# 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 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 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 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 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 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 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 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 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 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 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 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 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. Structural 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 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 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 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 $\gamma$-interferon priming on the ruffling behavior of human macrophages.

BP 15.16 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 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 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 scatter-

ing (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 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 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 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 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 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 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 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 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 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 700$\mu$m 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 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 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 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 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 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 100$\mu$m 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 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 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 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 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 experimen-

tal setup of CellMOUSE.

BP 15.37 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 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 $\mu m$ 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 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 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 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 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 3$\mu$m to 8$\mu$m. 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 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 possibil-

ity 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 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 Tue 14:00 Poster B

**Collective Hydration Dynamics in Binary Mixtures: A THz Time Domain Spectroscopic Study** — •Debasish Das Mahanta, Nirnay Samanta, Dipak Kumar Das, and Rajib Kumar Mitra — S. N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Saltlake, Kolkata-700106

We have studied the structure and dynamics of water in its binary mixture with two amphiphilic molecules 1,2-dimethoxy ethane (DME) and dimethyl sulfoxide (DMSO) by THz time-domain spectroscopy (TTDS) (0.3-1.6 THz region). In both the cases a non-ideal behaviour of the mixture is found owing to the formation of water clusters. The cooperative dynamics of water in those binary mixtures, obtained from Debye relaxation of TTDS data reveals a non-monotonous behavior as a function of water concentration (Xw).

BP 15.46 Tue 14:00 Poster B

**Photoinduced processes of free bilins in solution: fs TA absorption spectroscopy on phycocyanobilin and biliverdin IX$\alpha$** — •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 IX$\alpha$ (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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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 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. Semicon-

ducting 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 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 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 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.

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**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.

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**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.

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**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.