions are influenced by a detection noise. Estimating the stochastic trajectory properties requires the distinction between bacteria intrinsic randomness and the measurement noise. From the engineers it is known that the Kalmann filter algorithm provide this in an optimal way [2]. We adapted and implemented this filter for simulated as well as measured bacteria trajectories.

[1] Enhancing bacterial motility and search efficiency by genetic manipulation of flagellar number; Javad Najafi, M. Reza Shaebani, Thomas John, Florian Altegoer, Gert Bange & Christian Wagner; submitted to PNAS [2] Forecasting, structural time series models and the Kalman filter; Andrew C. Harvey; 1989; Cambridge University Press

BP 21.6 *(99)* Wed 16:30 H 1028

Phase diagram of a low Reynolds number swimmer near a wall — •Abdallah Daddi-Moussa-Ider[1], Maciej Lisicki[2,3], Christian Hoell[1], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, Düsseldorf 40225, Germany — [2]Department of Applied Mathematics and Theoretical Physics, Wilberforce Rd, Cambridge CB3 0WA, United Kingdom — [3]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

The hydrodynamic flow field generated by self-propelled active particles and swimming microorganisms is strongly altered by the presence of nearby boundaries in a viscous flow. Using a simple model swimmer composed of three-linked spheres, we show that the swimming trajectories near a non-slip wall reveal various interesting scenarios of motion depending on the initial orientation and the distance separating the swimmer from the wall. Accordingly, the swimmer can either be trapped by the wall, totally escape from the wall, or undergo an oscillatory gliding motion at a constant mean height above the wall. Using a far-field approximation, we find that the wall-induced correction at leading order has a quadrupolar flow structure where the translational and angular velocities of the swimmer decay as inverse third and fourth power with distance, respectively. The resulting equations of motion for the trajectories and the relevant order parameters fully characterize the transition between the phases and allow for an accurate description of the swimming behavior near a wall.

BP 21.7 *(402)* Wed 16:45 H 1028

Three-dimensional simulation of sperm in structured microfluidic channels — •Sebastian Rode, Jens Elgeti, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems (ICS-2) , Forschungszentrum Jülich, 52425 Jülich, Germany

Sperm cells propel themselves by a periodic wave-like beating of their flagellum [1-3]. At low Reynolds numbers and in confinement, the directed motion of sperm and other microswimmers is strongly influenced by steric and hydrodynamic surface interactions [1]. We model sperm motility in our mesoscale hydrodynamics simulations by imposing a planar traveling bending wave along the flagellum [2]. For swimming in zigzag shaped microchannels, we find that the deflection angle of a sperm cell at sharp corners depends on the orientation of its beating plane. Our results are in good agreement with recent microfluidic experiments, and help to improve the understanding of sperm cell navigation under strong confinement. We show that the emergence of a nonplanar component of the flagellar beat with increasing wavelength drastically increases surface attraction.

[1] J. Elgeti et al., Rep. Prog. Phys. 78, 056601 (2015) [2] J. Elgeti et al., Biophys. J. 99, 1018 (2010) [3] G. Saggiorato et al., Nat. Commun. 8, 1415 (2017)

BP 21.8 *(157)* Wed 17:00 H 1028

Altering diffusion by interaction of microalgae with micron-sized objects — •Francine Kolley[1,2], Patricia Dähmlow[2], Hajnalka Nadasi[2], Florian von Rüling[2], and Alexey Eremin[2] — [1]Technical University Dresden — [2]Otto-von-Guericke-University Magdeburg

The enhancement of passive particles, single silica spheres and their doublets, was studied in suspensions containing microswimmers Chlamydomonas reinhardtii. These green algae move with a flagellar motor, reaching typical velocities up to 150 μm/s. Stimulated by phototaxis, their motion is similar to humans doing breaststroke. The induced flow of the puller affects the translational as well as the rotational diffusion of the passive particles. The corresponding diffusion coefficients were obtained from the measurement of the mean square displacements of the passive particles for various concentrations of the algae. The Brownian Motion of the silica beads was observed in a quasi-2D system in flat cappilaries.To avoid cell immobilization by adsorption to the glass substrate the capillary surface was silanized. Additionally, a polymer was introduced to the suspension to optimize the diffusive behavior. In the range of small algae concentrations, the diffusion coefficients exhibited a linear dependence on the cell density of Chlamydomonas reinhardtii.

BP 21.9 *(323)* Wed 17:15 H 1028

Dynamics of chemotactic and chemokinetic bacterial populations — •Theresa Jakuszeit[1], James Lindsey-Jones[1], François J. Peaudecerf[2], and Ottavio A. Croze[1] — [1]Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — [2]Institute of Environmental Engineering, ETH Zürich, Stefano-Franscini-Platz 5, 8093 Zürich, Switzerland

Several motile bacteria are able to sense chemical gradients much larger than their own size, and perform a random walk biased up attractant gradients ('chemotaxis') by varying their reorientation rate. In addition to this well-known chemotactic behaviour, several soil and marine bacterial species are known to modify their swimming speed according to the local concentration of chemoattractant ('chemokinesis'). Therefore, a chemical field of attractant induces a spatially varying swimming speed, which results in a drift towards lower attractant concentrations – contrary to the drift created by chemotaxis.

Here, to explore the biological benefits of chemokinesis and investigate its impact on the chemotactic response, we extend a Keller-Segel type model to include a dependence of the swimming speed on the attractant concentration. Even though chemokinesis on its own results in a dispersion of the population away from high attractant concentrations, it can not only enhance the chemotactic response but also modify it qualitatively. We apply the model to predict the dynamics of bacteria capable of chemokinesis and chemotaxis in experimentally inspired chemoattractant fields, such as those generated in capillary migration assays and around environmental nutrient sources.

BP 22: Computational Biophysics II

Time: Wednesday 15:00–17:30 Location: H 1058

BP 22.1 *(374)* Wed 15:00 H 1058

anionic and cationic gold nanoparticles in model lipid membranes: experiments and simulations — ester canepa[2], •sebastian salassi[1], federica simonelli[1], riccardo ferrando[2], ranieri rolandi[1], chiara lambruschini[2], annalisa relini[2], and giulia rossi[1] — [1]Physics department — [2]Chemistry department, University of Genoa, Genoa, Italy

Designing metal nanoparticles (NPs) with biomedical applications requires the molecular understanding of their interaction with cell membranes. We use fluorescence spectroscopy measurements and molecular dynamics (MD) simulations to study the interaction between charged monolayer-protected AuNPs and model POPC lipid bilayer[1-2]. We consider cationic (NP+) and anionic (NP-) NPs. The anionic ligands differ from the cationic ones for their terminal group, which is a carboxylate or a quaternary ammonium ion. We use fluorescence leakage assays to quantify the damage induced by NP- and NP+ to liposomes, and find that NP+ are more disruptive. MD simulations offer a molecular interpretation of this result. Assuming no changes of the charge of NP+ and NP- they interact with the bilayer with the same mechanism[3] and bilayer deformation. Our simulations, though, show that anionic ligands can be protonated when interacting with the lipid head. Once protonated, the NP- interact with the bilayer in a less disruptive way, without deforming or damaging it. This change of the pKa of the anionic ligands can explain the smaller leakage induced by NP-.

1.Tatur, S et all. Langmuir 2013. 2. Van Lehn,R. C. et all. Nano Lett. 2013. 3. Salassi, S. et all. JPCC 2017.

BP 22.2 *(178)* Wed 15:15 H 1058

The effect of small molecules on lipid-domain formation studied by coarse-grained simulations — •Alessia Centi, Kurt Kremer, and Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany

The lateral organisation of cell membranes is believed to play a key role in many biological processes, including protein trafficking, signal transduction as well as transport of viruses and pathogens. Small molecules, such as alcohols and anesthetics, can alter this lateral arrangement by preferentially partitioning between lipid domains, hence significantly affecting both membrane properties and functionalities. The process of domain stabilization/destabilization induced by small molecules has been widely investigated, both at experimental and com-

putational level; however, its exact mechanism as well as the driving forces for it still remain elusive.

In this work, coarse-grained simulations based on the MARTINI force field have been used to try to shed light on the processes underlying domain reorganization mediated by small molecules. The approach used involves a combination of free energy calculations and replica exchange simulations; thereby, allowing to explore the effect of a multitude of parameters (e.g. type of lipids, solutes and relative concentrations) relevant for the process under evaluation at a reduced computational cost in comparison to atomistic simulations.

BP 22.3 *(281)* Wed 15:30 H 1058

Performing cell-based tissue simulations to explore the impact of cell mechanics on anisotropic epithelial tissue growth — •Anna Stopka and Dagmar Iber — D-BSSE, ETH Zürich, Schweiz

Understanding the anisotropic expansion of an embryonic tissue during organogenesis is a central challenge in developmental biology. Experimental studies increasingly provide quantitative data on cell behaviour during tissue growth. Computational models can help to interpret the acquired data and to infer underlying mechanisms. Our group has recently developed the 2D software framework LBIBCell to permit data-based simulations of tissue dynamics at cellular resolution [1]. LBIBCell represents cells as finely resolved polygons according to the Immersed Boundary (IB) method; membrane tension and cell-cell adhesion are represented via springs. The fluid behaviour inside and outside of the cells is described by the Lattice Boltzmann (LB) method. Cell growth is implemented via a fluid source inside the cells. Anisotropic outgrowth of epithelial tissues has been accounted to a range of mechanisms, including a bias in cell division orientation. We have used LBIBCell to investigate to what extent the mechanical properties of an epithelial tissue affect its capability to achieve anisotropic outgrowth via biased cell divisions. In our simulations we focused on the 2D apical plane where epithelial cells adhere tightly. We show that a bias in cell division orientation translates into a bias in outgrowth only for sufficiently stiff tissues. [1] S.Tanaka, D.Sichau, D.Iber, Bioinformatics (2015)

Invited Talk BP 22.4 *(14)* Wed 15:45 H 1058

Complex shapes and dynamics of red blood cells in shear flow under physiological conditions — Johannes Mauer[1], Simon Mendez[2], Luca Lanotte[3], Manouk Abkarian[3], Gerhard Gompper[1], and •Dmitry A. Fedosov[1] — [1]Institute of Complex Systems, Forschungszentrum Juelich, 52425 Juelich, Germany — [2]Institut Montpellierain Alexander Grothendieck, CNRS, University of Montpellier, 34095 Montpellier, France — [3]Centre de Biochimie Structurale, CNRS, University of Montpellier, 34090 Montpellier, France

Red blood cells (RBCs) constitute the major cellular part of blood and are mainly responsible for the transport of oxygen. They have a biconcave shape with a membrane consisting of a lipid bilayer with an attached cytoskeleton formed by a network of the spectrin proteins. The RBC membrane encloses a viscous cytosol (hemoglobin solution), so that RBCs possess no bulk cytoskeleton and organelles. Experiments on RBCs under shear flow reveal that the viscosity contrast between cytosol and blood plasma is an essential factor which determines their shape and dynamics. Under physiological conditions with a viscosity contrast of about five, RBCs first tumble, then roll, transit to a rolling and tumbling stomatocyte, and finally attain polylobed shapes at high shear rates. Our study based on microfluidic experiments and two different simulation techniques results in a complete diagram of RBC shapes and dynamics in shear flow as a function of shear rate and viscosity contrast. We will discuss potential mechanisms, which may lead to the variety of novel shapes, and compare the diagram for RBCs to that for vesicles.

BP 22.5 *(335)* Wed 16:15 H 1058

On how the CSF flows in the ventral third ventricle of brain — •Yong Wang[1], Christian Westendorf[1], Regina Faubel[2], Gregor Eichele[3], and Eberhard Bodenschatz[1] — [1]MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Department of Developmental Biology, U Pittsburgh, Pittsburgh PA 15201, USA — [3]MPI for Biophysical Chemistry, 37077 Göttingen, Germany

A complex transport network driven by coordinated motile cilia inside the ventral third ventricle (v3V) of mammalian brain was reported recently. This network generates cerebrospinal fluid (CSF) flow patterns such as a separatrix and a whirl that establish intraventricular boundaries. The CSF flow in the whole three-dimensional v3V cavity was studied numerically. Specifically, experimental trajectory data obtained by tracking fluorescent beads were converted to 2D velocity fields. The velocity maps were then refined by considering divergence-free and projected onto a curved virtual surface as boundary conditions. Three-dimensional flow features with likely physiological consequences were uncovered numerically. We thank the Max Planck Society for financial support. This work is conducted within the Physics and Medicine Initiative at Goettingen Campus between Max Planck Society and University Medicine Center.

BP 22.6 *(421)* Wed 16:30 H 1058

Memoryless navigation with limited sensing capacity — Luis Gómez Nava, •Robert Grossmann, and Fernando Peruani — Université Côte d'Azur, Nice, France

How should an active walker detect a target in a complex landscape, e.g. the maximal chemical concentration, given that (i) only local values of this external signal are instantaneously accessible, but no gradients, and (ii) there is no memory? This question is of broad relevance, from bacterial chemotaxis to the design of self-controlled microrobots that are supposed to perform complex tasks autonomously. The latter area of application is particularly important with regard to today's medicine aiming at fabricating micrometer-sized robots for target-specific drug-delivery, for example. Motion on the micronscale is, however, subject to a series of constraints: viscous forces dominate over inertial ones and thermal fluctuations are relevant. Navigation under these physical conditions is hence a nontrivial task. In this talk, we provide basic theoretical guidelines how to design active particles with internal states which are able to execute complex tasks such as adaptive gradient-following. We analytically link their internal dynamics of these particles to their motility properties such as drift and diffusivity enabling us to discuss how to tune the internal dynamics given a specific task. These findings are important in the design of simple navigation algorithms for robotic engineering and, moreover, may be present in various microbiological systems.

BP 22.7 *(120)* Wed 16:45 H 1058

How does reducible defense alter predator-prey dynamics? — •Tatjana Thiel, Andreas Brechtel, Adrian Brückner, Michael Heethoff, and Barbara Drossel — Technische Universität Darmstadt, Germany

In nature, numerous animal species use defense mechanisms like hardening or chemical secretions to defend against attacks of predators. However, there is yet no theoretical study of defensive mechanisms where protection is permanent, but diminished with attacks, which has been termed "reducible defense". This kind of defense mechanism is common among arthropods and is likely to change the dynamics and stability of the system.

We propose a predator-prey model where prey use a reducible defense mechanism (i.e. reservoir-based chemical defense). The prey excretes a certain amount of secretion upon attack and is therefore not consumable while it is armed. The predator has to attack often enough to disarm and consume prey, before the secretion is biosynthetically restored. We will discuss the behavior of our model under parameter changes and compare it to a conventional predator-prey system. We show that predator and prey can become considerably more abundant by taking reducible defense into account. Furthermore, we consider payoffs between fast replenishment of secretion and larger storage volume, and between investment in offspring vs investment in defense. For the latter, we find that prey should invest more in defense when resources are scarce, but completely in offspring when plenty of resources are available.

BP 22.8 *(301)* Wed 17:00 H 1058

Trade-off shapes diversity in eco-evolutionary dynamics — •Farnoush Farahpour[1], Mohammadkarim Saeedghalati[1], and Daniel Hoffmann[1,2,3] — [1]Bioinformatics and Computational Biophysics, Uni. Duisburg-Essen, DE — [2]CCSS, Uni. Duisburg-Essen, DE — [3]ZMB, Uni. Duisburg-Essen, DE

Over the last decades one of the main drivers of research in biodiversity has been to explain the naturally observed diversity and coexistence of competing species specially in well-mixed systems. In this project we propose a simple solutions for paradoxical question of diversity in competitive communities in a bare-bone and generic model. We introduce an Interaction and Trade-off based Eco-Evolutionary Model (ITEEM), in which species are competing for resources in a well-mixed system, and their evolution in interaction trait space is subject to a life-history trade-off between replication rate and competitive ability. We demon-

strate that the strength of the trade-off has a fundamental impact on eco-evolutionary dynamics, as it imposes four phases of diversity, including a sharp phase transition. Despite its minimalism, ITEEM produces without further ad hoc features a remarkable range of observed patterns of eco-evolutionary dynamics. Most notably we find self-organization towards structured communities with high and sustainable diversity, in which competing species form interaction cycles similar to rock-paper-scissors games. Our approach to study the role of trade-offs in diversity provides a general framework to study assembly process of competitive communities and investigate the mechanisms responsible for resistance and resilience of their networks.

BP 22.9 *(140)* Wed 17:15 H 1058

Interplay between Spatial Dynamics and Lifetime Distributions in an Evolutionary Food Web Model — •Tobias Rogge[1], Korinna T. Allhoff[2], David Jones[1], and Barbara Drossel[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Institute of Evolution and Ecology (EvE), University of Tübingen, Germany

We study the meta-network dynamics emerging in an evolutionary food web model on a system of coupled patches in space. Species are characterized by their body mass and the body-mass interval that specifies their prey. Each patch hosts a food web that contains several trophic layers, and the species composition in the patches changes due to ongoing processes of species addition ("mutation"), migration, and interaction-dependent extinction.

The model is able to sustain a complex food web structure on each patch, while undergoing continued species replacement dynamics. In particular, we evaluate species-lifetime distributions (how long is the time span that a species can survive in the system?) and species-area relationships SAR (how many species can we find in a given area?). All these relationships resemble power laws over appropriately chosen parameter ranges and thus agree qualitatively with empirical findings. We observe strong finite-size effects, and a dependence of the relationships on the trophic layer of the species. More precisely, we find that species with larger body masses on higher trophic position generate steeper SAR.

BP 23: Bioimaging and Biopspectroscopy II

Time: Wednesday 15:00–17:15 Location: H 2013

BP 23.1 *(110)* Wed 15:00 H 2013

Label-free, real-time monitoring of cytosolic composition and dynamics using digital holographic microscopy — •Daniel Midtvedt, Erik Olsén, Gavin Jeffries, and Fredrik Höök — Chalmers University of Technology

Cells continuously adapt their biophysical properties during their Life cycle as well as in response to changes in the environment. However, quantifying these biophysical changes on single cell level has only recently become possible. In this work we use a digital holographic microscope in combination with a millifluidic chip to study the response of microorganisms and mammalian cells to external stimuli. We demonstrate a label-free quantification of changes in both intracellular osmolarity and macromolecular concentration, on single cell level, in response to a change in medium osmolarity. This platform allows to disentangle cellular water fluxes from production and accumulation of higher molecular weight compounds, which suggests an applicability of this platform in studying a broad range of cellular processes.

BP 23.2 *(212)* Wed 15:15 H 2013

Structure and Dynamics of the Trypanosoma brucei Plasma Membrane — Marius Glogger, •Marie Schwebs, Markus Engstler, and Susanne Fenz — Universität Würzburg, Biocenter: Cell and Developmental Biology, Würzburg, Germany

African trypanosomes are the causative agents of sleeping sickness in human and Nagana in livestock. In the bloodstream of their host, they exhibit a dense coat of variant surface glycoproteins (VSG). Fluidity of the VSG coat is a fundamental for parasite survival. However, the diffusion behavior of the VSGs is also limited by the physical properties of their lipid matrix. We have recently introduced super-resolution imaging of intrinsically fast moving flagellates based on cyto-compatible hydrogel embedding [Glogger et al. JPD: Appl Phys 17]. Building on this work we employ leaflet-specific membrane probes and single-molecule fluorescence microscopy to elucidate the structure and dynamics of the plasma membrane and VSG coat in living trypanosomes. Using expressed lipid-anchored eYFP as a probe for the inner membrane leaflet, we found specific domains where the probe accumulates or appears diluted rather than being homogenously distributed. We hypothesize that this structuring of the membrane is associated with the underlying microtubule cytoskeleton. The next steps include employment of a more stable fluorescent label to resolve dynamic interaction of single probes with the observed domains. Moreover, we aim to track fluorescently labeled lipids in the outer leaflet to gain insight in inter-leaflet coupling in vivo, and we plan a two-color experiment to simultaneously investigate membrane and VSG dynamics.

BP 23.3 *(420)* Wed 15:30 H 2013

Enhanced fluorescence resonance energy transfer in G protein-coupled receptor probes by nano-coated microscopy coverslips — •Benjamin Schreiber[1], Michael Kauk[1,2,4], Hannah S Heil[1], Martin Kamp[3], Sven Höfling[3], Carsten Hoffmann[1,2,4], and Katrin G Heinze[1] — [1]Rudolf Virchow Zentrum, Universität Würzburg — [2]Institut für Pharmakologie und Toxikologie, Universität Würzburg — [3]Technische Physik, Universität Würzburg — [4]Institut für Molekulare Zellbiologie, Universität Jena

For probing biomolecular interactions in a live-cell setting the distance depending Fluorescence resonance energy transfer (FRET) is often the method of choice. G-protein-coupled receptors mediates cellular responses and communication across cellular membranes, and is the largest known class of molecular targets with proven therapeutic value. The design of FRET probes is crucial to ensure unhampered functionality and binding kinetics of the molecular complex. Thus, such FRET probes usually require labeling compromises with limited FRET efficiencies. Here, we present an approach to optimize the energy transfer without changing the design of the FRET probe. We show that gold coated glass cover slips allow reinforcing the otherwise forbidden donor-acceptor energy transfer by virtual optimization of the dipole orientation. We show resulting enhanced FRET on our nano-coatings for the ligand driven activation of M1 muscarinic acetylcholine receptors labeled with a CFP-FlAsH pair. We believe that our techniques has particular potential for pharmaceutical drug screening.

BP 23.4 *(440)* Wed 15:45 H 2013

Characterisation of Metabolic Dynamics by Fluorescence Lifetime Imaging Microscopy of NAD(P)H — •André Weber[1], Yury Prokazov[1], Marcus Hauser[2], and Werner Zuschratter[1] — [1]Leibniz-Institut für Neurobiologie Magdeburg, Germany — [2]Institut für Biometrie und Medizinische Informatik, Otto-von-Guericke- Universität Magdeburg, Germany

The energy metabolism of eucaryotic cells can show complex dynamics, i.e. glycolytic oscillations. Monitoring this intrinsic behaviour by fluorescence microscopy is influence the metabolism, which is sensitive to excitation light intensities, especially in UV range.

We show a low light imaging approach using a single photon counting position sensitive detector working with laser intensities below 3mW/cm^2 and a time resolution below 90ps. For excitation of intracellular NAD(P)H a 8 MHz pulsed frequency-tripled Nd:vanadate laser tuned at 355 nm was used. The analysis of the complex fluorescence decay of NAD(P)H in intact yeast cells revealed 4 molecular species with characteristic fluorescence lifetimes showing individual behaviour and glycolytic oscillations as response to glucose addition. Laser intensities higher 3mW/cm^2 did not lead to long lasting glycolytic oscillations.

BP 23.5 *(427)* Wed 16:00 H 2013

Cardiac Cells and Heart Tissue Studied by X-ray Imaging and Scanning X-ray Diffraction — •Jan-David Nicolas[1], Marten Bernhardt[1], Susanne Schlick[2], Malte Tiburcy[2], Wolfram-Hubertus Zimmermann[2], Amara Khan[3], Frauke Alves[3], Karl Toischer[4], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut für Pharmakologie und Toxikologie, Robert-Koch-Str. 40, 37075 Göttingen — [3]Max-Planck-Institut für Experimentelle Medizin, Hermann-Rein-Straße 3, 37075 Göttingen — [4]Klinik für Kardiologie und Pneu-

mologie, Institut für Pharmakologie und Toxologie, Robert-Koch-Str. 40, 37075 Göttingen

We have applied scanning x-ray diffraction on cardiac cells and tissue to characterize the cytoskeletal architecture and to localize potential structural defects due to disease. The method typically involves raster-scanning of a microfocused x-ray beam and collecting scattering patterns at each scan point. The collected data can then be analyzed in view of structural parameters such as the interfilament spacing or orientation of the myosin and actin filaments that are in almost crystalline arrangement in the sarcomere. We will show what signals can be extracted from cells and tissue and how nanoscale architecture develops with differentiation. Since many cardiomyopathies rely on the structural integrity of the sarcomere, the contractile unit of cardiac muscle cells, the present study can be easily extended to characterize cells and tissue from a diseased heart.

Invited Talk BP 23.6 *(11)* Wed 16:15 H 2013

Illuminating physical cues for the early embryogenesis of a simple model organism — •Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Embryogenesis is a remarkably robust, but still poorly understood self-organization phenomenon that is governed by a variety of biochemical and physical cues. Due to its simplicity, the small roundworm Caenorhabditis elegans is a superb model organism to study the role of physics during early developmental stages. Using single plane illumination microscopy (SPIM), we have explored how physical cues determine the cell arrangement during the early embryogenesis of C. elegans. In particular, we have studied the coupling of cellular volumes and cell cycle times, the nature of asymmetric cell divisions, and the mechanically driven cell arrangement process [1]. Going beyond mere imaging, we also have used pixel-wise fluorescence correlation spectroscopy (SPIM-FCS) to spatiotemporally quantify the diffusion of proteins in individual cells of the embryo in cytoplasm and on membranes [2]. As a result, we were able to monitor the emergence of intracellular diffusion and concentration gradients prior to the first cell division, which define the anterior- posterior body axis already in the single-cell state.

[1] Biophys. J. 105, 1805 (2013); Phys. Rev. Lett. 117, 188101 (2016); Sci. Rep. 7, 9369 (2017).

[2] J. Phys. D 49, 044002 (2016).

BP 23.7 *(231)* Wed 16:45 H 2013

Non-equilibrium forces drive the anomalous diffusion of vital cell constituents — •Lorenz Stadler, Konstantin Speckner, and Matthias Weiss — Experimentalphysik 1, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth

Diffusion is the basic mode of motion for supra-molecular assemblies in living cells, often with an anomalous scaling of the mean square displacement, with $ text $. Considerable effort has been invested to uncover the underlying types of subdiffusive processes, yet often with the tacit assumption that the involved random forces are mostly of thermal origin. Contrary to this simple assumption, our single-particle tracking data on the subdiffusive motion of telomeres in the nucleus of mammalian cells reveals an important role of cytoskeleton-associated non-equilibrium forces [1]. In line with this finding, we also have found strong non-equilibrium contributions in the trajectories of membrane domains in the cells' Endoplasmic Reticulum (so-called 'ER exit sites'). Due to the complex topology of the ER, exit sites not only are shaken by the cytoskeleton-driven motion of the entire ER network but they also show an (activated) subordinated motion on individual ER tubules. Altogether, our data show that even subdiffusive motion patterns in cells may not represent simple thermal transport process but rather are non-equilibrium events.

[1] Stadler & Weiss, New J. Phys. (in press) 2017

BP 23.8 *(414)* Wed 17:00 H 2013

Investigating Transient Peptide-Membrane Interactions with TIR-FCS — •Philipp Blumhardt[1,3], Jonas Mücksch[1,3], Henri G. Franquelim[1], Maximilian T. Strauss[1,2], Philipp Glock[1], Johannes Stein[1], Ralf Jungmann[1,2], and Petra Schwille[1] — [1]Max Planck Institute for Biochemistry, Martinsried, Germany — [2]Ludwig-Maximilians-Universität, Munich, Germany — [3]authors contributed equally

The accurate determination of binding rates to membranes or membrane-bound proteins is of key relevance for quantitative biology. Despite the existence of multiple methods to characterize surface interactions, there are still many experimental challenges regarding simplicity of use and general applicability. We developed a simple and versatile single-molecule fluorescence approach for the accurate determination of binding rates to surfaces or surface-bound receptors. Our approach combines Fluorescence Correlation Spectroscopy (FCS) with Total Internal Reflection (TIR) Fluorescence microscopy and a camera-based detection. This combination not only yields a high surface selectivity, but also resolves association and dissociation rates over a wide time range. Previously, we quantified the transient hybridization of single-stranded DNA to the complementary handles of immobilized DNA origamis. We varied the nucleotide overlap, yielding different transient binding times in the range of milliseconds to tens of seconds. Here, we present our latest results on the transfer of this assay to the otherwise challenging quantification of transient interactions between protein segments and lipid bilayers.

BP 24: Bioinspired Functional Materials, Biomaterials and Biopolymers (joint session CPP/BP)

Time: Wednesday 15:00–16:30 Location: PC 203

See CPP 52 for details of this session.

BP 25: Active Matter DY III (joint session DY/CPP/BP)

Time: Wednesday 15:30–18:45 Location: BH-N 243

See DY 52 for details of this session.

BP 26: Annual General Meeting of the BP Division (BP Mitgliederversammlung)

Time: Wednesday 18:00–19:00 Location: H 1028

Discussion

BP 27: Cell Mechanics II

Time: Thursday 9:30–12:45 Location: H 1028

Invited Talk BP 27.1 *(7)* Thu 9:30 H 1028

Size and Mechanical Scaling of Blood Platelets — Aastha Mathur, Sandra Correia, Serge Dmitrieff, Romain Gibeaux, Iana Kalinina, Tooba Quidwai, Jonas Ries, and •Francois Nedelec — EMBL Heidelberg

Blood platelets play a major role in hemostasis, the process of stopping blood loss from injured vessels. Platelets have a discoid shape while floating free in the blood in the so-called resting state but come in various sizes, ranging from 1.6 to 5 micrometers. I will argue that their size, in this case, can be understood from the competition between the elasticity of a circular bundle of microtubules, and surface tension at the cell edge. Such a mechanical equilibrium predicts a scaling law that is verified by imaging a large number of individual platelets live, from Mouse and Human blood samples. I will then discuss the dynamics that is observed at the onset of platelet activation, on the path towards platelet adhesion and aggregation. The microtubule ring maintaining the shape of platelets initially coils but is later able to recover within 30 minutes. This can be understood as the ring is made of multiple microtubules that are dynamically connected, and can respond both elastically or viscously. Importantly, given the mechanical properties of these components, we can explain why the overall mechanical response of platelets is dependent on their size, a fact that is known to be important for the physiology of platelets in vivo.

BP 27.2 *(23)* Thu 10:00 H 1028

Active prestress leads to an apparent linear stiffening of the cytoskeleton through geometrical coupling and shear-induced nematic alignment — •Elisabeth Fischer-Friedrich — Biotec, TU Dresden, Tatzberg 47-49, 01307 Dresden, Germany

Tuning of active prestress e.g. through activity of molecular motors constitutes a powerful cellular tool to adjust cellular stiffness through nonlinear material properties. Understanding this tool is an important prerequisite for our comprehension of cellular force response, cell shape dynamics and tissue organization. Experimental data obtained from cell-mechanical measurements often show a simple linear dependence between mechanical prestress and measured differential elastic moduli corresponding to a power law with exponent one. While these experimental findings could point to the theoretically predicted "pull-out" of soft bending modes, we propose here a surprisingly simple alternative explanation. In a theoretical study, we show how active prestress in the cytoskeleton gives rise to a linear increase of measured cellular force response and resulting apparent stress-stiffening through geometrical-coupling and shear-induced nematic alignment. We argue that a new experimental paradigm is required to separate this apparent stress-stiffening from actual nonlinearities in prestressed biological materials.

BP 27.3 *(227)* Thu 10:15 H 1028

Mechanical strain sensing in rod-shaped Escherichia coli — •Lars Renner[1], Felix Wong[2], Gizem Özbaykal[3], Sven van Teeffelen[3], and Ariel Amir[2] — [1]Leibniz Institute of Polymer Research Dresden — [2]Harvard University, Cambridge, USA — [3]Institut Pasteur, Paris, France

Why bacteria have evolved and maintained their specific shapes is a central question in bacterial cell biology. Bacteria are remarkably successful in achieving a precise shape and tightly coordinating cellular processes such as DNA replication, protein production and cell division, yet the underlying biophysical cues and the evolutionary advantage for one shape over another are largely unknown. We are setting out to understand how rod-shaped bacteria maintain their shape when subjected to mechanical deformation. In particular, we explore how mechanical force changes the bacteria morphology and consequently affects the bacterial shape after the mechanical force is released. We combine microfabrication tools and mathematical models to analyse cell shape recovery of E. coli with intentionally modified cell morphology under mechanical stress. When confined, cells are readily adapting to the new morphology. When released, bacterial cells recover their straight, rod-shaped morphologies. We find a straightening rate that is approximately twice the growth rate. By developing a theory of residual stresses, we identify mechanical stress-based nucleation of new growth sites to explain the enhanced straightening rate. Our results indicate a stress-based mechanism for shape regulation in rod-shape bacteria.

BP 27.4 *(325)* Thu 10:30 H 1028

Poroelastic two-phase model for moving droplets of Physarum polycephalum with free boundaries — •Dirk Alexander Kulawiak[1], Jakob Löber[3], Markus Bär[2], and Harald Engel[1] — [1]Institut für Theoretische Physik, TU Berlin, Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden Germany

Motivated by recent experiments, we model the flow-driven amoeboid motility that is exhibited by protoplasmic droplets of Physarum. Here, a feedback loop between a chemical regulator, active mechanical deformations, and induced flows give rise to spatio-temporal contraction patterns that result in directed motion. Our model describes the droplet's cytoskeleton as an active viscoelastic solid phase that is permeated by a passive viscous fluid representing the cytosol. The active tension in the solid phase depends on the concentration of a regulating agent that is advected by the fluid phase. Previously, it was shown that under rigid boundary conditions that impose a fixed shape, this model reproduces a large variety of mechano-chemical patterns such as antiphase oscillations and rotating spirals. This in line with experimental observations of contraction patterns in these droplets. Here, we present an approach that includes free boundary conditions, nonlinear friction between droplet and substrate and a nonlinear reaction kinetic for the regulator to model the movement of these droplets. We find deformations of the droplet boundary as well as oscillatory changes in the droplets position with a net motion in each cycle.

BP 27.5 *(104)* Thu 10:45 H 1028

The Mechanics of Vesicle Blebbing — •Sebastian Hillringhaus, Gerhard Gompper, and Dmitry A. Fedosov — Institute of Complex Systems, Forschungszentrum Jülich, Jülich, Germany

A broad range of *in silico* models, including liquid and viscoelastic drop models, has been introduced for simulating the complex mechanical properties of different cell types. These models are used to understand and quantify experimental measurements. In this work, we employ a coarse-grained cell model in two and three dimensions which incorporates the membrane properties similar to the RBC-model and an elastic inner mesh to include the cytoskeletal properties. The model is formulated in the framework of the dissipative particle dynamics simulation method. It is used to investigate cell-blebbing, which is observed in synthetic vesicles. Cell-blebbing describes the dissociation of the membrane from the inner network, in this case as result of inner stress. We analyze the influence of different parameters on the blebbing process and show that the occurrence of blebbing is a result of the instability of the connection between membrane and actin-network.

30 min. break

BP 27.6 *(114)* Thu 11:30 H 1028

Simulations of stem cells in microjets — •Carina Bezold, Christian Bächer, and Stephan Gekle — Biofluid Simulation and Modeling, Bayreuth, Germany

3D bioprinting offers the opportunity to create tissues and organs which could be used for transplantation. The tissue is built up layer for layer by a continuous jet containing stem cells.We develop a model for stem cells as elastic spheroids, using tools of the finite element method. We validate our model using the Hertzian theory for small deformations. To simulate the fluid, we use 3D Lattice-Boltzmann simulations including the transition from the printer nozzle into the free liquid jet. This region is of particular interest since high extensional forces are present. Due to the different flow profiles at the transition we observe a change in the cell shape.

BP 27.7 *(299)* Thu 11:45 H 1028

Induction of cytoplasmic flows reveals: asymmetric cell division is a digital decision based on gradually varying PAR polarization states — M. Mittasch[1], M. Nestler[2], P. Gross[3], A. Fritsch[1], M. Kar[1], S. Grill[3], A. Voigt[2], and •M. Kreysing[1] — [1]MPI-CBG — [2]Dept. of Mathematics, TUD — [3]Biotec, TUD (all Dresden)

Throughout the last decades, access to genetic perturbations boosted our molecular-level understanding of cell biological processes. However, it was suggested that the spatio-temporal organization of cells and developing embryos also depends on physical transport processes, which remains an experimental challenge to confirm.

Here we present *Focused light induced cytoplasmic streaming* (FLUCS) which enables the dynamic control of cytoplasmic flows in cells and developing embryos via thermoviscous expansion phenomena (Weinert & Braun, J Appl Phys 2008). FLUCS allows to systematically dissect the role of flows during PAR polarization. We find that i) cytoplasmic flows towards the membrane drive PAR loading locally, ii) cytoplasmic flows parallel to the membrane induce cortical flows. iii) Control over cortical flows enables to move pre-established PAR domains. iv) We find that small displacements of PAR domains are self-corrected and cells divide normally. v) For rotations beyond 90 degrees, however, we observe a flip of the PAR defined body axis, followed by inverted asymmetric cell divisions. Our results suggest that asymmetric cell division is a digital decision based on a gradually varying PAR polarization states. Ref: Mittasch et al (accepted).

BP 27.8 *(362)* Thu 12:00 H 1028

Entropic swelling of chromatin drives neutrophil extracellular trap release — •Daniel Meyer[2,3], Elsa Neubert[1,2], Luise Erpenbeck[1], and Sebastian Kruss[2,3] — [1]Department of Dermatology, Venereology and Allergology, University Medical Center, Goettingen University, Germany — [2]Institute of Physical Chemistry, Göttingen University, Germany — [3]Center for Nanoscale Microscopy and Molecular Physiology of the Brain (CNMPB), Göttingen, Germany

Neutrophilic granulocytes are the most abundant immune cells in humans and essential to defeat pathogens. They can release their own DNA as neutrophil extracellular traps (NETs) to capture and eliminate bacteria, fungi and viruses. DNA expulsion (NETosis) has also been documented for other immune cells but also for amoebas and plant cells, and has been implicated in many diseases, including cancer, vascular and chronic inflammatory disorders.

During NETosis, neutrophils undergo dynamic and dramatic alterations of their cellular as well as sub-cellular morphology whose biophysical basis is poorly understood. We investigated NETosis in real-time on the single-cell level using high-resolution fluorescence and atomic force microscopy. Our results show that NETosis is highly organized into distinct phases with a clearly defined point of no return. Entropic chromatin swelling is the major driving force and the reason for cell morphology changes, mechanical changes and the rupture of both nuclear envelope and plasma membrane. Through its material properties, chromatin thus directly and actively orchestrates this biological process.

BP 27.9 *(267)* Thu 12:15 H 1028

Effect of Arp2/3 on 3D migration and cellular mechanical properties — •Stefanie Puder, Tom Kunschmann, and Claudia Tanja Mierke — Biological Physics Division, Peter Debye Institute for Soft Matter Physics, University of Leipzig, Germany

Cellular motility is essential in many physiological processes such as tissue repair during wound healing. The migration of cells in 3D extracellular matrices (ECM) is regulated by the actin cytoskeleton. The actin related protein complex Arp2/3 facilitates nucleation and polymerization of new actin branches, which is supposed to impact cellular mechanical properties. However, whether Arp2/3 affects cellular mechanical properties and subsequently migration of cells is not well understood. We suggested that the Arp2/3 complex facilitates 3D motility into ECM by regulating cellular mechanical properties. Our study focuses on Arp3 conditional knock-down fibroblast cells induced by 4-OH-tamoxifen. Cells are analyzed for their ability to migrate in dense 3D ECM. The knock-down of Arp3 accompanies with a significant reduced invasiveness. Cellular mechanical properties are quantified by an optical cell stretcher and AFM resulting in comparable characteristics of cellular deformability and Young's modulus. We found that Arp3 knock-down cells are less deformable (stiffer) compared to control treated cells in both presented techniques. In conclusion, Arp2/3 complex and its subunit Arp3 are essential for providing mechanical cellular stiffness regulating motility into 3D ECM. We demonstrated that Arp2/3 regulates cellular deformability, stiffness and transmission promoting Arp2/3-dependent cell invasion.

BP 27.10 *(253)* Thu 12:30 H 1028

Influence of matrix and cellular properties on human cancer cell migration in 3D biomimetic matrices — •Tony Fischer and Claudia Tanja Mierke — Universität Leipzig, Peter-Debye-Institut

3D cellular motility in connective tissue is a fundamental process during tissue development and cancer progression, mostly studied in biomimetic in vitro models. Crucial factors for cancer metastasis are cellular motility and mechanical properties of the migrating cell and topology and elasticity of the surrounding matrix. ECM and cell properties are altered in many tumors as stiffness of the matrix and cells is linked to malignancy and metastasis. Different ECM models and quantifying algorithms exist to measure matrix topology, cell elasticity, motility and cell-matrix interactions. We used a collagen I ECM model comprised of rat tail collagen building elongated fibrils and bovine dermal collagen building node-shaped scaffolds to adapt to local inhomogeneities. Pore-size and topology was analyzed using a euclidean distance map approach to bubble analysis and a gel reconstruction algorithm using fuzzy-connectedness. Elastic properties of both cells and gels were determined using AFM. Cellular motility was analyzed using an invasion assay. Cell-mediated fiber displacement was determined using optical flow measurements. Our findings show that stiffer matrices indeed enhanced cellular motility. Malignant MDA-MB-231 cancer cells were softer, more motile and deformed their surrounding ECM more than less invasive MCF-7 cells. We are able to study cancer cell migration and mechanotransduction in our ECM model with tunable topology and mechanics and measure topological influences.

BP 28: Single Molecule Biophysics

Time: Thursday 9:30–13:00 Location: H 1058

BP 28.1 *(42)* Thu 9:30 H 1058

Cell free protein synthesis systems and single molecule fluorescence studies: a perfect marriage — Alexandros Katranidis[1], Mayuri Sadoine[1], Noemie Kempf[1], Michael Gerrits[2], Michele Cerminara[1], and •Jörg Fitter[1,3] — [1]Research Centre Juelich, ICS-5, Juelich, Germany — [2]TU Berlin, Biocatalysis Group, Department of Chemistry, Berlin, Germany — [3]RWTH Aachen University, I. Physikalisches Institut (IA), AG Biophysik, Aachen, Germany

Protein synthesis is a fundamental cellular process, by which ribosomes decode genetic information and convert it into an amino acid sequence. This highly complex process does not necessarily require cell integrity, but can also proceed in so called cell-free protein systems. This opens the door for comprehensive studies to obtain a deeper understanding of individual steps of the translation cycle and of the folding of de novo synthesized proteins. The use of cell-free protein synthesis (CFPS) systems allowed us to watch some of these essential steps in real time and on single molecule level [1,2]. On the other hand the open nature of the CFPS system allows the production of tailor-made protein samples, perfectly suited for single molecule Förster resonance energy transfer (smFRET) studies [3]. Examples from both above mentioned topics will be presented and demonstrate the strength of combining CFPS with single molecule fluorescence studies.

[1] A. Katranidis et al., Angewandte Chemie Int. Edit., 48, 1758-1761, (2009); [2] N. Kempf et al., Sci. Rep., 7, 46753, (2017); [3] M. Sadoine et al., Anal. Chem., 89, 11278-11285, (2017)

BP 28.2 *(55)* Thu 9:45 H 1058

Coiled Coils as structural building blocks: A sequence-based approach towards tuning Coiled Coil mechanics — •Patricia López-García, Melis Göktas, and Kerstin G. Blank — Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

The natural abundance of coiled coil (CC) motifs in cytoskeleton and extracellular matrix proteins suggests that CCs play an important role as passive (structural) and active (regulatory) mechanical building blocks. It is well established that modifications in CC sequence, e.g. in hydrophobic core or solvent-exposed residues, are responsible for the thermodynamic stability of CCs; however, nothing is known

about how these factors affect CC mechanics.

With the goal of shedding light on the sequence-structure-mechanics relationship of CCs we have chosen thermodynamically well-characterized sequences and analyzed their mechanical stability using single molecule force spectroscopy, applying force parallel to the helical axis in the shear geometry. Modifications in the hydrophobic core or the helix propensity alter the binding potential with different outcomes: a less tightly packed hydrophobic core increases the potential width without significantly affecting the barrier height (koff). In contrast, a reduced helix propensity decreases both potential width and barrier height. Our goal is to use this information for developing a library of mechanically characterized CCs that can be applied as calibrated building blocks for a wide range of applications: from molecular force sensors to mechanosensitive material crosslinks in protein nanostructures and synthetic ECM mimics.

BP 28.3 *(153)* Thu 10:00 H 1058

Tuneable reversibility in force probe simulations — •Stefan Jaschonek and Gregor Diezemann — Institut für Physikalische Chemie, Duesbergweg 10-14, 55128 Mainz

In this talk a detailed study of the dependence of force probe molecular dynamics (FPMD) simulations on the pulling parameters is presented. As a model system, the well studied calix[4]arene catenane dimer was chosen. This system consists of two "cups", the calixarene structure, which are mechanically locked by aliphatic loops of tuneable length, realized by a catenane structure. The dimer shows reversible rebinding meaning that the opening and the rebinding transition can be monitored. Due to the tuneable loop length it is possible to gain full control over the energy landscape. The kinetics of the system can be understood in terms of a two state model for shorter loops (≤ 14 CH_2 units) and a three state model for longer loops (≥ 17 CH_2 units).

The impact of a systematical variation of the pulling parameters, the pulling velocity V and the stiffness K, of the externally applied potential and the loop length of the system are discussed. Furthermore the characteristic unbinding and rebinding forces are analyzed and the kinetic rates are extracted.

BP 28.4 *(384)* Thu 10:15 H 1058

Non-Markovian bond kinetics and its application in dynamic force spectroscopy — •Jakob Tómas Bullerjahn[1,2], Sebastian Sturm[2], and Klaus Kroy[2] — [1]Max-Planck-Institut für Biophysik, Frankfurt am Main, Germany — [2]Universität Leipzig, Institut für theoretische Physik, Leipzig, Germany

Single-molecule force spectroscopy data are conventionally analyzed using a schematic model, wherein a molecular bond is modeled as a virtual particle diffusing in a one-dimensional free-energy landscape. This simplistic but efficient approach is unable to account for the "anomalous" bond-breaking kinetics increasingly observed in high-speed force spectroscopy experiments and simulations, such as a non-exponential distribution of bond lifetimes under constant load. In the traditional framework, the only remedy has been to postulate a multitude of intermediate states. Here, we introduce a complementary approach, namely a rigorous extension of the one-dimensional standard theory that accounts for the transient dynamics of a generic set of coupled degrees of freedom. These "hidden modes" affect the reaction dynamics in various ways, depending on their relaxation spectrum. We find exact analytical expressions for pertinent experimental observables, such as the mean rupture force and the rupture force distribution, in two asymptotic limits. They become unconditionally exact at high loading rates, thus providing us with a microscopically consistent theory of rapid force spectroscopy that avoids the usual Markov assumption.

Invited Talk BP 28.5 *(12)* Thu 10:30 H 1058

Multiplexed Magnetic Tweezers: From DNA Mechanics to Retroviral Integration — •Jan Lipfert, Franziska Kriegel, Willem Vanderlinden, and Philipp Walker — Department of Physics and Center for Nanoscience, LMU Munich, Germany

Magnetic tweezers are a powerful tool to probe single DNA molecules and their complexes with proteins under controlled forces and torques at the single molecule level. Using a parallelized version of magnetic tweezers that can measure torque directly, we have carried out high-precision torque measurements of DNA mechanics. Our results indicate that the intrinsic torsional stiffness does not change with mono- or divalent ion concentration and is approximately independent of temperature, for temperatures well below the melting temperature. Quantitative comparison of high-resolution single molecules measurements to coarse-grained simulations of DNA mechanics shows that taking into account the anisotropy of DNA and introducing a non-zero twist-bend coupling significantly improves agreement with torque measurements. In addition, we demonstrate that all-atom molecular dynamics simulations correctly predict the temperature-dependence of DNA twist and of DNA torsional stiffness, if the most recent force fields are used. Going beyond bare DNA, we have developed a magnetic tweezers assay to follow retroviral integration in real time, revealing several critical steps along the integration free energy landscape. In particular, we find an ultra stable strand transfer complex that suggests the role of a resolving factor in vivo.

15 min. break

BP 28.6 *(75)* Thu 11:15 H 1058

Interaction of DNA structures with ectoine: a molecular dynamics simulation study — •Ewa Anna Oprzeska-Zingrebe and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

In nature, the cellular environment of DNA composes not only of water and ions, but also of salts, lipids and other cosolutes, which can exert both stabilizing and destabilizing influence on the formation and existence of particular DNA higher-order forms. Among them, ectoine, known as osmoprotectant occurring naturally in halophilic bacteria and other microorganisms exposed on severe osmotic stress, turns out to be of particular importance. In our research, we investigate the behavior of a short 7-bp DNA oligonucleotide with the sequence d(GCGAAGC) in both linear and folded form, as well as 24-bp B-DNA duplex in aqueous solution with various concentrations of ectoine. Our results demonstrate a DNA conformation-dependent binding behavior, which allows us to rationalize the structure-stabilizing influence of ectoine.

BP 28.7 *(395)* Thu 11:30 H 1058

Pressure effect on the conformational landscapes of a large loop DNA hairpin in the presence of osmolyte and salt — Satyajit Patra[1], Vitor Schuabb[1], •Irena Kiesel[1], Jim Marcel Knop[1], Rosario Oliva[2], and Roland Winter[1] — [1]Fakultät für Chemie und Chemische Biologie, TU Dortmund, Otto-Hahn-Str. 6 — [2]Department of chemical sciences, University of Naples Federico II, Via Cinita, 80126 Naples, Italy

The conformational landscapes of a large loop DNA hairpin model system has been investigated in absence and presence of salt and osmolytes at both ambient and extreme conditions (high hydrostatic pressure and high temperature) using primarily single molecule Förster resonance energy transfer (smFRET) technique. We use cationic salts (K^+, Mg^{2+}, Co^{3+}) and TMAO and urea as osmolytes. Introduction of pressure favors the open state (low FRET species) of this DNA hairpins thus facilitates the unfolding. Addition of the salt in the solution populates the high FRET species and counteract the pressure and temperature effect. The order of stabilizing effect of the salt against pressure and temperature follows the order $Co^{3+} > Mg^{2+} > K^+$. Introduction of urea and temperature favors the formation of intermediate state populations which is further supported by smFRET measurement under immobilized condition. This is indicating that the free energy landscapes of this large loop DNA hairpin is actually a rugged one. Further smFRET measurement under immobilized condition provides a deeper insights into the differential stabilization mechanism of salt and osmolytes.

BP 28.8 *(24)* Thu 11:45 H 1058

DNA strand break yields by OH-radicals, low energy electrons and prehydrated electrons — •Marc Benjamin Hahn[1,2], Tihomir Solomun[2], and Heinz Sturm[2,3] — [1]Freie Universität Berlin — [2]Bundesanstalt für Materialforschung und -prüfung — [3]Technische Universität Berlin

Radiation damage to biomolecules such as DNA, is the reason to treat cancer *via* radiation therapy. The understanding of the molecular processes and the quantification of the underlying damaging mechanisms is necessary to develope more efficient irradiation protocols for cancer therapy. Thereby damage to DNA is of key interest due to its central role in reproduction and mutation. Due to the high amount of water in biological tissue, most of the damage is caused by the secondary particles which are produced by the interaction of ionizing radiation with water. Thereby a multitude of species are produced, e.g. kinetic low energy electrons, prehydrated electrons, OH-radicals and ions. The quantification of the contribution to DNA damage by

the various species is of interest. Here we present an experimental approach to disentangle their relative DNA strand break yields. Plasmid DNA (*pUC19*) is irradiated in water with electrons under the presence of different scavengers. The presented preliminary results reveal the relative contributions of OH-radicals, low energy electrons and prehydrated electrons and their DNA single and double strand break yields.

BP 28.9 *(216)* Thu 12:00 H 1058

Detection of nanoscale biological samples using Nanocapillaries — •Tobias Jäckering[1], Marco Radukic[2], Dario Anselmetti[1], and Martina Viefhues[1] — [1]Experimental Biophysics, Physics Faculty, Bielefeld University, Bielefeld, Germany — [2]Biotechnological Faculty, Bielefeld University, Bielefeld, Germany

Filamented borosilicate glass capillaries can be pulled down to 40 nm diameter nanopipettes with the ability of easy filling the nanopipette via capillary forces. These nanopipettes were used for the detection and analysis of nanometer sized biological analytes by monitoring the electric (ionic) current during translocation through the nanopipette. We applied either electrophoretic or hydrodynamic driving forces to investigate different types of analytes like DNA and adeno-associated viruses (AAV).

To differentiate the detected signal from the background it is essential to adjust the nanopore-size of the nanopipette to the respective analytes size. Additionally the respective buffer has a significant effect on the measurement. We will demonstrate that these nanoscopic coulter-counter experiments allow to distinguish various analytes like DNA and AAV.

BP 28.10 *(129)* Thu 12:15 H 1058

Antenna-enhanced fluorescence correlation spectroscopy resolves calcium-mediated lipid-lipid-interactions — •Stephan Block[1,2], Srdjan S. Aćimović[1], Nils Odebo Länk[1], Mikael Käll[1], and Fredrik Höök[1] — [1]Chalmers University of Technology, Göteborg, Sweden — [2]Freie Universität Berlin, Berlin, Germany

Fluorescence correlation spectroscopy (FCS) has provided a wealth of information on the composition, structure, and dynamics of cell membranes. However, it has proved challenging to reach the spatial resolution required to resolve biophysical interactions. Herein, we form artificial cell membranes on dimeric, nanoplasmonic antennas, which shrink the FCS probe volume down to the 20 nm length-scale. By analysing fluorescence bursts from individual fluorescently tagged lipids moving through the antenna hot spots, we show that the confinement of the optical readout volume below the diffraction limit allows the temporal resolution of FCS to be increased by up to 3 orders of magnitude. Employing this high spatial and temporal resolution to probe diffusion dynamics of individual dye-conjugated lipids, we further show that lipid molecules diffuse either as single entities or as pairs in the presence of calcium ions. Removal of Ca2+ by addition of EDTA almost completely removes the complex contribution, in agreement with previous theoretical predications on the role of Ca2+ in mediating transient interactions between zwitterionic lipids. We envision that antenna-enhanced FCS will enable to resolve a broad range of challenging membrane biophysics questions, such as stimuli-induced lipid clustering and membrane protein dynamics.

BP 28.11 *(176)* Thu 12:30 H 1058

Visualizing cellular secretion dynamics with single protein sensitivity — •Katharina König[1,2], André Gemeinhardt[1], Matthew P. McDonald[1], and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen — [2]Friedrich Alexander University Erlangen-Nuremberg, Erlangen

Cellular secretion of proteins and exosomes into the extracellular environment is an essential mediator of critical biological mechanisms, including cell-to-cell communication, immunological response, targeted delivery, and differentiation. Here, we report a novel methodology that allows for the real-time detection and imaging of single unlabeled proteins and exosomes that are secreted from individual living cells. This is accomplished via interferometric detection of scattered light (iSCAT), and is first demonstrated with human B cells that are found to actively secrete IgG antibodies at a rate of ca. 100 molecules per second. Importantly, iSCAT signals can be measured at extremely high speeds (up to MHz for small nanoparticles), enabling the measurement of single cell secretion dynamics with sub-second temporal resolution and single protein sensitivity. Such experimental capabilities are unmatched by any contemporary proteomic method. We furthermore show the generality of the technique through the study of T cell cytokine secretion, Leishmania parasite exosome release, and single-cell lysate analysis. Our results establish iSCAT imaging as a powerful label-free tool for studying the real-time exchange between cells and their immediate environment with single protein sensitivity.

BP 28.12 *(251)* Thu 12:45 H 1058

Reductive caging and photoactivation in single-molecule Förster resonance energy transfer experiments — •Atieh Aminian Jazi[1], Evelyn Ploetz[2], Muhamad Arizki[1], Christine Ziegler[4], Reinhard Krämer[4], and Thorben Cordes[1,3] — [1]Zernike Institute for Advanced Materials, Groningen, The Netherlands — [2]Department of Chemistry and CeNS, Ludwig Maximilians-Universität, Munich, Germany — [3]Department Biology I, Ludwig-Maximilians-Universität München, Germany — [4]Institute of Biophysics and Biophysical Chemistry, Universität Regensburg,Germany

Förster-resonance energy transfer(FRET), in combination with single-molecule detection, has become a powerful tool to investigate the structural dynamics of biomolecular systems. We used caging of fluorophores by reversible chemical deactivation of fluorescence.

The diffusing molecules can be reactivated by ultraviolet (UV) light. UV-reactivation allows retrieving both FRET-related distances and sorting of multiple intramolecular spices in solution-based smFRET. We employed caged FRET to investigate the structure of a membrane transporter BetP, as multi-subunit protein, and nucleic acids containing more than two fluorescent labels. The results revealed that chemical caging and photoactivation (uncaging) by UV light allows temporal uncoupling of convoluted fluorescence signals from multiple donors or acceptor molecules.Caged FRET also can be used in a further application to study the intermolecular details of low-affinity binding interactions with diffusion-based smFRET.

BP 29: Statistical Physics of Biological Systems I (joint session BP/DY)

Time: Thursday 9:30–13:00 Location: H 2013

BP 29.1 *(43)* Thu 9:30 H 2013

Thermodynamic bounds on the ultra- and infra-affinity of Hsp70 for its substrates — •Basile Nguyen[1,2], David Hartich[1], Paolo De Los Rios[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany — [2]Laboratory of Statistical Biophysics, Institute of Physics, School of Basic Science and Institute of Bioengineering, School of Life Sciences, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

The 70 kDa heat shock protein Hsp70 has several essential functions in living systems, such as protecting cells against protein aggregation, assisting protein folding, remodeling protein complexes, and driving translocation into organelles. These functions require high affinity for nonspecific amino acid sequences that are ubiquitous in proteins. It has been recently shown that this high affinity, called ultra-affinity, depends on a process driven out of equilibrium by ATP hydrolysis. Here, we establish the thermodynamic bounds for ultra-affinity, and further show that the same reaction scheme can in principle be used both to strengthen and to weaken affinities (leading in this case to infra-affinity). We show that cofactors are essential to achieve affinity beyond the equilibrium range. Finally, we consider small GTPases which can benefit from infra-affinity to optimize intracellular signal transduction.

[1] B. Nguyen, D. Hartich, U. Seifert and P. De Los Rios (2017), *Biophys. J.* 113, 362-370

BP 29.2 *(81)* Thu 9:45 H 2013

A reaction center driven by entropy — •Franz-Josef Schmitt, Zuleyha Yenice Campbell, Mai Vi Bui, and Thomas Friedrich — Technische Universität Berlin, Sekr. PC 14, Straße des 17. Juni 135, 10623 Berlin

The phototrophic cyanobacterium *Halomicronema hongdechloris* contains chlorophyll *a* and *f* in photosystem II. The ratio of Chl *f* to Chl

a is reversibly changed from 1:8 under illumination with far red light (720-730 nm) to a very low level of Chl f under white-light culture conditions. Phycobiliproteins exhibit highly efficient excitation energy transfer (EET) to Chl a and from there to Chl f within 200 ps apparent transfer time if *H. hongdechloris* grown under far red light is illuminated with 630 nm laser radiation which is absorbed by phycobilisomes. However excitation energy localized on Chl f shows long lifetime of more than 1 ns. Questions arise about composition of the reaction center and possible primary charge separation driven by Chl *f*. Our Simulations and thermodynamic considerations suggest that the time- and wavelength-resolved ps fluorescence data can be explained assuming light-induced far red-shifted traps of excitation energy localized on Chl f in the light harvesting antenna while the large majority of Chl a is strongly coupled to these Chl f traps driving the uphill EET from Chl f to Chl a by entropic force.

BP 29.3 *(193)* Thu 10:00 H 2013

Shape of pinned polymer loops in an external force field — •Wenwen Huang[1], Yen Ting Lin[2], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Los Alamos National Laboratory, New Mexico, USA

We studied the shapes of pinned polymer loops subjected to a constant external force field. We show that the polymer density profile can be calculated analytically in agreement with the simulation results. Moreover, we calculated the distribution of gyration radius and found it to vary non-monotonically with the strength of the external force field: the distribution is broader for moderate forces and more narrow for strong and weak forces. Furthermore, we analyzed the gyration tensor of the polymer loop characterizing its overall shape and in particular two parameters called asphericity and the nature of asphericity. These parameters, along with the gyration radius, can be used to quantify experimental data.

BP 29.4 *(83)* Thu 10:15 H 2013

The labyrinth-like shapes of nasal cavities arise from physical and geometrical constraints — •David Zwicker[1,2], Rodolfo Ostilla-Mónico[2], Daniel E. Lieberman[2], and Michael P. Brenner[2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Harvard University, Cambridge, USA

Although the nasal cavity is vital for heating and humidifying inhaled air in all vertebrates, its shape varies widely across animals. To understand this variability, we here connect nasal geometry to its function by theoretically studying the airflow and the associated scalar exchange that describes heating and humidification. We show that optimal geometries, which have minimal resistance for a given exchange efficiency, are narrow with a uniform gap width. Our prediction for the gap width matches measured values over a large range of animal sizes. Moreover, we show that geometric constraints imposed by the head can be satisfied with the observed labyrinth-like geometries, which perform almost as well as the optimal shapes without the constraints. Taken together, our theory explains the geometric variations of natural nasal cavities quantitatively and we hypothesize that the trade-off between high exchange efficiency and low resistance to airflow is the main driving force shaping the nasal cavity.

BP 29.5 *(197)* Thu 10:30 H 2013

Cell polarization in elliptical geometry: how does C. Elegans determine its first axis? — •Raphaela Gessele, Jacob Halatek, and Erwin Frey — Department of Physics, Ludwig-Maximilians-Universität München, 80333 Munich, Germany

Cell polarity defines axes that guide cell differentiation and division. In the single cell state of the Caenorhabditis Elegans embryo, PAR protein patterns determine the anterior-posterior axis which further guides the first cleavage. Experiment and theory have indicated that mutual binding inhibition of (anterior) aPAR and (posterior) pPAR proteins is the key mechanism of polarity maintenance by the PAR reaction-diffusion network. Strikingly, our analysis of the reaction-diffusion dynamics in (elliptical) cellular geometry shows that mutual inhibition alone does not lead to a stable polarity along the long (anterior-posterior) axis of the cell but generically favors polarity by aPAR and pPAR protein domains aligned with the short axis. We find that the geometry adaption of the patterning process depends on an intricate interplay between attachment-detachment dynamics on the one hand, and cytosolic reactivation on the other hand. Our findings show that the local ratio of membrane surface to cytosolic bulk volume is the main geometric cue to which patterns adapt. Furthermore, an inactive phase after membrane detachment can switch the preferred polarity axis - The decisive parameter for switching is the diffusion length of the inactive phase. In conclusion, our studies reveal the crucial role of geometry for self-organized pattern formation. Geometry should be explicitly considered in models for intracellular pattern formation.

BP 29.6 *(385)* Thu 10:45 H 2013

A Spheroidal Squirmer in Shear Flow — •Kai Qi[1], Elmar Westphal[2], Gerhard Gompper[1], and Roland G. Winkler[1] — [1]Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Jülich Centre for Neutron Science, Forschungszentrum Jülich, D-52425 Jülich, Germany

Squirmers are generic models for microswimmers like bacteria and algae. The behavior of a spheroidal squirmer [1, 2] in shear flow is studied by hydrodynamic simulations via the multiparticle collision dynamics [3] approach. Due to the elongated shapes of spheroids, alignment along the shear direction is observed for both passive spheroidal colloids and squirmers in the weak shear flow. When the shear rate exceeds a critical value, alignment changes from the shear to the vorticity direction. The alignment transition reveals a clear dependence on the hydrodynamic dipole of the swimmer's flow field. Pullers with a large positive force-dipole coefficient exhibit gradual variations of the alignment direction, whereas abrupt changes are found for pushers with a large negative coefficient. Comparison between elongated and spherical squirmers reveals a significant shape dependence of their behaviors in shear flow.

[1] M. Theers, E. Westphal, G. Gompper, and R. G. Winkler, Soft Matter **12**, 7372 (2016).

[2] J. Elgeti, R. G. Winkler, and G. Gompper, Rep. Prog. Phys. **78**, 056601 (2015).

[3] G. Gompper, T. Ihle, D. M. Kroll, and R. G. Winkler, Adv. Polym. Sci. **221**, 1 (2009).

15 min. break

Invited Talk BP 29.7 *(15)* Thu 11:15 H 2013

Protein Pattern Formation: Rethinking Nonlinear Dynamics — •Erwin Frey — Ludwig-Maximilians-Universität München, München, Germany

Protein pattern formation is essential for spatial organization of many intracellular processes like cell division, flagellum positioning, and chemotaxis. More generally, these systems serve as model systems for self-organization, one of the core principles of life. We present a rigorous theoretical framework able to generalize and unify pattern formation for quantitative mass-conserving reaction-diffusion models. Within this framework, separation of diffusive mass redistribution on the level of conserved species provides a general mathematical procedure to decompose complex reaction-diffusion systems into effectively distinct functional units, and to reveal the general underlying bifurcation scenarios. We apply this general framework to a range of specific intracellular pattern forming protein networks, and show how it facilitates the identification of general self-organisation principles.

BP 29.8 *(100)* Thu 11:45 H 2013

Self-organised length oscillations of cellular protrusions — Mareike Bojer[1,2], •Isabella Graf[1], and Erwin Frey[1] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Munich, Germany — [2]present address: Department of Physics, Technische Universität München, Garching, Germany

We consider a stochastic non-equilibrium model which is inspired by the interplay of directed transport and diffusive motion of molecular motors in growing and shrinking cellular protrusions like filopodia. Based on this model we investigate the effect of finite diffusion in a half-closed geometry and show that it can lead to temporal patterns in the form of oscillating system length. We examine the dynamics of the system length in terms of the growth rate of the protrusion and identify two different limits: For small growth rate, the system length changes very stochastically and our analytic prediction, using a so-called adiabatic assumption, agrees well with the result from numerical simulations. For larger growth rate, however, temporal patterns occur. More concretely, we observe quasi-periodic changes in length in a parameter regime where motor mixing (diffusion) is slow compared with the shrinkage dynamics. We provide an intuitive picture for the origin of this pattern-forming mechanism which relies on the closure

of the system at the dynamic end of the protrusion and the resulting particle conservation.

BP 29.9 *(130)* Thu 12:00 H 2013

Force sharing between elastically coupled molecular motors — •Mehmet Can Ucar and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14476 Potsdam, Germany

Molecular motors are nano-scale machines that drive many essential processes within the living cell such as the organization of the mitotic spindle, the powering of flagella and cilia, and the long-distance transport of cellular cargos. These motor proteins frequently work in teams of multiple motors and can collectively generate large forces, but the underlying mechanism of force generation and force sharing remains controversial. Here we address this question by introducing a new model for cargo transport by elastically coupled molecular motors. For a system of two identical motors acting against an antagonistic motor or an optical trap, we find that motors share the generated forces almost equally among the members of the same team. The model furthermore provides a new explanation for observed forces in different in vitro studies.

BP 29.10 *(145)* Thu 12:15 H 2013

Statistical inference of bacterial chemotaxis strategies — •Maximilian Seyrich[1], Zahra Alirezaei[2], Carsten Beta[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam, Germany

Bacteria like *E. coli* move with alternating runs and tumbles. Modern imaging techniques provide a high-throughput access to these run-and-tumble trajectories. However, good tumble recognition analysis is still a bottleneck and needs to set a-priori threshold parameters. We present a high-throughput inference technique, which allows to infer all swimming parameters of the bacterium without such a need.

We set up a random-walk model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed extending our previous work [1]. The dynamics of the swimming direction is described by enhanced rotational Brownian motion during tumbling, while thermal and shot noise together with a relaxational drift analogously to an Ornstein-Uhlenbeck process govern the speed dynamics. In order to infer the relevant swimming parameters, moments and autocorrelation functions are calculated for our model and matched to the ones determined from experimental trajectories. We first show that our method identifies the classical bacterial chemotaxis strategy of *E. coli*, i.e., the tumble rate decreases when swimming along the chemical gradient. We also find evidence that a fast subpopulation of *E. coli* reduces its mean tumble angle in this direction.

[1] O. Pohl *et al.*, PLoS Comp. Biol. **13**, 1 (2017).

BP 29.11 *(180)* Thu 12:30 H 2013

Chemoattractant induced transient adaptation in the oscillatory cytoskeleton of motile amoeboid cells. — •Jose Negrete JR[1,2], Alain Pumir[3,4], Christian Westendorf[4], Marco Tarantola[4], Eberhard Bodenschatz[4,5,6], and Carsten Beta[7] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [3]École Normale Supérieure de Lyon, Lyon, France — [4]Max Planck Institute for Dynamics and Selforganization — [5]University of Göttingen, Göttingen, Germany — [6]Cornell University, Ithaca, USA — [7]University of Potsdam, Potsdam, Germany

Dictyostelium discoideum presents oscillatory actin polymerization cycles which amplitude is mostly given by noise. We investigate the transient response on the actin polymerization activity in Dictyostelium discoideum induced by a short pulse of cAMP. The stimulation induces a transient response, of reduced amplitude and frequency, which time duration is stochastic and varies between cells. To model the observed actin behavior, we extend the description of noisy oscillator by introducing an inhibitory variable that acts as a timer for the transient phase.

BP 29.12 *(179)* Thu 12:45 H 2013

Evolution of carrying capacity and extinction of populations in a stochastic system — •Hye Jin Park[1], Yuriy Pichugin[1], Weini Huang[2], and Arne Traulsen[1] — [1]Max Planck Institute for Evolutionary Biology, Plön, Germany — [2]Barts Cancer Institute, London, United Kingdom

Once a mutant emerges in the population, new interactions are drawn between types, which may lead to changes in the population size. Using the game theory, we implement this population dynamics in a stochastic system. Since interactions between types are described by a game payoff matrix, the emergence of a mutant is interpreted as extending the payoff matrix. New equilibria can emerge by the change of the payoff matrix. If the population settles to a new equilibrium state, the population size changes. We examine the change of population size in time and quantify the extinction risk by the mean time to extinction.

BP 30: Focus Session: Complex Contagion Phenomena I (joint session SOE/DY/BP)

Contagion processes are stochastic dynamical systems that are ubiquitous in natural and engineered systems and their fundamental understanding is of crucial importance for prediction and control of large-scale system behavior. A classical example of a contagion process is the spread of infectious diseases. In addition, in recent years, there has been also an increased scientific interest in so-called social contagion phenomena, which is largely fueled by the rise of digital communication in online social platforms. New challenges that arise due to the digital transformation of communication can be addressed by developing new concepts like collective risk perception.

(Session organizers and chairs: Philipp Hövel, Pawel Romanczuk, and Jonathan Donges)

Time: Thursday 9:30–13:15 Location: MA 001

See SOE 18 for details of this session.

BP 31: Microswimmers DY II (joint session DY/CPP/BP)

Time: Thursday 10:00–13:15 Location: BH-N 243

See DY 59 for details of this session.

BP 32: Anomalous Diffusion (joint session DY/BP)

Time: Thursday 10:00–13:15 Location: BH-N 334

See DY 60 for details of this session.

BP 33: Cytoskeletal Filaments II

Time: Thursday 15:00–17:15 Location: H 1028

BP 33.1 *(109)* Thu 15:00 H 1028

High resolution three-dimensional tracking with optical tweezers reveals protofilament switching of the kinesin-8 Kip3 — •Michael Bugiel and Erik Schäffer — Zentrum für Molekularbiologie der Pflanzen (ZMBP), Universität Tübingen, Auf der Morgenstelle 32, 72076 Tübingen, Germany

The budding yeast kinesin-8 Kip3 is a highly processive motor protein that walks to the ends of cytoskeletal microtubules and shortens them in a collective manner. Microtubules consist of circularly arranged tubulin polymer chains, called protofilaments. How exactly Kip3 reaches the end is unclear. Left-handed rotations of microtubules in Kip3 gliding assays indicated sideward motion of Kip3 perpendicular to the microtubule axis, i.e. switching between single protofilaments. We used high resolution optical tweezers in a force-feedback mode to track the trajectories of single Kip3 motors. Previous 2D assays with alternating sideward loads showed that Kip3 performs sideward steps in both directions, consistent with a diffusive sideward motion on the microtubule lattice. Here, we topographically suspended microtubules such that Kip3-coated microspheres can freely rotate around the microtubules in three dimensions. Tracking these motor driven microspheres with a 3D, zero-load force-clamp showed that Kip3 switched protofilaments in discrete steps equally frequent in both directions. A statistical analysis confirmed a diffusive sideward motion of Kip3, consistent with the 2D results. The diffusive protofilament switching may enable Kip3 to bypass obstacles and reach the microtubule end for length regulation.

BP 33.2 *(319)* Thu 15:15 H 1028

Visualizing acto-myosin dynamics and vortices at a membrane surface using interferometric scattering microscopy — •Darius V Köster[1,2], Nikolas Hundy[3], Gavin Young[3], Adam Fineberg[3], Philipp Kukura[3], and Satyajit Mayor[1,4] — [1]NCBS, Bangalore, India — [2]Warwick Medical School, Warwick, UK — [3]University of Oxford, Oxford, UK — [4]InStem, Bangalore, India

The plasma membrane and the underlying cytoskeletal cortex constitutes an active platform for many cellular processes. Recent work has shown that acto-myosin dynamics modify the local membrane organization, but the molecular details are not well understood due to difficulties with experimentally accessing the associated time and length scales. Here, we use interferometric scattering (iSCAT) microscopy to investigate a minimal acto-myosin network linked to a supported lipid bilayer membrane. Using the magnitude of the interferometric contrast, which is proportional to molecular mass, we detect, image and distinguish actin and myosin filaments. As a result, we can follow the diffusion of single actin filaments attached to the bilayer revealing different types of diffusion depending on filament length and quantify binding kinetics and processivity as a function of ATP concentrations, providing new evidence for the theoretically predicted behavior of ensembles of myosin head domains. Simultaneous observation of long-term network flow and organization enables us to link changes in myosin II filament dynamics with decreasing ATP concentrations to a switch in the acto-myosin network from a remodeling, fluid state to a contractile, and observe the formation of vortices as predicted by theory.

BP 33.3 *(111)* Thu 15:30 H 1028

Size-dependent phagosomal transport depends on microtubules, actin filaments and associated motors — •Steve Keller, Konrad Berghoff, and Holger Kress — University of Bayreuth, Bayreuth, Germany

The internalization and intracellular degradation of pathogens by macrophages is an essential part of the mammalian immune response. The associated intracellular transport of the phagosome from the cell periphery to the perinuclear region is crucial for the phagosome maturation. To date biochemical factors are known to influence the fate of phagosomes. Here we show that the phagosomal transport is also strongly influenced by the size of the phagosomes and that this size-dependent transport depends on microtubules, actin filaments and associated motors. We found that large phagosomes are transported very persistently to the nucleus with almost no centrifugal motion, whereas small phagosomes show strong bidirectional transport. Our investigation of the molecular basis of this size-dependent transport suggests that dynein motors and the intracellular distribution of microtubules strongly influence the centripetal transport of large phagosomes. Additionally, our findings indicate that actin filament-associated motors and the distribution of actin filaments strongly influence the bidirectional transport of small phagosomes. Our findings suggest that a simple size-dependent cellular sorting mechanism might exist that supports inward transport of large phagocytosed bacteria for facilitating their digestion and that simultaneously supports outward transport of small bacterial fragments for example for antigen presentation.

Invited Talk BP 33.4 *(4)* Thu 15:45 H 1028

Dynamics and instabilities of contractile actin networks in artificial cells — •Kinneret Keren — Physics Department, Technion-Israel Institute of Technology, Haifa 32000, Israel

Contractile actin network have an essential role in many cellular processes including cell division, intracellular transport and cell motility. While the molecular components involved are largely known, we still do not understand what controls the large scale properties of these networks. We generate bulk actin networks by introducing cytoplasmic Xenopus egg extracts, which contain all the components of the actin machinery, into cell-sized water-in-oil droplets. Importantly, the presence of turnover in our system allows these networks to attain a dynamic steady state characterized by contractile actin flows which persist for hours. We find that under a broad range of conditions, the network undergoes homogenous contraction despite large spatial variations in network density, and that this contraction rate is inversely proportional to the actin disassembly rate. We observe either a symmetric state in which the network contracts towards the center of the droplets and exhibits a spherically symmetric density and flow pattern, or a polar state in which the contraction center is localized near the droplet's boundary. In the symmetric state, the contraction center is actively maintained near the middle of the droplet, reminiscent of actin-based centering mechanisms found in living cells. During symmetry breaking, the system transitions from this symmetric state to a polar state, mimicking cellular symmetry breaking as seen for example during motility initiation or spindle migration in mammalian oocytes.

BP 33.5 *(166)* Thu 16:15 H 1028

Rotational movement of microtubules driven by thermal forces and by kinesin-5 motors leads to mitotic spindle formation — •Ivana Ban[1], Marcel Prelogović[1], Lora Winters[2], Iva Tolić[2,3], and Nenad Pavin[1] — [1]Faculty of science, University of Zagreb, Croatia — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Division of Molecular Biology, Ruder Bošković Institute, Zagreb, Croatia

During mitosis, the spindle divides chromosomes between two daughter cells. In the fission yeast Schizosaccharomyces pombe, the rod shaped mitotic spindle is composed of antiparallel microtubules (MTs) emanating from two opposite spindle poles, whose formation is mediated by motor proteins. A key question is what are the physical principles underlying the formation of a mitotic spindle. Here we show, experimentally and theoretically, that MTs at one pole search for a MT from the other pole by performing random rotational movement around the spindle pole. When MTs from opposite poles get into close proximity, motor proteins start to accumulate in the region where MTs are close to each other. In our model, minus end directed motors generate forces that drive the formation of an antiparallel MT bundle, thereby forming the mitotic spindle. We identified experimentally the kinesin-5 motor Cut7 as the main force generator in this process. In conclusion, random rotational motion helps MTs from opposite poles to find each other and subsequent accumulation of kinesin-5 motors allows them to generate forces that drive spindle formation.

BP 33.6 *(274)* Thu 16:30 H 1028

Bistability and oscillations in cooperative microtubule and kinetochore dynamics in the mitotic spindle — •Felix Schwietert and Jan Kierfeld — TU Dortmund University, 44221 Dortmund, Germany

In the mitotic spindle microtubules attach to kinetochores via catch bonds during metaphase. We investigate the cooperative dynamics of a one-sided spindle model consisting of a microtubule ensemble which is attached to a kinetochore via elastic linkers. The model includes

the dynamic instability of microtubules, forces on microtubules and kinetochores from elastic linkers, and an external force on the kinetochore. We use a mean-field approach based on Fokker-Planck equations to analytically solve the one-sided spindle model, which establishes a bistable force-velocity relation of kinetochore motion. All results are in agreement with stochastic simulations. We derive constraints on linker stiffness and microtubule number for the occurrence of bistability. In the full two-sided spindle model, two such bistable systems are coupled in a tug-of-war. This leads to stochastic chromosome oscillations in metaphase (directional instability), which have been observed in several experiments. We also derive constraints on linker stiffness and microtubule number for metaphase chromosome oscillations. With certain modifications the model can be used to explain the effects of additional processes, e.g. microtubule poleward flux or polar ejection forces.

BP 33.7 *(309)* Thu 16:45 H 1028

Bending dynamics of single-walled carbon nanotubes in viscoelastic media — •Kengo Nishi[1], Fred MacKintosh[2,3,4], and Christoph Schmidt[1,5] — [1]Third Institute of Physics - Biophysics, University of Göttingen, 37077 Göttingen, Germany — [2]Department of Chemical & Biomolecular Engineering, Rice University, Houston, TX 77005, USA — [3]Center for Theoretical Biological Physics, Rice University, Houston, TX 77030, USA — [4]Department of Physics and Astronomy, Vrije Universiteit, 1081HV Amsterdam, The Netherlands — [5]Department of Physics, Duke University, Durham, NC 27707, USA

The mechanics and dynamics of cells and tissues are dominated by semi-flexible polymer networks, whose bending stiffness leads to non-trivial dynamics. Micron-sized beads are commonly used in microrheology approaches to measure the viscoelasticity of such systems. Insertion of such probes can lead to artefacts and is often not possibly in confined geometries in living cells. Here we introduce the use of single-walled carbon nanotubes (SWNTs), themselves semi-flexible polymers with non-photobleaching near-infrared fluorescence, as multiscale stealth probes for microrheology. We investigate the bending dynamics of SWNTs embedded in viscoelastic media and analyze their thermally driven shape fluctuations. We find that we can describe the bending dynamics of SWNTs by a Langevin equation with a bending term and a time-dependent memory function.

BP 33.8 *(50)* Thu 17:00 H 1028

Tensile elasticity of a hinged wormlike chain — •Panayotis Benetatos — Kyungpook National University, Daegu, South Korea

It is known that local defects in the bending rigidity of double-stranded DNA, such as denaturation bubbles or singe-stranded nicks, significantly affect its configurational properties and elastic response. In this talk, we present an analytic calculation (within the weak bending approximation) of the force-extension relation of a wormlike chain with a fixed hinge defect. We show that the gain in configurational entropy allowed by the defect has a significant effect on the stretching compliance of the polymer. Our results apply to any pair of semiflexible segments connected by a hinge. As such, they may also be relevant to cytoskeletal filaments (F-actin, microtubules), where one may treat the cross-link connecting two filaments as a hinge defect.

P. Benetatos, Phys. Rev. E 96, 042502 (2017)

BP 34: Neuroscience

Time: Thursday 15:00–17:30 Location: H 1058

Invited Talk BP 34.1 *(20)* Thu 15:00 H 1058

How do we learn? Synaptic Plasticity across multiple time scales — •Wulfram Gerstner — EPFL Lausanne

If we memorize a French word that is new to us, if we learn to play table tennis, if we meet our new boss, at all these occasions the connections between neurons in our brains change. These changes, called synaptic plasticity, happen on several different time scale: induction can be rapid (sometimes a single event is sufficient), but the stabilization of changes takes much longer. In this talk, I will overview mathematical models of synaptic plasticity that cover different temporal scales - and I will indicate how plasticity models can (or cannot) lead to functional memories.

BP 34.2 *(34)* Thu 15:30 H 1058

Spike rate models derived from recurrent networks of adaptive neurons — •Moritz Augustin, Josef Ladenbauer, Fabian Baumann, and Klaus Obermayer — Technische Universität Berlin, Germany

The spiking activity of single neurons can be well described by a nonlinear integrate-and-fire model that includes somatic adaptation. When exposed to fluctuating inputs sparsely coupled populations of these model neurons exhibit stochastic collective dynamics that can be effectively characterized using the Fokker-Planck equation. Here we derive from that description four simple models for the spike rate dynamics in terms of low-dimensional ordinary differential equations using two different reduction techniques: one uses the spectral decomposition of the Fokker-Planck operator, the other is based on a cascade of two linear filters and a nonlinearity, which are determined from the Fokker-Planck equation and semi-analytically approximated. We evaluate the reduced models for a wide range of biologically plausible input statistics and find that both approximation approaches lead to spike rate models that accurately reproduce the spiking behavior of the underlying adaptive integrate-and-fire population. The low-dimensional models also well reproduce stable oscillatory spike rate dynamics that are generated either by recurrent synaptic excitation and neuronal adaptation or through delayed inhibitory synaptic feedback. The derived spike rate descriptions retain a direct link to the properties of single neurons, allow for convenient mathematical analyses of network states, and are well suited for application in large-scale brain network models.

BP 34.3 *(171)* Thu 15:45 H 1058

Modeling the electrical activity of pacemaker neurons: from milliseconds to days — •Pablo Rojas and Martin Garcia — Theoretical Physics, Universität Kassel, 34132 Kassel, Germany

Molecular circadian oscillators in pacemaker neurons consist of interlocked feedback loops in gene transcription. Membrane electrical activity is regulated by genetic, and consequently exhibits a circadian pattern, but the mechanisms for this are object of current research [1]. Despite the usefulness of Hodgkin-Huxley model, few work has been done to account for a long-time behavior of membrane electrical activity[2]. Pacemaker neurons show autonomous circadian oscillations, but new properties emerge in the collective behavior [3]. Several properties found in electrophysiology recordings have been suggested to be linked to functional biological implications [4]. We propose an extension of the Hodgkin-Huxley scheme, that allows for computing the dynamics of electrical activity over long times, enabling inputs from molecular clock as well as coupling between neurons. Our results and predictions are discussed with the analysis of long-term in vivo electrophysiology recordings from Leucophaea maderae accessory medulla. Our model has been able to reproduce distinct patterns found in experimental data, and hint possible functional implications for the described behavior.

[1] CN Allen et al. Cold Spring Harb Perspect Biol 2017;9:a027714
[2] C Vasalou and MA Henson . PLoS Comput Biol 6(3) (2010)
[3] DK Welsh et al. Annu Rev Physiol. 2010 ; 72: 551-577.
[4] G Werner. Front Physiol. 2010; 1: 15.

BP 34.4 *(390)* Thu 16:00 H 1058

Optimal detection of a localized perturbation in random networks of integrate-and-fire neurons — •Davide Bernardi[1,2] and Benjamin Lindner[1,2] — [1]Bernstein Center for Computational Neuroscience, Berlin, Germany — [2]Humboldt University, Berlin, Germany

Cortical networks operate in a chaotic regime, as both theoretical and experimental studies have shown. Therefore, neural coding is believed to rely on the mean activity of many cells. However, there is evidence that the brief stimulation of a single neuron can elicit a behavioral response, a theoretically unexplained result. We study how large recurrent networks of integrate-and-fire neurons react to the perturbation of one single cell and propose a simple readout mechanism to detect the perturbation. Biasing the readout towards specific neurons leads to detection rates similar to experimentally observed values, as our numerical simulations and analytical estimates show. We observe

near-optimal detection for intermediate values of the mean coupling between neurons. Current research aims to capture how detection rates depend on the temporal structure of the stimulation.

Ref: Bernardi and Lindner, *Phys. Rev. Lett.* **118** (2017)

BP 34.5 *(386)* Thu 16:15 H 1058

Nonlinear response of noisy neurons — •Benjamin Lindner and Sergej Voronenko — Humboldt Universität Berlin

We study the firing rate modulation of stochastic neurons in response to mixtures of periodic signals. For the leaky integrate-and-fire neuron with white Gaussian background noise, we calculate analytically the second order (weakly nonlinear) response of the instantaneous firing rate. We inspect several situations in which the nonlinear contributions shape the response significantly and a purely linear analysis would fail qualitatively. We demonstrate that similar effects are observed for a biophysically more realistic system, the NaK Izhikevich model endowed with channel noise.

Ref.: Voronenko & Lindner New J. Phys. 19, 033038 (2017)

BP 34.6 *(88)* Thu 16:30 H 1058

A memristive plasticity model of voltage-based STDP suitable for recurrent bidirectional neural networks in the hippocampus — •Nick Diederich[1,2], Thorsten Bartsch[2], Hermann Kohlstedt[1], and Martin Ziegler[1] — [1]Technische Fakultät, Christian-Albrechts-Universität zu Kiel — [2]Neurologie, Universitätsklinikum Schleswig-Holstein

Memristive systems have gained considerable attention in the field of neuromorphic engineering, since they allow the emulation of synaptic functionality in solid state nano-physical systems. In this talk it will be shown that memristive behaviour provides a working framework for the phenomenological modelling of cellular synaptic mechanisms. For this purpose, the basic characteristics of memristive systems, i.e. the volatility and history-dependence of prior applied electrical signals, are used to derive a voltage-based plasticity rule. We show that this model is suitable to account for a variety of electrophysiology plasticity data. To show the network capabilities of the plasticity model, the plasticity model was incorporated into the circuitry of the hippocampal subfields. The obtained results are discussed in the framework of the processing of mnemonic information in the hippocampus.

Financial support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

BP 34.7 *(139)* Thu 16:45 H 1058

Interkinetic nuclear migration as a stochastic process in the zebrafish retina — •Anne Herrmann[1], Afnan Azizi[2], Salvador J. R. P. Buse[2], Yinan Wan[3], Philipp J. Keller[3], William A. Harris[2], and Raymond E. Goldstein[1] — [1]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge, United Kingdom — [2]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, United Kingdom — [3]Howard Hughes Medical Institute, Janelia Research Campus, Ashburn, VA, USA

In recent years evidence has been increasing that retina development is governed by stochastic processes rather than being tightly regulated. In this context, both the varying numbers of offspring from a single progenitor cell as well as the distributions of final cell fates have been explained using simple probabilistic models. We focus on interkinetic nuclear migration (IKNM), a movement of nuclei between the apical and basal surfaces of the cells in developing pseudostratified epithelia, that was first observed more than 80 years ago. Since, IKNM has been studied in multiple organisms but despite these efforts many questions about the role and precise mechanism of this process remain unsolved. We combine *in vivo* light sheet microscopy and theoretical models and develop a quantitative description of IKNM in the zebrafish retina. Our findings support the hypothesis of IKNM as a stochastic process. Given that IKNM has been suggested to play a regulatory role in cell differentiation, these results have important implications for understanding the organisation of developing vertebrate tissues.

BP 34.8 *(337)* Thu 17:00 H 1058

Control of Wave Propagation in Neural Field Equations — Alexander Ziepke, •Steffen Martens, and Harald Engel — Technische Universität Berlin, Institut für Theoretische Physik, 10623 Berlin, Germany

The investigation of neural fields, describing dynamics of large networks of synaptically coupled neurons by means of continuous field equations, has gained interest over the last decades. In particular, neural field systems exhibit self-organized spatio-temporal structures, such as stationary and traveling fronts and pulses, spiral waves, and localized spot-like bump solutions. This makes them a convenient tool to describe various neural processes, such as working memory, motion perception and visual hallucinations, to name a few. Due to the important applications of neural field models, the question arises how to effectively control solutions in these systems.

In order to address this problem, we extend analytic control techniques, previously derived for reaction-diffusion systems [J. Löber, PRL **112**, 148305; arXiv:1703.04246], to neural field equations. The proposed open-loop control scheme enables shifting and rotating traveling bump and wave solutions according to a prescribed protocol of motion while simultaneously conserving their shape. Noteworthy, the control signal solely depends on the profile and velocity of the unperturbed solution, and thus, for applying the control scheme, a detailed knowledge of the internal dynamics is not required.

BP 34.9 *(258)* Thu 17:15 H 1058

Predicting animal behavior from neural dynamics — •Monika Scholz, Ashley N. Linder, and Andrew M. Leifer — Department of Physics and Princeton Neuroscience Institute, Princeton, NJ, USA

How does a nervous system control animal behavior? While models of behavior and neural computation exist, investigating the connection experimentally is challenging in even the simplest organisms. It is only recently that tools have become available to image the behavior and neural dynamics simultaneously in the roundworm *C. elegans*. Its small nervous system with only 302 neurons and stereotyped behaviors allow us to probe how well simple models perform in predicting behavior from neural dynamics alone. We use a suite of microscopy tools and a calcium-sensitive fluorescent protein to image the activity of a large number of neurons in the animal's brain during locomotion. Using a linear model, we predict forward and backward velocity as well as turns and turn direction from neural activity. I will show our progress and discuss the implications for understanding neural computation in a model organism.

BP 35: Statistical Physics of Biological Systems II (joint session BP/DY)

Time: Thursday 15:00–17:15 Location: H 2013

BP 35.1 *(222)* Thu 15:00 H 2013

Do Predator attacks tune a collective of interacting agents to criticality and why? — •Pascal Klamser[1,2] and Pawel Romanczuk[1,2] — [1]Institute for Theoretical Biology, Department of Biology, Humboldt-Universität zu Berlin — [2]Bernstein Center for Computational Neuroscience, Humboldt-Universität zu Berlin

Based on theoretical considerations it is hypothesized that biological systems self-tune to criticality [1]. Motivated by this, we investigate the collective behavior of self-propelled agents at the phase transition from an ordered (parallel moving agents = *school*) to a disordered movement (*swarm*) and their reaction to a predator. Systematic numerical simulations show that at the phase transition the performance of the predator decreases. However, this decrease is not only caused by a better response of individuals to the predator, but also by complex spatial structures of the collective at the transition. This finding emphasizes the need of explicitly considering spatial models to describe biological systems, e.g. fish swarms. Beside different interaction-networks (voronoi, k-nearest neighbor, visual-field) an evolutionary algorithm was used to check for the relevance of the results.

[1] Mora, T. and Bialek, W. J Stat Phys (2011) 144: 268.

BP 35.2 *(397)* Thu 15:15 H 2013

Intermittent collective behavior in small groups of gregarious animals — •Luis A. Gómez[1], Richard Bon[2], and Fernando Peruani[1] — [1]Laboratoire J. A. Dieudonné, Université Côte d'Azur, Nice, France — [2]Centre de Recherches sur la Cognition Animale, Université Paul Sabatier, Toulouse, France

Collective behavior of small groups of gregarious animals is our subject of interest. Experiments with small groups of merino sheep showed interesting features like periodicity of moving and resting phases, synchronization of these phases at the individual level, collective stick–slip dynamics and cohesivity of the group around the center of mass. We show some experimental evidence obtained from the tracking of individual sheep that suggests that the no motion phase of the individuals is qualitatively different to the motion phase. In particular, we discover that a refractory period can be associated to the no motion phase. We propose the introduction of a 3-state model in order to describe the experimental observations for several group sizes (2, 3, 4 and 8 individuals) and study the temporal evolution. Although the model is proposed at the individual level, repercussions at the collective level emerge.

BP 35.3 *(270)* Thu 15:30 H 2013

How a well-adapting immune system remembers — •Andreas Mayer[1], Vijay Balasubramanian[2], Thierry Mora[3], and Aleksandra Walczak[3] — [1]Princeton University, Princeton, USA — [2]University of Pennsylvania, Philadelphia, USA — [3]Ecole normale superieure, Paris, France

The adaptive immune system uses its past experience of pathogens to prepare for future infections. How much can the adaptive immune system learn about the statistics of changing pathogenic environments given its sampling of the antigenic universe? And how should it best adapt its repertoire of lymphocyte receptor specificities based on its experience? Here, to answer these questions we propose a view of adaptive immunity as a dynamic Bayesian machinery that predicts optimal repertoires based on past pathogen encounters and knowledge about typical pathogen dynamics. Two key experimentally observed characteristics of adaptive immunity emerge naturally from this model: (1) a negative correlation between fold change of protection upon a challenge and preexisting immune levels and (2) differential regulation of memory and naive cells. We argue that to explain the benefits of immune memory, antigenic environments need to be highly sparse. We derive experimentally testable predictions about the diversity of the memory repertoire over time in such sparse antigenic environments. The Bayesian perspective on immunological memory provides a unifying conceptual framework for a number of features of adaptive immunity and suggests further experiments.

BP 35.4 *(313)* Thu 15:45 H 2013

Asymmetric Link detection via a generalized ESABO approach — •Jens Christian Claussen — Computational Systems Biology, Jacobs University Bremen, Germany

Mutualisms in biological populations are widespread from bacteria to mammals. Mutualistic interactions can be positive (synergistic) or negative. Often even in microbial data the number of available samples is marginally sufficient to allow for detection of interactions, especially for the low-abundance species that may carry important information in clinical context. The recently introduced ESABO method (PloS Comp Biol 13: e1005361 (2017)) utilizes an information-theoretic approach to evaluate binarized abundances and was demonstrated to detect interaction links that were not apparent in the classical correlation analyses. ESABO provides high (resp. low) scores if joint occurence is higher (resp. lower that in surrogate data. As so far, ESABO concludes on negative interactions when co-occurrence is lower than expected. However, this can be due to asymmetric (unidirectional parasitic) interaction in any of two directions, or due to symmetric interactions. Here we generalize the ESABO method to analyze co-abundance data resolving for asymmetry between the interactions.

BP 35.5 *(330)* Thu 16:00 H 2013

Modelling the Emergence of Robustness and Evolvability in Genotype-Phenotype Maps — •Marcel Weiss[1,2] and Sebastian E. Ahnert[1,2] — [1]Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, UK — [2]Sainsbury Laboratory, University of Cambridge, UK

Genotype-Phenotype (GP) maps play an important role in evolution and their properties fundamentally affect the outcome of evolutionary processes. A striking property found in several GP maps, such as that of RNA secondary structure, is the positive correlation between the robustness and evolvability of phenotypes, meaning that a phenotype can be strongly robust against mutations and at the same time evolvable to a diverse range of alternative phenotypes. By introducing two analytically tractable GP map models that follow the principles of real biological GP maps, we study the characteristics that cause this positive correlation between phenotype robustness and evolvability. We find that it only emerges if mutations can have non-local effects on sequence constraints, highlighting that these effects are likely to be an important feature of many biological GP maps.

Invited Talk BP 35.6 *(16)* Thu 16:15 H 2013

Out-of-equilibrium response of soft and biological matter to forces and deformation — •Claus Heussinger — Institut für theoretische Physik, Universität Göttingen

In the talk I will give a few examples from our research concerning the complex dynamical response of soft and biological materials to perturbations via forces or deformation. The systems we study are, in general, far from thermal equilibrium. Phenomena will range from the emergence of flow instabilities (shear-banding, rheo-chaos) in complex fluids, over the visco-elasto-plastic behavior of biological cells and their sub-cellular components, to the fluid-to-solid jamming transition in a-thermal granular particles. The goal is to define suitable model systems where the relevant physical mechanisms can be identified and understood. To this end we use different simulation tools going hand in hand with analytical modeling and, whenever possible, experimental verification.

BP 35.7 *(383)* Thu 16:45 H 2013

Mechanical tuning of synaptic patterns enhances immune discrimination — •Milos Knezevic[1,2] and Shenshen Wang[1] — [1]Department of Physics and Astronomy, University of California Los Angeles, Los Angeles, CA 90095, USA — [2]Institut fur Theoretische Physik, Technische Universitat Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

An immunological synapse is an adhesive intercellular junction that forms between B cells and antigen-presenting cells (APCs) during recognition. This dynamic surface contact is patterned with complementary receptors and ligands on the apposing membranes, thus specifically regulating directed information transfer. Via synapses, B cells use mechanical pulling forces to extract antigen (Ag) from APCs for subsequent processing and presentation. Recent experiments show that, depending on the stage in its life cycle, a B cell exhibits distinct synaptic patterns accompanied with different strength and timing of force usage, which appears to lead to varied stringency of affinity discrimination. Using a minimal model of membrane adhesion, we study how the observed synaptic architectures can originate from normal mechanical forces coupled to lateral organization of mobile receptors, and show how this coupling might affect the efficiency and selectivity of Ag acquisition. We conclude that cytoskeletal forces could play an important role in tuning the synaptic patterns, which in turn enlarges the dynamic range of immune recognition with enhanced discrimination.

BP 35.8 *(416)* Thu 17:00 H 2013

Specialisation and plasticity in interacting biological populations — Solenn Patalano[1], •Adolfo Alsina[2], Steffen Rulands[2], and Wolf Reik[1] — [1]Babraham Institute, Cambridge, UK — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The structure and dynamics of biological systems are tightly regulated on multiple scales, from transcriptional and epigenetic regulation to population level feedback. While many biological systems are surprisingly robust against environmental fluctuations they, simultaneously, exhibit a remarkable plasticity in response to changes in their environment. Using the social wasp Polistes as an example we combine experimental and theoretical methods to study how a primitive society simultaneously achieves phenotypic specialisation and a remarkable degree of plasticity. After perturbing the society by queen removal, we experimentally follow the relaxation dynamics into the social steady state across scales, from social and behavioural measurements to physiological measurements and detailed molecular characterisations of single wasps. We develop a theoretical framework that explains the emergence of the social structure of Polistes as a result of opposing dynamics on the molecular and the population scales. We show that such dynamics provide a general principle of how both specialization and plasticity can be achieved in biological systems. As well as elucidating mechanisms of epigenetic plasticity in wasps and other biological systems this study shows that the multiscale dynamics in primitive social insects provide a laboratory for non-equilibrium physics.

BP 36: Cell Adhesion and Migration, Multicellular Systems II

Time: Friday 9:30–12:00 Location: H 1028

Invited Talk BP 36.1 *(8)* Fri 9:30 H 1028

Physical forces driving migration, division and folding in epithelial sheets — •Xavier Trepat — IBEC, Baldiri Reixac 15-21, 08028 Barcelona

Biological processes such as morphogenesis, tissue regeneration, and cancer invasion are driven by collective migration, division, and folding of epithelial tissues. Each of these functions is tightly regulated by mechanochemical networks and ultimately driven by physical forces. I will present maps of cell-cell and cell-extracellular matrix (ECM) forces during cell migration and division in a variety of epithelial models, from the expanding MDCK cluster to the regenerating zebrafish epicardium. These maps revealed that migration and division in growing tissues are regulated cooperatively. I will also present direct measurements of epithelial traction, tension, and luminal pressure in three-dimensional epithelia of controlled size and shape. By examining epithelial tension over time-scales of hours and for nominal strains reaching 300%, we establish a remarkable degree of tensional homeostasis mediated by cellular adaptations.

BP 36.2 *(307)* Fri 10:00 H 1028

Simultaneous Modeling of Random Crawling and Internal Polarization of Motile Amoeboid Cells — •Sergio Alonso[1], Maike Stange[2], and Carsten Beta[2] — [1]Department of Physics, Universitat Politecnica de Catalunya, Barcelona, Spain — [2]Institute of Physics and Astronomy, Universität Potsdam, Potsdam, Germany

The amoeboid motion of certain cells gives rise to different dynamics depending on the level of starvation. This motion is correlated with the patterns of diverse biochemicals in the interior of the cells. We compare first the displacement and the velocity of vegetative and starving cells of Dictyostelium discoideum with a simple model of individual cells. Second, the deformations of the membrane is studied in the numerical model and in the living cells, and finally, we study the patterns originated in the interior of the simulated cells and compare them with the actin patterns observed in the experiments. Therefore, we fit and adapt the parameter values of the model to correctly account for the motion of the centre of mass of the cell and the intracellular pattern formation.

BP 36.3 *(239)* Fri 10:15 H 1028

Intricate features of 3D cancer cell invasion — •Frank Sauer[1], Steffen Grosser[2], Josef A. Käs[2], and Claudia T. Mierke[1] — [1]Biological Physics Division, Peter Debye Institute for Soft Matter Physics, University of Leipzig, Germany — [2]Soft Matter Physics Division, Peter Debye Institute for Soft Matter Physics, University of Leipzig, Germany

The invasion and the motility of cells into 3D tissues is often connected to cell shape changes and pathologists typically diagnose cancer from cell shape or tissue architecture anomalies. However, the correlation between cell shapes and tissue properties and their influence on cancer cell motility is still not well understood. We developed live invasion assays that allow us to analyze the 3D migration pathway of single cells or cells invading from spheroids into tunable collagen gels on statistically relevant cell numbers. Cell shape information can be correlated with migration patterns, invasion depth and matrix properties. Our results show that the invasiveness and the aspect ratio of single invasive MDA-MB-231 cells is drastically reduced by increasing collagen concentration, whereas clusters of the same cells show a distinct contraction and densification of the collagen network prior to invasion followed by a subsequent degradation. On spheroids from non-invasive MCF7 cells only minor network deformations and no invasion or fiber degradation was observed. Our findings support the view that the mechanical properties of the extracellular matrix are a key factor to initiate cancer cell evasion from cell masses such as spheroids, however, they can also act as an obstacle for single cell migration.

BP 36.4 *(294)* Fri 10:30 H 1028

The Physics of Blastoderm Flow during Early Gastrulation of Tribolium castaneum — •Stefan Münster[1,2,3], Alexander Mietke[1], Akanksha Jain[2], Pavel Tomancak[2], and Stephan Grill[1,3] — [1]MPI for Physics of Complex Systems — [2]MPI of Molecular Cell Biology and Genetics — [3]TU Dresden

The early embryo of the red flour beetle, Tribolium castaneum, initially consists of a single-layered blastoderm covering the yolk uniformly that differentiates into an embryonic rudiment as well as extraembryonic amnion and serosa. The germband anlage forms inside the egg during gastrulation when the embryonic rudiment condenses and folds along the ventral midline; this process is accompanied by large-scale flow and expansion of the extraembryonic serosa which ultimately covers the entire surface of the egg, thus engulfing the growing embryo. The mechanical properties of these tissues and the forces governing these processes in Tribolium, as well as in other species, are poorly understood. Here, we present our findings on the dynamics of myosin in the early blastoderm of Tribolium using multiview lightsheet live imaging of transiently labeled wild type embryos. We quantitatively measure the global distribution of myosin throughout the flow phase and present a physical description that couples the contractile forces generated by myosin to the mechanical properties of the blastoderm. In particular, we describe the overall tissue as a thin, actively contractile, viscous bulk medium that exhibits friction with the vitelline membrane. This description accurately captures the large-scale deformation the tissue undergoes during the initial stages of gastrulation.

BP 36.5 *(339)* Fri 10:45 H 1028

Force generation during collective migration of bacteria — •Benedikt Sabass — Forschungszentrum Jülich, Germany

Bacterial migration, aggregation, and even host infection depend on the generation of mechanical force. Here, we present a first study of bacterial cell-substrate traction using Myxococcus xanthus as a model organism. M. xanthus exhibits two common mechanisms of motility, namely, twitching and gliding. We find that these two mechanisms lead to complementary dynamics and traction patterns. Twitching leads to local, uncoordinated traction while gliding in groups allows for collective emergence of directional traction. The forces generated by each cell are significantly upregulated when cells contact each other in groups, which highlights the importance of cell-cell signaling for collective motility.

Force generation by groups of migrating bacteria
B. Sabass, M.D. Koch, G. Liu, H.A. Stone, J.W. Shaevitz
PNAS, 114(28) : 7266, 2017

BP 36.6 *(373)* Fri 11:00 H 1028

Integrated Heart-on-a-Chip systems: *In situ* characterization of contractile forces in 3D cardiac μ-tissues — •Oliver Schneider, Stefanie Fuchs, Christopher Probst, and Peter Loskill — Department of Cell and Tissue Engineering, Fraunhofer Institute for Interfacial Engineering and Biotechnology IGB, Stuttgart, Germany

Human induced pluripotent stem (iPS) cells possess the power to revolutionize medicine and basic biological research by opening pathways for individualized medicine and large-scale animal-free drug testing. Over the last years, microfluidic Organ-on-a-Chip (OoC) systems evolved from a conceptual idea to a feasible alternative for animal models. OoCs combine iPS-based tissues with microfabrication technologies to create microphysiological *in vitro* models featuring human genetic background, physiologically relevant tissue structure and "vasculature-like" perfusion. Most of these systems, however, lack the ability to thoroughly analyze the integrated tissues and their response to administered drugs. We present a novel integrated device enabling the parallelized cultivation and characterization of human cardiac microtissues in a physiological, precisely controlled environment. By combining traction force microscopy with microfluidic OoC-systems, we are able to extract *in situ* information about the spatial and temporal force distribution in cardiac microtissues. The developed system enables the multiplexed automated analysis of many individualized tissues in parallel, thus bridging the gap from basic tissue creation to viable big data collection.

BP 36.7 *(380)* Fri 11:15 H 1028

Dynamics of Cell Jamming: Disentangling the Shape and Density Dependences — •Jürgen Lippoldt, Steffen Grosser, Paul Heine, Linda Oswald, and Josef Käs — Peter Debye Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Cellular dynamics have been shown to display characteristics of jamming transitions, which originally had been observed as a function of

cell number density (Angelini et al., PNAS 2011). Recently, the Self-Propelled Voronoi (SPV) model has predicted a density-independent transition as a result of the counter play of adhesion and contractile forces (Bi et al., Nat. Phys. 2015), visible in the dimensionless shape parameter.

We use cell tracking combined with Voronoi tessellation of the nuclei to estimate the probability of T1 transitions and neighborhood exchanges. Thereby, we can describe the local fluidity of a cell layer and look for the onset of cellular jamming. A moderately high density is required for epithelial-like MCF-10A cells to jam. Within this high-density regime, the correlation of fluidity and shape of the individual local cells is stronger than the correlation of fluidity and local density. Mesenchymal-like MDA-MB-231 cells stay fluid even for very high densities and never reach the round configurations that correlate to jamming for epithelial-like MCF-10A. In co-culture, both cell types demix and MDA-MB-231 cells form unjammed islands within the jammed collective of MCF-10A cells.

BP 36.8 *(391)* Fri 11:30 H 1028

Temperature gradients characterize, counteract and rescue P granule segregation in *C. elegans* — •Anatol W. Fritsch[1], Matthäus Mittasch[1], Carsten Hoege[1], Frank Jülicher[2], Anthony Hyman[1], and Moritz Kreysing[1] — [1]MPI-CBG, Dresden, Germany — [2]MPI-PKS, Dresden, Germany

Recent studies report on membrane-less condensates in cells, that are formed by liquid-liquid phase separation. In *C. elegans* zygotes condensates, named P granules, segregate asymmetrically to one daughter cell during the first cell division. This process is involved in the development of a functional germ line. More specifically, the asymmetric localization of P granules depends on a protein gradient of MEX-5 along the long axis of the zygote. MEX-5 in turn, is thought to act through an mRNA competition mechanism and locally regulates the phase separation of the of the condensates.

Using a strategy based on the physical principles of phase-separation, we are able to rescue the asymmetric localization of P granules in MEX-5 RNAi mutants with defective segregation *in vivo*. We replace the protein gradient with a localized temperature gradient that mimics the physical mechanisms of the local regulation in phase separation. Furthermore, with this approach, we are able to invert the endogenous spatial distribution of P granules in zygotes. This enables us to study the dynamics of *in vivo* phase separation via controlled physical perturbations. In this study we conclude, that P granule segregation is a spatially tuned, diffusive-flux dependent, evaporation-condensation phenomenon.

BP 36.9 *(401)* Fri 11:45 H 1028

Inversion of rod photoreceptor nuclei improves retinal light transmission by 50% — •Kaushikaram Subramanian[1], Martin Weigert[1], Heike Petzold[1], Marius Ader[2], Irina Solovei[3], and Moritz Kreysing[1] — [1]MPI-CBG, Dresden, Germany — [2]CRTD, Dresden, Germany — [3]LMU, Munich, Germany

Vertebrate retina has a puzzling inverted structure, with 100s of microns of living neural tissue in the light path before its detection by rods and cones. Large number of rods result in densely packed, light scattering nuclei. In nocturnal mammals rods postnatally undergo a hallmark process of nuclear architecture inversion [1]. Previous studies suggest,reduced forward light scattering in isolated rod nuclei and their predicted light focusing was experimentally verified [2].

Now, with high-throughput analysis of wild type and transgenic mouse retina nuclei we establish causality in large angle light scattering and sub nuclear architecture. Using modulation transfer analysis at tissue level, we demonstrate nearly 50% reduction in image detail transfer (Strehl ratio) in transgenic retina lacking nuclear inversion. Modelling and simulation of light propagation reveal a mechanistic relation between single cell scattering and emergent tissue optics. Finally, behavioral studies confirm the visual benefit of inverted nuclear organization for motion detection in low light conditions. Thus, inverted nuclear architecture in mouse retina conclusively improves retinal image transfer and visual function.

References: [1] Solovei et al, Cell(2009) [2] Błaszczak et al, Opt Express(2014) [3] Solovei, et al, Cell(2013)

BP 37: Active Matter (joint session BP/CPP/DY)

Time: Friday 9:30–12:00 Location: H 1058

BP 37.1 *(78)* Fri 9:30 H 1058

Collective cell behavior - a phase field active polar gel model — •Axel Voigt, Simon Praetorius, and Dennis Wenzel — TU Dresden, Institut für Wissenschaftliches Rechnen

We consider a continuum model for collective cell movement. Each cell is modeled by a phase field active polar gel model and the cells interact via steric interactions. We provide a finite element implementation with a parallel efficiency in the number of cells. This is achieved by considering each cell on a different processor and various improvements to reduce the communication overhead to deal with the cell-cell interactions. We demonstrate results for up to 1.000 cells.

BP 37.2 *(97)* Fri 9:45 H 1058

Statistical physics and hydrodynamics of passive/active mixtures — •Raphaël Jeanneret[1], Arnold Mathijssen[2], and Marco Polin[3] — [1]IMEDEA-UIB, Esporles, Spain — [2]Stanford University, Stanford, US — [3]Warwick University, Coventry, UK

In this talk I will present a series of experimental and theoretical results regarding the dynamics of passive particles in liquid bath of active ones. The active particles act here, via the flows they generate, as localized and erratic sources of momentum for the passive beads leading to non-trivial dynamics. Beyond their exciting features for the physicist, active/passive systems are worth studying quantitatively for applications as diverse as the transport of passive entities in cells, biogenic mixing (i.e. mixing of the ocean by living creatures), virus infection, cargo transport (e.g. drug delivery) or self-assembly (e.g. via motility-induced phase separation). The model system I consider is composed of the motile micro-alga Chlamydomonas reinhardtii, a model organism at numerous levels, and polystyrene beads. I will first show that the effective diffusion of micron-sized beads embedded in homogeneous suspensions of algae is greatly enhanced compared to their thermal counterpart. I will then demonstrate how this coarse-grained dynamics can be understood from the near-field hydrodynamics of the swimming organisms via hydrodynamical entrainment events. Finally I will talk about recent results regarding systems of weakly Brownian colloids in spatially heterogeneous suspensions of algae and show how our findings can be used to induce the spontaneous demixing of the two kinds of particles.

BP 37.3 *(184)* Fri 10:00 H 1058

Got worms? Collective feeding in C. elegans — Robert Endres, •Linus Schumacher, Serena Ding, and Andre Brown — Imperial College, London, United Kingdom

Collective behaviour, a hallmark of complex living systems, is often studied in groups of large animals or small cells, but less at the mesoscopic scale. Here, we investigate the collective feeding of the nematode C. elegans, known for its easy genetic manipulation and stereotypic worm postures. In this system, small genetic perturbations can lead to strikingly different population-level behaviors. First, we quantified behavioral differences between the 'solitary' lab strain and a 'social' aggregating mutant strain, using fluorescence imaging and many-worm tracking to probe the dynamics inside aggregates. Second, to understand the mechanism of aggregation, we drew on concepts from motility-induced phase transitions and developed a minimal model. Finally, using this model, we investigated the potential benefits of collective feeding to explain the predominance of aggregating strains in the wild.

BP 37.4 *(269)* Fri 10:15 H 1058

A continuum model to study coordination of tissue growth — •Maryam Aliee, Damir Vurnek, Sara Kaliman, and Ana-Sunčana Smith — Cluster of Excellence: Engineering of Advanced Materials, Friedrich-Alexander-University of Erlangen-Nürnberg

Living organisms represent fascinating and precise structures. It is still a big challenge to understand the mechanisms though which cells interact with each other and the environment to form reproducible patterns. We analyze how tissue growth is controlled by cell properties putting

together a theoretical model and quantitative analysis of experiments. We measure carefully growth properties of a single-layered epithelium, cultured MDCK cells. In these experiments a group of several cells grows to a bigger colony. We observe the density of cells increases and a bulk region with a high constant density is established in the center, surrounded by the edge where cell density decreases. Our results demonstrate a gradual transition from an early exponential growth to a non-linear regime when growth speed increases with colony size.

We develop a continuum model to take into account cell mechanics and growth to study dynamics of tissues. We consider balance of cell number and forces for viscoelastic materials modified by active terms coming from cell division and apoptosis. We solve the equations with analytical and numerical methods. Our results show establishment of bulk and edge regions independent of many details. We study how the dynamics of the colony is controlled by cell characteristics and their interactions with surroundings. Remarkably, our model reproduces the nontrivial properties of MDCK growth in different experiments.

BP 37.5 *(302)* Fri 10:30 H 1058

Synthetic reconstitution of beating cilia — •Isabella Guido, Smrithika Subramani, Christian Westendorf, and Eberhard Bodenschatz — Max Planck Institute for dynamics and self-organization, Göttingen, Germany

Cilia are microscopic hair-like structures that present a rhythmic waving or beating motion and are found on the surface of almost all mammalian cells and on the body of some protozoan organisms. They are used for fluid flow based transport (e.g. removal of pollutants in the trachea) or for the locomotion in viscous fluid environments.

In our work we aim to develop synthetic ciliated systems able to propel themselves or to move fluids across a fixed surface. For this purpose we employ a bottom-up approach for assembling a simple system made of few building blocks adapted from natural cilia, namely microtubules and motor proteins. Using Kinesin-1, a processive motor powered by ATP hydrolysis, we synthesized a system containing MT bundles that are free to move in all planes, deviating from the conventional gliding assay. By binding them to a surface using a suitable anchor system, we are able to observe the microtubules-motor protein system oscillations in a manner that closely mimics ciliary movement.

The issue that we are addressing in our experiments is: how simple is the simplest system that is able to beat?

BP 37.6 *(318)* Fri 10:45 H 1058

DNA in the cell nucleus is organized similar to an active microemulsion — •Lennart Hilbert[1,2,3], Yuko Sato[4], Hiroshi Kimura[4], Frank Jülicher[1,3,5], Alf Honigmann[2], Vasily Zaburdaev[1,3], and Nadine Vastenhouw[2] — [1]Center for Systems Biology Dresden — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Max Planck Institute for the Physics of Complex Systems — [4]Tokyo Institute of Technology — [5]Center for Advancing Electronics Dresden

Inside cell nuclei, DNA is stored in the form of chromatin. Chromatin is three-dimensionally organized in response to transcription of DNA into RNA. Here, we studied the mechanisms by which transcription organizes chromatin, using experiments in zebrafish embryonic cells and theory. We show that transcription establishes an interspersed pattern of mutually exclusive chromatin-rich domains and RNA-rich domains. Ongoing transcriptional activity stabilizes the interspersed domain pattern by establishing contacts between the RNA and transcribed parts of chromatin. We explain our observations with an active microemulsion model based on two macromolecular mechanisms: (i) RNA/RNA-binding protein complexes and chromatin undergo phase separation, while (ii) transcription tethers RNA/RNA-binding proteins to chromatin and thereby forms amphiphile particles that intersperse the phases. Thus, three-dimensional DNA organization in the cell nucleus is an example of an unconventional, active microemulsion, stabilized by a catalytically active amphiphile that produces one of the emulsified phases.

BP 37.7 *(408)* Fri 11:00 H 1058

Size increases produce coordination trade-offs in a simple multicellular animal near criticality — Mircea R. Davidescu[1], •Pawel Romanczuk[2,3], Thomas Gregor[4], Corina E. Tarnita[1], and Iain D. Couzin[5,6] — [1]Dept. of Ecology and Evol. Biology, Princeton University ,USA — [2]Institute for Theoretical Biology, Dept. of Biology, Humboldt Universität zu Berlin, Germany — [3]Bernstein Center for Computational Neuroscience, Berlin, Germany — [4]Joseph Henry Laboratories of Physics, Princeton University, USA — [5]Dept. of Collective Behavior, MPIORN, Konstanz, Germany — [6]Dept. of Biology, University of Konstanz, Germany

Based on theoretical arguments from statistical physics, it has been suggested that collective systems in biology should operate close to criticality in order to maximize their susceptibility to external signals [Mora & Bialek, J Stat Phys, 144, 2 (2011)]. Recently, this hypothesis received increased attention in the context of collective behavior in biology. However, it is still rather controversial and up to know most support for it comes from idealized mathematical models and few experimental systems. Here, we will discuss some recent experimental observations of Placozoa (*Trichoplax Adhaerens*), a simple multicellular animal effectively corresponding to a quasi two-dimensional cellular sheet. By combining experimental data with simple mathematical model of Placozoa motion as a collective system, we find that the observed dynamics are indeed consistent with the criticality hypothesis, but as a consequence these simple animals without a central nervous system have to face a fundamental size-coordination trade-off.

BP 37.8 *(124)* Fri 11:15 H 1058

Harnessing emergence in bacterial populations: From biological mixing to active mechanics — •Anupam Sengupta — Institute for Environmental Engineering, ETH Zurich, Switzerland — Physics and Materials Science Research Unit, University of Luxembourg

At the scale of a single cell, interactions between a bacterium and its micro-environment represent a complex biophysical interface between phenotypic states (free-living planktonic or surface-attached sessile state) and external cues. In this talk I will discuss two recent works where we use experiments and modeling to elucidate how bacterial phenotype cross-talks with immediate micro-environment, and harnesses the emergent physics for biological functions. In the first case, we will see how Chromatium okenii, a 10 μm long purple sulphur bacterium, is capable of mixing over a meter thick layer of water in the Swiss Alpine lake, Lago di Cadagno. By changing the local fluid density, C. okenii is able to trigger convection rolls, creating a sustained well-mixed nutrient layer within an otherwise stratified lake. In the second instance, we will examine emergent geometrical and mechanical properties of a bacterial colony growing on a soft substrate. We show that such an expanding colony self-organizes into a "mosaic" of micro-domains consisting of highly aligned cells, before emerging into an active nematodynamic system. Interestingly, phenotypic traits - motility in the first and growth-induced stresses in the latter - couple with local hydrodynamics, to elicit important ecological functions at scales that can be orders of magnitude higher than single cells.

BP 37.9 *(433)* Fri 11:30 H 1058

Hydrodynamic theory of aster positioning by motor proteins — •Andrej Vilfan — J. Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

In fertilized egg cells of certain species the male pronucleus is transported to the center of the cell by growing an asymmetric microtubule aster, which then serves as a track for motor proteins carrying vesicles towards the center. Because these vesicles experience a viscous drag in the surrounding cytoplasm, the motors exert the opposite force on the microtubules. The asymmetry of the aster then leads to a net pulling force towards the cell center. Yet hydrodynamic interactions make the understanding of the process difficult.

Here we discuss a coarse-grained approach where we describe the aster as a porous medium and the moving vesicles as sources of an active pressure gradient. In parallel, we use computational models to determine the parameters of the continuum model. For realistic parameters, we show that a significant proportion (10-20%) of the motor force is converted to a pressure gradient and contributes to aster centering. We conclude that vesicle transport in a viscous environment is a surprisingly efficient way of force generation.

BP 37.10 *(438)* Fri 11:45 H 1058

Active polymer models for the 3D organization of chromosomes — •Johannes Nuebler[1], Geoffrey Fudenberg[2], Maxim Imakaev[1], Nezar Abdennur[1], and Leonid Mirny[1] — [1]Institute for Medical Engineering and Science, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — [2]University of California, San Francisco, Gladstone Institutes, San Francisco, CA 94158, USA

Eukaryotic chromatin is far from being a randomly arranged polymer in the cell nucleus. Rather, a high degree of spatial organization on various length scales is revealed by Hi-C and imaging techniques.

We show that the organization on intermediate scales emerges from the interplay of two mechanisms, one active and one passive: first, on the scale of one million basepairs and below, active formation of growing chromatin loops emerges as a general organizational principle throughout the cell cycle. Second, a block-copolymer based phase separation explains chromatin compartmentalization on larger scales. Interestingly, these processes interact: only the interplay of loop extrusion and spatial segregation explains a large number of experimental perturbations, namely removal of the loop extruder cohesin, removal of the cohesin boundary element CTCF and removal of the cohesin unloader Wapl, and it makes specific predictions for variations in the compartmental interaction and topological constraints (bioRxiv: https://doi.org/10.1101/196261).

BP 38: Membranes and Vesicles II (joint session BP/CPP)

Time: Friday 9:30–12:00 Location: H 2013

BP 38.1 *(379)* Fri 9:30 H 2013

Change of thermodynamic state of cell membrane during an action potential — •Simon Fabiunke, Christian Fillafer, and Matthias Schneider — Medizinische und Biologische Physik, TU-Dortmund

Nonlinear pulses like action potential are considered to be purely electrical phenomena. However, it has been shown that thermal, mechanical, chemical and optical changes also occur at the excitable membrane. From a thermodynamic perspective such pulses have been described as a propagating state change in the cell membrane.

In the present work, we investigated the emission properties of a commonly used potential-sensitive dye (di-4-ANEPPDHQ) as a function of state in phospholipid vesicles and cell membranes. When the thermodynamic state of vesicles made from di-myristoyl-phosphatidylserine (DMPS) was changed by temperature or pH, the fluorescence intensity and spectrum of the embedded dye underwent characteristic changes. During the transition from the liquid-disordered to the liquid-ordered phase, the fluorescence intensity exhibited a maximum and the emission spectrum shifted to shorter wavelengths (by about 26 nm). Subsequently, the same dye was incorporated into the plasma membrane of an excitable cell (Chara Braunii). When an action potential was triggered the emission spectrum shifted to shorter wavelengths. This indicates that propagation of an action potential is associated with a significant change of state of the excitable cell membrane.

BP 38.2 *(409)* Fri 9:45 H 2013

Vesicle adhesion and fusion studied by small-angle x-ray scattering — •Karlo Komorowski[1], Annalena Salditt[1], Yihui Xu[1], Halenur Yavuz[2], Martha Brennich[3], Reinhard Jahn[2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Neurobiology, Max-Planck-Institute for Biophysical Chemistry, Göttingen, Germany — [3]European Molecular Biology Laboratory, Grenoble, France

Membrane fusion takes place in numerous physiological processes on the cellular and subcellular level as in the case of synaptic neurotransmission. The merger of two membranes generally involves a highly complex interplay on the molecular level among lipids, membrane fusion proteins, ions of the aqueous environment and water molecules. We aim at the structure of intermediate states of a vesicle and membrane fusion pathway. A main emphasis is laid on adhered vesicles. Recent observations indicate that such a docking state, showing two flattened membranes in close proximity, plays a role in vesicle fusion. For this purpose, we have studied adhesion and fusion of lipid vesicles induced by $CaCl_2/MgCl_2$, and show that a stable adhesion state can be induced under certain conditions. The bilayer structure and the inter-bilayer distance between adhered vesicles was analyzed by small-angle x-ray scattering (SAXS). From the obtained structural parameters we aim at an understanding of inter-membrane potentials in adhesion and in fusion. Finally, we have studied structural dynamics of lipid vesicle fusion using time-resolved SAXS techniques, and show that intermediate states can be distinguished over time.

Invited Talk BP 38.3 *(2)* Fri 10:00 H 2013

The role of dynamin twist in membrane fission — Martina Pannuzzo[1], Zachary A. McDargh[1,2], and •Markus Deserno[1] — [1]Department of Physics, Carnegie Mellon University — [2]Department of Chemical Engineering, Columbia University

The final step of many biological membrane fission events involves the GTPase dynamin, which assembles into a helical filament around the neck of a nascent vesicle and somehow severs this remaining connection. But despite about two decades of research, the actual physical processes that lead to fission are still a matter of debate. Dynamin's action occurs on the scale of a few tens of nanometers over just a few milliseconds, which is too small and fast for many experimental techniques, but too large and slow for atomistic simulations. Here we present coarse-grained simulations that are specifically designed to capture the interplay of geometry and elasticity. We argue that, within reasonable experimental limits, the two widely discussed conformational changes of shrinking the radius or increasing the pitch of a dynamin helix are insufficient to trigger fission. However, a third change, reminiscent of an effective twist of the filament, which accounts for the experimentally observed asymmetric unbinding of dynamin's PH-domains, turns out to efficiently drive the neck into the hemifission state. Following the retraction of the substrate, the remaining dynamin coat can unbind, and the tensile force in the connecting micellar string draws the almost severed membranes together one more time, until bilayer contact catalyzes the scission of the micelle.

BP 38.4 *(417)* Fri 10:30 H 2013

Appling forces to model cells using microfluidic systems — •Tom Robinson — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Biological cells in their natural environment experience a variety of external forces such as fluidic shear stress, osmotic pressures, and mechanical loads. While membrane proteins are a crucial part of the cellular response to external stimuli, in recent years so called *lipid rafts* have been thought to play an important role in the spatial organization of membrane proteins. Synthetic membranes such as giant unilamellar vesicles (GUVs) offer a reduced cell model, whereby individual components can be isolated and studied without interference from the complexity of the natural cell. However, applying specific forces to these delicate objects in a controllable manner is non-trivial. To this end, we report a microfluidic method to capture GUVs and apply a variety of forces. The first device contains micro-patterned electrodes which allows the application of electric fields and observations of the subsequent membrane fusion (Robinson et al. Lab on a chip 2014). The second device uses a valve-based system to apply specific fluidic shear forces to membranes (Sturzenegger et al. Soft Matter 2016). Our latest microfluidic design comprises an integrated micro-stamp which is able to mechanically compress GUVs to study the effects of deformation. We investigate the effects of these forces on the behaviour of lipid domains as a model for lipid rafts in cells.

BP 38.5 *(429)* Fri 10:45 H 2013

Design of a switchable DNA origami structure for shaping lipid membranes — •Alena Khmelinskaia[1], Megan Engel[2,3], Garima Mishra[3], Jonathan Doye[3], and Petra Schwille[1] — [1]Max Planck Institute of Biochemistry, Planegg, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom — [3]Department of Physical and Theoretical Chemistry, University of Oxford, Oxford, United Kingdom

Biological membranes are dynamic cellular barriers that suffer deformation and bending. In recent years, due to its exclusive nanoengineering properties, the DNA origami technology has been vastly used to build synthetic scaffolds that partially recapitulate curvature-inducing mechanisms. Nonetheless, the control over such shaping phenomena is yet scarce. Here, we design a DNA based nanostructure with an integrated conformational switch, with the goal to deform free-standing lipid membranes. Using site-directed single-strand displacement reactions as force elements, DNA nanostructures change their conformation into a bent state. Simulations of the DNA-based nanostructures using the oxDNA coarse-grained model confirm the experimentally observed bending. A complementary approach of nucleotide sequence variation and simulation is used to balance the implemented

force elements and consequently optimize the conformational switch. We show that bent DNA-based structures are capable of inducing large scale deformations on free-standing lipid bilayers. Furthermore, our results may confirm theoretical predictions of membrane bending based on the free energy changes of the bound DNA structures.

BP 38.6 *(437)* Fri 11:00 H 2013

FCS analysis of protein mobility on lipid monolayers — •Jonas Mücksch[1,2], Alena Khmelinskaia[1,2], Franco Conci[1], Grzegorz Chwastek[1], and Petra Schwille[1] — [1]Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Martinsried — [2]authors contributed equally

In vitro membrane model systems are used to study complex biological phenomena under controlled unadulterated conditions. Lipid monolayers are particularly suited to study lipid packing in an unbiased manner. To explore the effect of lipid packing on protein mobility, we used miniaturized chambers instead of conventional Langmuir-Blodgett troughs. This assay requires only minute amounts of protein and is ideally suited to be combined with single molecule sensitive fluorescence correlation spectroscopy (FCS) to characterize diffusion dynamics. Our results confirm the influence of lipid packing on lipid mobility and validate the use of FCS as an alternative to conventional surface pressure measurements. Furthermore, we study the effect of lipid density on the diffusion of membrane binding biomolecules, ranging from small peptides to large DNA-based nanostructures. We exploit the sensitivity of FCS to characterize protein interactions with the lipid monolayer in a low concentration regime, which is inaccessible to conventional surface pressure measurements. Finally, we relate our measurements to the characteristic hydrodynamic length of the lipid monolayer. Our work provides a detailed strategy for the conduction of point FCS experiments on lipid monolayers, which is the first step towards extensive studies of protein-monolayer interactions.

BP 38.7 *(94)* Fri 11:15 H 2013

Structure and Conformation of Single and Interacting Bacterial Surfaces — •Ignacio Rodriguez Loureiro[1], Victoria Latza[1], Giovanna Fragneto[2], and Emanuel Schneck[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Institut Laue-Langevin, Grenoble, France

The outer surfaces of Gram-negative bacteria are composed of lipopolysaccharide (LPS) molecules exposing oligo- and polysaccharides to the aqueous environment. This unique, structurally complex biological interface is of great scientific interest as it mediates the interaction of bacteria with antimicrobial agents as well as with neighboring bacteria in colonies and biofilms. Structural studies on LPS surfaces, however, have so far dealt almost exclusively with rough mutant LPS of reduced molecular complexity and limited biological relevance. Here, using neutron reflectometry we structurally characterize planar monolayers of wild-type LPS from Escherichia Coli O55:B5 featuring strain-specific O-side chains in the presence and absence of divalent cations and under controlled interaction conditions. For interacting LPS monolayers we establish pressure-distance curves and determine the distance-dependent saccharide conformation.

BP 38.8 *(135)* Fri 11:30 H 2013

Osmotic instabilities and organelle biogenesis — •Sami Al-Izzi[1,2], George Rowlands[2], Pierre Sens[1], and Matthew Turner[2] — [1]Institut Curie (UMR 168), Paris, France — [2]University of Warwick, Coventry, Uk

We study theoretically a membrane tube with unidirectional ion pumps driving an osmotic pressure difference. A pressure driven peristaltic instability is identified, quantitatively distinct from similar tension-driven Rayleigh type instabilities on membrane tubes. We discuss how this instability could be related to the function and biogenesis of membrane bound organelles, in particular the contractile vacuole complex found in protists. The unusually long natural wavelength of this instability is in close agreement with that observed in cells. We also consider extensions of this result to more complex/realistic systems.

BP 38.9 *(297)* Fri 11:45 H 2013

Cholesterol effects on lateral structure formation — •Fabian Keller, Davit Hakobyan, and Andreas Heuer — Institut für Physikalische Chemie, Münster, Deutschland

Cholesterol is essential for, e.g. , the domain formation of lipid membrane mixtures and is thus at the heart of many basic properties of lipid membranes.

In recent studies we could show that cholesterol is able to intercalate between DPPC molecules without changing the mean distance of their head groups and, surprisingly, not changing the number of DPPC or DLiPC neighbors. Additionally the presence of cholesterol was found to decrease the lipid-lipid interactions of nearby lipids, indicating the complex interaction mechanisms in cholesterol containing bilayers. Our findings support the observations of cholesterol's condensing capabilities and DPPC-cholesterol interaction to be the driving force for domain formation.

To further understand the underlying mechanisms of cholesterols unique properties it is an essential step to include cholesterol to a formerly introduced Monte Carlo lattice model mapping MD data of DPPC and DUPC bilayers to a lattice [1]. Using this model one will be able to study cholesterol structure formation for decisively greater length and time scales, thereby completely resorting to input from short-time MD data.

[1] D. Hakobyan, A. Heuer, J. Chem. Phys. 146, 064305 (2017)

BP 39: Focus Session: Complex Contagion Phenomena II (joint session SOE/DY/BP)

Session organizers and chairs: Philipp Hövel, Pawel Romanczuk, and Jonathan Donges. See part I of the session for a synopsis.

Time: Friday 9:30–13:15 Location: MA 001

See SOE 23 for details of this session.