

BP 12: Poster II

Topics: Bioimaging and biospectroscopy (12.1 - 12.24); Computational biophysics (12.25 - 12.33); Membranes and vesicles (12.34 - 12.46); Neurosciences (12.47 - 12.49); Focus session: Collective dynamics in neural networks (12.50 - 12.56); Focus session: Physics of Cilia: Dynamics of synchronized oscillators across scales (12.57 - 12.58); Protein structure and dynamics (12.59 - 12.61); Single molecule biophysics (12.62 - 12.75); Systems biology & Gene expression and signaling (12.76 - 12.80)

Time: Tuesday 14:00–16:00

Location: Poster B2

BP 12.1 Tue 14:00 Poster B2

High-statistics SAXS of desmin-expressing cells — ●CHIARA CASSINI¹, MANFRED BURGHAMMER², HARALD HERRMAN³, and SARAH KÖSTER¹ — ¹IRP, Georg-August-Universität Göttingen, Germany — ²ESRF, Grenoble, France — ³DKFZ, Heidelberg, Germany

Desmin is the main intermediate filament (IF) protein in muscle cells. Recently, a large number of mutations in the desmin gene have been discovered to be pathogenic. In order to assess the structures formed in cells by normal and mutant desmin, a high resolution method, capable of retrieving structural information at sub-cellular length scales, without the need for slicing the cells, is preferable. Thus, we performed scanning small angle X-ray scattering (SAXS) experiments on three different cell lines generated from IF-free mouse fibroblasts: one expressing wild type desmin, one expressing R406W-desmin, and the IF-free mother cell clone itself. The cells were grown on Si₃N₄ windows and measured in freeze-dried state. Each window contained tens to hundreds of cells. In the past, each cell scan took minutes to hours. Recently, we were able to employ a special fast scanning mode that allowed us to image an entire window within a single scan in about 8 hours only. This approach ensured the collection of a statistically significant pool of data in a reasonable time span. However, the data analysis became more challenging: the selection of the different regions of interest needed to be automated. This was achieved by segmenting the dark field image of a scan with Bradley's and Otsu's thresholding; it was subsequently possible to compare local structure-related parameters of the three cell lines in a statistically relevant way.

BP 12.2 Tue 14:00 Poster B2

Studying molecular interactions under flow — ●ELEONORA PEREGO and SARAH KÖSTER — Institute for X-Rays physics, University of Göttingen

In recent years the investigation of assembly and aggregation of proteins attracted attention in the scientific community. These processes are the basis of important cellular mechanisms, thus it is important to gain a complete knowledge of the interactions between molecules. Here, we focus on studying the ordered assembly of intermediate filament proteins (IFs), a cytoskeletal component. Although in human more than 70 types of IFs exist, the assembly pathway is common to all of them. The assembly starts with the lateral association of small rod-shaped monomers forming a so called unit length filament (ULF), that is the starting point for the elongation step. We combine photon counting histogram (PCH) to study this process with high spatial resolution, with microfluidics to achieve high temporal precision. We use a multi-layer microfluidics device that prevents the protein from come in contact with the channel walls. This type of device also provides a controlled mixing of assembly buffer and protein solution. Employing PCH on these devices enables us to precisely measure the labelling stoichiometry of the assembling protein, helping us to understand the first steps of vimentin assembly. Our results show that the combination of microfluidics and single molecule fluorescence provides a suitable approach for studying the aggregation of biomolecules in real time, which is important for understanding cellular behaviour.

BP 12.3 Tue 14:00 Poster B2

Quantification of DNA by Combined X-ray Scanning Nanodiffraction and Holography — ●ANDREW WITTMER, MAREIKE TÖPPERWIEN, TIM SALDITT, and SARAH KÖSTER — Uni Göttingen. Institute for X-ray Physics. Göttingen, Germany.

Imaging nanostructures within a cell presents several challenges. Although traditional optical imaging techniques, such as visible light phase contrast or fluorescence microscopy, are widely used, they cannot access the necessary length scales of subcellular structures such as nuclear DNA. Techniques such as electron microscopy can image the necessary length scales but at the invasive expense of slicing the cells. These two challenges are overcome by x-rays: with their short

wavelengths and high penetration depths, they are capable of imaging nanostructures in whole cells. Measurements can be performed on both living and lyophilized cells but, when compared to living cells, the electron density contrast between the sample and environment is higher when the cells are lyophilized. Here, we perform both x-ray scanning nanodiffraction and holography measurements on lyophilized 3T3 fibroblasts. The presented analysis supplies information concerning the morphology, aggregation state and projected electron density of nuclear material within distinguishable regions of the nucleus. The relationship between the number of scattered photons (nanodiffraction) of a distinguished region and its corresponding electron density (holography) is investigated.

BP 12.4 Tue 14:00 Poster B2

Photo-induced force microscopy (PiFM) - a promising new spectroscopic imaging technique for chemical information of biomaterials — ●ANIKA STRECKER^{1,2,3}, NILA KRISHNAKUMAR^{1,3,4}, ANURADHA RAMOJI^{1,5}, UTE NEUGEBAUER^{1,4,5}, ANNE-DOROTHEA MÜLLER⁶, HEIDEMARIE SCHMIDT^{1,4}, and DANIELA TÄUBER^{1,4} — ¹Leibniz-IPHT, Jena, Germany — ²Ernst-Abbe University of Applied Science, Jena — ³Abbe Center of Photonics, Jena — ⁴Friedrich-Schiller-University Jena — ⁵Center for Sepsis Control and Care, Jena University Hospital — ⁶Anfatec Instruments GmbH, Oelsnitz, Germany

Staining-free imaging methods are advantageous for revealing chemical information of biomedical materials. PiFM is a promising new spectroscopic imaging method, which combines excitation in the mid infrared by quantum cascade lasers with detection using a conductive AFM tip, thereby, enabling nanoscale lateral resolution. Here we present PiFM and discuss advantages and disadvantages compared to established IR- and Raman spectroscopy imaging methods.

BP 12.5 Tue 14:00 Poster B2

Metal Induced Energy Transfer reveals nanostructure of an focal adhesion complex — ●FABIAN PORT, LYDIA REBEHN, and KAY-E. GOTTSCHALK — Institute of Experimental Physics, Ulm University, Germany

Cell adhesion to the extracellular matrix does not only function as an anchor, it also enables cells to sense their environment [1]. The focal adhesion complex, which is responsible for these adhesions, is a complex structure consisting of a multitude of different proteins. Despite this important role its structure remains difficult to resolve [2]. Knowing the exact position of these proteins in the focal adhesion complex is necessary to understand the sensing mechanisms of the cell. For a detailed analysis of the focal adhesions, 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 various focal adhesion proteins and the underlying surface in different cell lines and demonstrate the usefulness of MIET for analyzing molecular structures close to the basal membrane with nm accuracy in life cells.

[1] Geiger, B., Spatz, J. P., & Bershadsky, A. D., *Nature Reviews. Molecular Cell Biology*, 10(1), 21-33 (2009)

[2] Kanchanawong, P., Shtengel, G., Pasapera, A. M., Ramko, E. B., Davidson, M. W., Hess, H. F., & Waterman, C. M., *Nature*, 468(7323), 580-584 (2010)

[3] Chizhik, A. I., Rother, J., Gregor, I., Janshoff, A., & Enderlein, J., *Nature Photonics*, advance on(January), 1-8 (2014)

BP 12.6 Tue 14:00 Poster B2

Tunable nanoplasmonic substrates for biosensory applications — ●PETER KOLB and KAY-E. GOTTSCHALK — Institute for Experimental Physics, Ulm University, Germany

Arrays of metallic nanoparticles show specific electromagnetic resonances which are strongly dependent on their geometry. Coupling

between closely spaced plasmonic particles leads to a strong resonance dependence on the inter-particle distance. By combining gold nanoparticles with a soft PDMS substrate, resonances can be mechanically tuned [1] or used to detect substrate strain [2]. As gold and PDMS are both biocompatible they are frequently used in biological applications.

Utilizing electron beam lithography, electron beam evaporation, and lift-off procedures, we produce gold nanodisc arrays on soft PDMS substrates. We investigate the optical properties of these substrates by simulation and experimentation, with further testing of suitability for biosensing applications.

References:

[1] Liu, Wenjie, et al., Mechanically tunable sub-10 nm metal gap by stretching PDMS substrate. *Nanotechnology* 28.7 (2017): 075301.

[2] Gao, Li, et al., Optics and nonlinear buckling mechanics in large-area, highly stretchable arrays of plasmonic nanostructures. *ACS nano* 9.6 (2015): 5968-5975.

BP 12.7 Tue 14:00 Poster B2

Fluorescent nanodiamonds as a nanoscopic magnetic field detector — ●FREDERIKE ERB and KAY-E. GOTTSCHALK — Institute of Experimental Physics, 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. A nanodiamond sensor can be smaller than 50 nm in diameter and read-out optically without contact, also in biological samples. As they are biocompatible and non cytotoxic, they can be used for many experiments *in vivo*.

We present experiments using the NV-center in nanodiamond as a magnetic field detector. Gd^{3+} ions in the surrounding of the nanodiamond introduce magnetic field fluctuations, which affect the NV's spin relaxation time T_1 [1]. Reading-out this T_1 -Time with a commercial confocal microscope gives a measure of the Gd^{3+} concentration in the sample.

References:

[1] Kaufmann, S. et al. (2013): Detection of atomic spin labels in a lipid bilayer using a single-spin nanodiamond probe. In: *Proceedings of the National Academy of Sciences* 110 (27), S. 10894-10898.

BP 12.8 Tue 14:00 Poster B2

Developing a fast microrheological sensor device with live tracking — ●JONAS PFEIL, DANIEL GEIGER, TOBIAS NECKERNUS, and OTHMAR MARTI — Institute of Experimental Physics, Ulm University, Ulm, Germany

Passive microrheology (PMR) based on tracking of incorporated coated polystyrene beads is an established technique to measure physical properties of biological tissue. PMR works by imaging the beads at very high frame rates in the kHz range and observe the brownian motion with sub-pixel resolution. From this motion the rheological properties of the tissue are computed. Some of the issues are the high speed imaging requirements and the needed tracking to calculate the information. We present a new device consisting of an image sensor and a field programmable gate array (FPGA) to lower the bandwidth requirements of the sensor and to track the beads in real time. This drastically reduces the storage requirements and bandwidth needed for the measurement, allowing very long duration, continuous measurements with cost efficient hardware.

BP 12.9 Tue 14:00 Poster B2

Cyclic olefin copolymer microfluidic devices for SAXS studies on protein assembly — ●GERRIT BREHM and SARAH KÖSTER — Universität Göttingen, Institut für Röntgenphysik

Protein assembly is essential in cellular mechanics and, in particular, the mechanical properties of assembled proteins in higher-ordered structures. The mechanical properties of bundles and networks, for example, are directly encoded by the specific hierarchical architecture of protein structures. Therefore, understanding the assembly pathway of proteins is essential in determining their biological function.

Combining the high spatial resolution of small angle X-ray scattering (SAXS) with the precise, controllable sample environment inside microfluidic devices enables investigation of such processes, as they take place on nanometer and micrometer length scales and occur on sub-second to second times scales. We present a straightforward fabrication method for X-ray compatible microfluidic devices made solely

from cyclic olefin copolymers. Furthermore, no gluing between interfaces is necessary, rendering the production very reliable.

As a biophysical application we investigate the early time points of the assembly of vimentin intermediate filament proteins into higher-order structures. We benchmark the performance of the devices against other devices including more commonly used Kapton windows and obtain data of equal quality using SAXS. This weakly scattering protein system leads to high quality data in the new devices, thus opening up the way for numerous future applications.

BP 12.10 Tue 14:00 Poster B2

X-ray diffraction studies on bovine red blood cells in microfluidic devices — ●JAN-PHILIPP BURCHERT¹, GERRIT BREHM¹, RITA GRACEFFA¹, MANFRED BURGHAMMER², and SARAH KÖSTER¹ — ¹Institut für Röntgenphysik, Universität Göttingen, Germany — ²European Synchrotron Radiation Facility, Grenoble, France

Red blood cells (RBCs) belong to the major cellular components of blood. They possess a very flexible but stable cytoskeleton below their membrane that is based on an actin-spectrin network. This cortex structure allows them to deform under shear stress and to pass through blood vessels with diameters smaller than their own size. In contrast to other cells, erythrocytes possess no cell organelles. Consequently, their cytoplasm is made up from water and proteins only. One important protein is hemoglobin which is, due to its high volume fraction, proposed to play a role in cell volume regulation. It is suggested that shear forces alter the equilibrium between aggregated and single hemoglobin inside the cell resulting in a change of cytoplasmic properties close to the cell membrane. Thereby, membrane proteins such as pumps and channels might be influenced. In our experiments, bovine RBCs flow through a microfluidic capillary device that simulates shear forces of different magnitudes. Moreover, different osmotic conditions are taken into consideration. To examine the aggregation state of hemoglobin for these experiments, small angle X-ray scattering (SAXS) is applied at different positions within the device. The resulting scattering images are related to the concentration and velocity fields simulated by finite element simulations.

BP 12.11 Tue 14:00 Poster B2

Imaging of folded proteins deposited via soft-landing native electrospray ion beam deposition — ●SVEN SZILAGYI¹, HANNAH OCHNER¹, LUKAS KRUMBEIN¹, JOSEPH GAULT², ALBERT KONIJNENBERG³, ESTHER MARTIN^{3,4,5}, JUSTIN BENESCH², FRANK SOBOTT^{3,4,5}, CAROL ROBINSON², SABINE ABB¹, STEPHAN RAUSCHENBACH^{1,2}, and KLAUS KERN^{1,6} — ¹Max-Planck-Institut für Festkörperforschung, Stuttgart — ²Department of Chemistry, University of Oxford — ³Department of Chemistry, University of Antwerp — ⁴Astbury Centre, University of Leeds — ⁵School of Molecular and Cellular Biology, University of Leeds — ⁶École Polytechnique Fédérale de Lausanne

Imaging techniques provide valuable information on the structure of proteins. Gaining reliable data strongly depends on the sample preparation technique, such as shock-freezing and staining of proteins or drop casting of samples. Here, we present the soft landing electrospray ion beam deposition (ES-IBD) as an alternative sample preparation approach in (ultra) high vacuum for imaging of protein samples. To this end, native electrospray ionization brings the proteins into the gas phase while preserving their folded state [1]. In this poster, we present successfully deposited proteins of different size which were imaged using different techniques, such as TEM, AFM, STM and Low Energy Electron Holography (LEEH) [2]. We further discuss the substrate influence on the folded state of the proteins from metal surfaces to free-standing graphene. [1] *Nat. Meth.*, 5(11), 2008, 927-933. [2] *PNAS*, 114(7), 2017, 1474-1479.

BP 12.12 Tue 14:00 Poster B2

Force microscopy studies of mechanically loaded albumin films — ●LUKAS BÖTTCHER¹, SVEN KRAFT¹, REGINA LANGE¹, INGO BARKE¹, JESSICA HEMBUS², CARMEN ZIETZ², RAINER BADER², and SYLVIA SPELLER¹ — ¹Institute of Physics, University of Rostock, 18051 Rostock — ²Biomechanics and Implant Technology Research Laboratory, University Medical Center Rostock, 18057 Rostock

In humans articulating joints such as hip or knee contain synovial fluid for sufficient lubrication. Major components are polysaccharides, lipids and proteins such as albumin. During walking oscillating pressure is applied leading to structural changes of the proteins. Under dynamic pressure the proteins might be partially unfolded or even formation of amyloid may occur. Such degraded protein possibly contributes to

lubrication. Typical tip-sample pressures in atomic force microscopy are in the same regime as macroscopic joints. Our research question is whether a parameter can be derived from force spectra and be established as a measure for protein degradation. In an initial stage we use albumin as a model protein. This approach requires substantial energy transfer from an oscillating cantilever tip to the protein. In this work we present first results of topographic and spectroscopic analysis of mechanical-loaded albumin films on surfaces.

BP 12.13 Tue 14:00 Poster B2

Towards Label Free Imaging of Action Potentials by Deep Learning — ●STEPHAN RINNER¹, ALBERTO TRENTINO¹, HEIKE URL², BERNHARD WOLFRUM², and FRIEDEMANN REINHARD¹ — ¹Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany — ²Munich School of Bioengineering, Technische Universität München, Boltzmannstrasse 11, 85748 Garching, Germany

Imaging of action potential signals in cells thus far requires fluorescence labels. Interestingly, it is plausible that action potentials could also induce small intrinsic changes in the optical properties of a cell. We aim to develop a label-free imaging method by searching for such signatures, capitalizing on the emergence of powerful cameras and image recognition schemes over the past years. On this poster, I will present our efforts to resolve such signals using high resolution polarized light microscopy of heart cells. I will introduce the key features of our setup, namely high-powered LED illumination, a high framerate slow-motion camera and an incubation system for keeping cells alive. Furthermore, the poster will summarize data processing methods to identify patterns in small fluctuations, such as different filtering methods. If successful, this experiment will provide a new method to observe action potentials in a label-free and non-invasive manner.

BP 12.14 Tue 14:00 Poster B2

Targeted near infrared sensing and imaging with GFP-nanobody nanotube hybrids — FLORIAN MANN, JÖRG GROSSHANS, FELIPE OPAZO, and ●SEBASTIAN KRUSS — Göttingen University, Göttingen, Germany

Fluorescent nanomaterials have many advantages in terms of their photophysics but it is difficult to target them to specific locations in living systems. In contrast, the green fluorescent protein (GFP) can be genetically targeted to proteins in cells or animals. Therefore, GFP can be seen not only as a fluorophore but as a universal target/handle. Moreover, many transgenic organisms or transfected cells are available. We wanted to combine the advantage of GFP targeting and fluorescent nanomaterials. Therefore, we conjugated a GFP nanobody to near infrared (nIR) fluorescent single-walled carbon nanotubes (SWCNTs). SWCNTs fluoresce in the nIR tissue transparency window (900 nm -1700 nm) and do not bleach. The GFP nanobody serves as recognition unit for GFP and the SWCNT serves as superior nIR fluorophore. These hybrids were then used in biological experiments to demonstrate the versatility of this approach. First, we demonstrated that it is possible to label single GFP-tagged kinesin motors in living drosophila embryos and track their directional movement during embryogenesis. Second, we labeled the cytoskeleton in mammalian cells in the nIR. Finally, we targeted cell surface receptors and used the SWCNTs fluorescence for sensing and to detect the neurotransmitter dopamine. In summary, we show that GFP nanobody conjugated SWCNTs show great potential for targeted nIR imaging, sensing and labeling.

BP 12.15 Tue 14:00 Poster B2

Nanomorphology of living sinus nodal cells — ●MAX ULBRICH¹, MIRCO WENDT¹, JULIA J. JUNG², CHRISTIAN VÖLKNER¹, REGINA LANGE¹, HEIKO LEMKE², CHRISTIAN RIMMBACH², ROBERT DAVID², INGO BARKE¹, and SYLVIA SPELLER¹ — ¹Institute of Physics, University of Rostock, 18051 Rostock — ²Reference and Translation Center for Cardiac Stem Cell Therapy, University Medical Center Rostock, 18057 Rostock

Cardiomyocytes exhibit electro-mechanical activity and may therefore be envisioned as sensor or actuator cells. Sinus nodal cells form the pacemaker of the heart and exhibit autonomous activity while working myocardial cells follow their pace. In our studies, we use scanning ion conductance microscopy (SICM) [1] to observe the live-cell morphology and surface dynamics of individual sinus nodal cardiomyocytes derived by forward programming of pluripotent stem cells [2]. Here, we focus on the question whether the sinus nodal cell subtype exhibits characteristic features on its surface which can help to conclude on their origin as well as functionality.

[1] C-C Chen et al., *Annu. Rev. Anal. Chem.* 5, 207 (2012)

[2] J.J. Jung et al., *Stem Cell Rep.* 2, 592 (2014)

BP 12.16 Tue 14:00 Poster B2

Myofiber orientation in a whole mouse heart — ●MARIUS REICHARDT and TIM SALLDITT — Institut für Röntgenphysik, Göttingen, Deutschland

Heart contractility is one of the most important physiological functions and relies on an intricate, hierarchical molecular- and cytoarchitecture. With recent advances in high-resolution imaging techniques, most notably computed tomography (CT) and magnetic resonance imaging (MRI), the cardiac cytoarchitecture and muscle fiber arrangement can now be resolved in three-dimensions with micrometer resolution. The resolution offered by such conventional means, i.e. ultrasound, diffusion-tensor MRI or clinical CT, is however still not sufficient to resolve the full fiber network down to the level of a single muscle fiber. We performed experiments on an entire mouse heart at a liquid-metal jet μ CT laboratory setup with an effective pixel size of $5.5 \times 5.5 \mu\text{m}^2$. Based on the reconstructed 3D electron density the fiber orientation, degree of filament alignment and thickness of single muscle bundles in the whole heart could be determined by applying an algorithm based on the 3D Fourier transform of sub-volumes of the reconstruction. The results will be very useful for structural and dynamical models of cardiac tissue as electromechanical finite element models in order to increase the precision and the way they represent the geometry of the heart. This information may also be used in the future to differentiate healthy and pathological heart tissue in clinical computed tomography as we could already show for neuronal tissue.

BP 12.17 Tue 14:00 Poster B2

Surface relief scanning beyond the diffraction limit with optically trapped probes — ●MATTHIAS ALLKEMPER, LARS FRIEDRICH, and ALEXANDER ROHRBACH — Laboratory for Bio- and Nano-Photonics, Department of Microsystems Engineering - IMTEK, University of Freiburg, Germany

Optical traps play an increasing role in the bio-nano-sciences due to their ability to flexibly apply forces on tiny structures in fluid environments. Combined with particle tracking techniques they allow sensing miniscule forces exerted on these structures. Similar to atomic force microscopy (AFM), but much more sensitive, an optically trapped probe can be scanned across a structured surface to measure the height profile from the displacements of the probe. Here we demonstrate that by a combination of a time-shared twin-optical trap and nanometer-precise three-dimensional interferometric particle tracking reliable height-profiling and surface imaging is possible with a spatial resolution below the diffraction limit. The technique exploits the high energy thermal position fluctuations of the trapped probe, leading to a sampling of the surface 5000 times softer than in AFM. The measured height and force profiles from test structures and helicobacter cells illustrate the potential to uncover specific properties of hard and soft surfaces. We present a novel approach to minimize sticking events between surface and probe, by driving the trapped sphere in tapping mode.

BP 12.18 Tue 14:00 Poster B2

Perceptual evaluation studies of a multisensory interface for exploring nanomechanical tissue properties — ●MÓNICA TAMARA HEREDIA MUÑOZ¹, ANDREAS OTTO¹, MATTHIAS LÖW¹, SOPHIE NEUMANN¹, STEPHEN BARRASS², MARTIN DEHNERT¹, THOMAS BAUMANN¹, ALEXANDRA BENDIXEN¹, and ROBERT MAGERLE¹ — ¹TU Chemnitz, Chemnitz, Germany — ²sonification.com, Canberra, Australia

Biological tissues display a very complex spatial structure and their mechanical properties remain largely unexplored on the nanometer scale. We are building an interface that allows humans to explore the spatially complex data of nanomechanical force fields interactively and with multiple senses simultaneously (visual, auditory, and haptic). From a technological viewpoint, the multisensory display has to translate the user's hand motion fluently and quasi in real time into a haptic, visual, and auditory presentation of the data. Avoiding a perceivable delay between the different display channels is essential, since humans are very sensitive to asynchronies between the senses and to delays between perception and action. Of equally high importance as the technical challenge is the question of how particular nanomechanical properties—such as different types of adhesive and repulsive forces—can be translated to the human senses and represented so that they can be efficiently explored. Here we report on our implementation

of the multisensory interface, its multisensory information design, and perceptual evaluation studies.

BP 12.19 Tue 14:00 Poster B2

Analysis of Organic Molecules in the THz Regime using Whispering-Gallery Mode Resonators — ●FELIX LAMMERMAN, MARIA TH. SCHLECHT, STEFAN MALZER, and HEIKO B. WEBER — Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg, Germany

Distinguishing small amounts of organic or biomolecules like single- and double-stranded DNA in aqueous solutions in a fast and non-destructive way is of great interest for bioanalysis [1]. For this task, we present a measurement scheme based on whispering-gallery mode resonators (WGMR) and continuous-wave THz-radiation in the frequency range from 80 GHz to > 1 THz. The evanescent field of a PTFE THz-waveguide couples to a WGMR made of PE (disk $\varnothing$ 10 mm). A hole in this disk allows to insert a cannula filled with the fluid to be examined.

This local disturbance of the refractive index of the disk severely shifts the resonance frequencies of the WGMR such that the organic molecules can be identified. In a first step, the frequency shifts of short-chained alcohols and organic materials with a high refractive index like glycerine were investigated. We were able to distinguish 1- and 2-propanol which only differ by the position of the -OH group. We verified our results with finite element method simulations. To differentiate various sucrose concentrations of aqueous solutions the sensitivity of our setup had to be improved. Thus, the transmission through larger volumes of the corresponding fluid was measured to determine its specific absorption frequencies. Studying the resonance shifts of the resonator close to those should severely increase our selectivity.

[1] Weisenstein, DOI: 10.1109/IRMMW-THz.2018.8510052 (2018)

BP 12.20 Tue 14:00 Poster B2

Open-source 3D-printed Digital Inline Holographic Microscope for microscopic cell analysis — STEPHAN AMANN^{1,2}, MAX VON WITZLEBEN¹, and ●STEFAN BREUER¹ — ¹Institute of Applied Physics, Technische Universität Darmstadt, Schlossgartenstraße 7, 64289 Darmstadt, Germany — ²Department of Physics, Norwegian University of Science and Technology, Høgskoleringen 5, NO-7491 Trondheim, Norway

Digital inline holographic microscopy (DIHM) is a promising cellular object imaging modality. We demonstrate two cost-efficient DIHM experiments set-ups comprising of standard LED and semiconductor laser light sources and a Raspberry Pi Camera for image acquisition. The DIHM is 3D-printed yielding a highly compact and portable microscope. Imaging of cellular micro objects including tobacco cells and human red blood cells is performed by the use of open-source reconstruction software. Spatial resolutions of 3.96 micrometer and 1.98 micrometer are achieved. The developed DIHM is cost-efficient (<\$200), compact and portable and constitutes a highly flexible tool to be used in science and education that can be tailored flexibly to the researchers demand.

BP 12.21 Tue 14:00 Poster B2

Nanomechanical sub-surface mapping of cells by atomic force microscopy — ●LUKAS STÜHN, ANNA FRITSCHEN, and CHRISTIAN DIETZ — Physik der Oberflächen, Materialwissenschaften, TU-Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt

We aim to visualize nanomechanical properties of the cell's interior with the atomic force microscope. Compared to optical methods, the atomic force microscope can sense the mechanical properties of cells with high spatial and depth precision. In combination with fluorescence microscopy methods cell processes can be specifically investigated. We demonstrate how the atomic force microscope can be utilized to produce nanomechanical maps of human breast cancer epithelial cells.

To this end, we exploit conventional force-distance techniques or dynamic approaches where we force the cantilever to oscillate in several cantilever eigenmodes (flexural/torsional) simultaneously and record the cantilever motion as function of the tip-sample indentation at each pixel. Thus, tip-sample interactions in different spatial directions can be reconstructed and mapped in various sample depths.

We can mechanically distinguish several components of the cell's interior. The nucleus and cytoskeleton are clearly visible. Within the nucleus, nucleoli appear as mechanically stiffer, small round objects. In cross-sections drawn through the three-dimensional maps, the stiff cytoskeleton that mechanically stabilizes the cell becomes apparent in

the proximity of the membrane. Strikingly, the soft gel-like cytosol within the cell can be detected beneath this stiff enclosure.

BP 12.22 Tue 14:00 Poster B2

Probing mitochondrial dynamics and heterogeneity during cell state switching using multiplexed, environment-sensitive fluorescent dyes — ●SUFU O. RAJA^{1,2}, GANDHI SIVARAMAN¹, CHRISTOPH F. SCHMIDT², and AKASH GULYANI¹ — ¹Technology for Advancement of Science, Institute for Stem Cell Biology & Regenerative Medicine, Bellary Road, Bangalore-560065, India — ²Drittes Physikalisches Institut - Biophysik, Fakultät für Physik, Georg-August-Universität Göttingen, 37077 Göttingen

Mitochondria are known as power house of the cell also play significant role in regulating cellular metabolism, calcium and ROS signaling as well as in programmed cell death. Despite decades on research, precise and real-time information on mitochondrial dynamics and functionality, is still limiting. To better visualize the functional dynamics of mitochondrion, we have developed red-emitting, multi-functional, novel mitochondrial probes that are sensitive to local environment, specifically parameters like micro-viscosity, pH, ROS, etc. The developed dyes have low toxicity and very high photo-stability, allowing their use in long term imaging. These dyes have yielded new insights into mitochondrial dynamics in embryonic stem cells as well as during onset of differentiation. In a different example, we have also used our new dyes to probe mitochondrial heterogeneity within primary *activated* cells. These results would be placed in the context of our larger efforts to build new ways of probing *cellular dynamics* with a focus on physico-chemical changes in the intra-cellular compartments.

BP 12.23 Tue 14:00 Poster B2

In-line DNA optical mapping in nanochannels for biomedical applications — ●FRANZISKA ESMEK — Center for Hybrid Nanostructures

On-chip DNA optical mapping allows studying intact individual molecules with higher throughput than conventional sequencing techniques. In optical mapping, typically a "fluorescent barcode-like" pattern is first created, then the DNA molecules are elongated and the fluorescent signal is read out to get information about the genomic structure for biomedical applications. We explore a technique to selectively label the DNA molecules with organic fluorophores as well as by competitive binding at specific locations of interest. The DNA molecules are then stretched in nanofluidic devices made by nanoimprint lithography in a two-minute process. The signal is read out in real time in a home made confocal set up. We perform in-line detection of DNA molecules as they pass through the nanochannels with a focused laser as point excitation and a photon counter, without using a camera. In this configuration, the molecules are detected as step-like peaks in time scans, allowing for real time read-out, with high throughput. Peak analysis (as intensity and duration) gives information about the molecule length, as well as its sequence-dependent barcode. Here there is no limitation with the length of the molecules, or the resolution due to the thermal drift and molecule movement.

BP 12.24 Tue 14:00 Poster B2

Modern data workflow management providing new insights into biomedical data — HENRIK TOM WÖRDEN^{1,2}, ●ALEXANDER SCHLEMMER^{1,3}, DANIEL HORNUNG¹, TIMM FITSCHEN^{1,2}, ULRICH PARLITZ^{1,2,3}, and STEFAN LUTHER^{1,2,3,4,5} — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Institute for Nonlinear Dynamics, Georg-August-Universität, Göttingen, Germany — ³German Center for Cardiovascular Research (DZHK), partner site Göttingen, Germany — ⁴Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — ⁵Department of Physics and Department of Bioengineering, Northeastern University, Boston, USA

The progress in measurement and imaging technologies, such as multichannel EEG, 4D ultrasound imaging or real-time MRI, results in unprecedented amounts of high-resolution, multi-modal data. The processing, analysis, and interpretation of this complex data is a major scientific challenge and a significant bottleneck. Links and interdependencies can exist between all kinds of data on multiple levels, possibly spanning single experiments, experiment series or even larger collaborative projects. Although analysis procedures in biomedical sciences are often advanced, limits in data management may constrain their application. Using data from cardiac research we show how a modern data workflow management allows for a more effective and versatile interface to the data. The workflow also supports the connection of

experimental data to simulation data and analysis results, ensuring a high flexibility of data access and reusability for the researcher.

BP 12.25 Tue 14:00 Poster B2

Computational optimization of compound selectivity to different membrane environments — BERNADETTE MOHR and •TRISTAN BEREAU — Max Planck Institute for Polymer Research

Current virtual screening approaches reduce the computational cost by using simplified representations and approximations, statistical mechanical effects are excluded. We investigate one way to include the effects determining the selectivity of a molecule to a specific target into virtual screening by using physics-based models. Coarse-grained simulations are introduced as a preliminary step to allow the effective screening of a large number of molecules. As a test case, the physical and chemical properties of the fluorescent dye 10-N-nonyl acridine orange are modified to increase its binding affinity to Cardiolipin. In eukaryotes, Cardiolipin is almost exclusively found in the inner mitochondrial membrane. Mitochondria are the location of important metabolic pathways and are linked to diseases and apoptosis. Therefore, targeting a lipid specific to mitochondria is of great interest. In the coarse-grained representation, the bead types at selected positions of the acridine orange molecule are changed and the difference in binding affinity between the original and modified structures are determined by free energy calculations. The present results from the coarse-grained simulations indicate that hydrogen bonding has the desired effect. As a next step, the information lost in the coarse-graining process is to be reintroduced to a small subset of the screened molecules by repeating the free energy calculations in atomistic detail.

BP 12.26 Tue 14:00 Poster B2

Applying microwaves on a cellular level — •SIMON STREIT and STEPHAN GEKLE — Theoretische Physik VI, Universität Bayreuth, Germany

The influence of microwaves in the range of MHz and GHz on the human body and particular cellular components are still not fully understood. For new treatment methods in the medical field like hyperthermia, absorption characteristics need to be understood on the cellular level. Therefore we present our cell model which uses prior work on the specific absorption rate (SAR) of a cell membrane to calculate SAR values for different common cell sizes and frequencies. In addition we take a look into the absorption behaviour of short DNA pieces by means of molecular dynamic simulations and dipole correlation calculations for spectral analysis.

BP 12.27 Tue 14:00 Poster B2

Simulation of visco-elastic behavior of cells in a microfluidic device — •RALF SCHUSTER, TOBIAS NECKERNUSS, DANIEL GEIGER, JONAS PFEIL, KAY GOTTSCHALK, and OTHMAR MARTI — Institute of Experimental Physics, Ulm University, D-89081 Ulm

Variations of structure and shape of cells play an important physiological role. For instance, tumor and normal cells can be distinguished by elasticity, indicated by the amount of deformation under given stress. The mechanical characterization of a certain cell type is meaningful to obtain (patho-) physiological insight. Simulations help to understand, verify and improve the analysis of deformation based cell characterization such as CAOS (1) or flow based cytometry (2). We aim to provide a simulation-based database for the mechanical deformation of cells in microfluidic channels. The variation of parameters of the viscoelastic models for the cells results in a library of possible cell deformation classes. The cell develops characteristic shapes, while moving through a microfluidic channel with varying width. We compare the cell's deformation with measurements. We achieve efficient computations using a 2D-rotational symmetric model, based on Fluid-Structure-Interaction with a hyper-elastic material. Distortions of the mesh, due to strong deformations of the cell, often lead to computational instabilities. This challenge was mastered and our model is able to describe the deformation of the cell along the entire channel.

(1) Neckernuss (2018): Stretching adherent cells with light. Dissertation. (2) Otto et al., Real-time deformability cytometry: on-the-fly cell mechanical phenotyping, Nat. Methods, 2015

BP 12.28 Tue 14:00 Poster B2

Optimization of the Ligase Cycling Reaction (LCR) via Rule-Based Modeling — •LARA BECKER, NIELS SCHLICHTING, JOHANNES FALK, JOHANNES KABISCH, and BARBARA DROSSEL — TU Darmstadt, Germany

Synthetic biologists are working to find a way for efficient and robust implementation of complex genetic circuits into living systems. One approach to this is the employment of computer-aided design tools and the exploitation of automatization procedures, e.g. for DNA assembly. The Ligase Cycling Reaction (LCR) is a powerful method for automated and modularized assembly of DNA. Our goal is to further optimize the LCR based on insights from computer simulation models that mimic, in a simplified fashion, the main steps of the LCR.

To this end, we built a rule-based model of the LCR in Kappa (κ) - a language for modeling systems of interacting agents. The dynamics of the LCR is stochastically simulated in κ , and we explore how changing parameters, concentrations, and timing affects the efficiency. This is done in close collaboration with synthetic biologists from our team who perform assays in the wet lab to validate our findings and predictions, which in turn causes the modelers to include additional features that appear to be relevant in the experiments.

BP 12.29 Tue 14:00 Poster B2

Binding properties of SIM/SUMO complexes — •ALEXANDER KÖTTER and ANDREAS HEUER — Institut für Physikalische Chemie, WWU Münster

The interaction between the small ubiquitin related modifier (SUMO) and different sumo interacting motifs (SIMs) has been the subject of a number of studies in the past few years (e.g., [1]). We investigate complexes formed by the SUMO protein and SIMs by means of atomistic molecular dynamics simulations. We calculate the standard binding free energies for a number of SIMs and find that their relative order agrees well with experiments [1]. We quantify the importance of acidic residues in the neighborhood of the SIMs for the binding and measure the contribution of single residues in the SIM to the interaction energy. Furthermore we find, that, in general, two binding modes exists for the considered SIMs. Their relative importance however varies strongly. [1] Xu et al. Nat. Comm. 5

BP 12.30 Tue 14:00 Poster B2

Fundamentals of domain formation in lipid bilayers: Analyzing atomistic molecular dynamics simulations — •FABIAN KELLER and ANDREAS HEUER — Westfälische Wilhelms-Universität, Münster, Germany

The complex interplay of the myriad of different lipid species as well as membrane proteins that are found in plasma membranes and the resulting unique properties still remain elusive and not well understood. A cell's ability to tune phase behavior clearly is crucial for sustaining vital functionality.

Efforts have been made simulating lipid bilayers with a close-to native lipid composition to shed light on this behavior. [1] Nevertheless the underlying mechanisms remain unidentified.

In this work we approach the problem from a fundamental point of view, analyzing the interaction enthalpies of different lipid species as well as of one candidate of a transmembrane domain to get a better understanding of the driving forces of domain formation. These results can directly be used to expand a recent lattice model of lipid bilayers. [2]

[1] H. I. Ingólfsson, et al. JACS, 136, (2014)

[2] D. Hakobyan, A. Heuer, J. Chem. Phys. 146, (2017)

BP 12.31 Tue 14:00 Poster B2

Generalized Markov State Modeling of Electric Field Induced Conformational Changes in the HIV-1 V3 Loop Peptide — BERNHARD REUTER^{1,2}, •DAUNGTHAI JARUKANONT², SINA ZENDEHROUD², and MARTIN E. GARCIA² — ¹Zuse Institute Berlin (ZIB), Berlin, Germany — ²University of Kassel, Kassel, Germany

Conformational changes regulate the physiological functionality of proteins. The influence of environmental conditions on the function and, therefore, on the conformation of proteins is being studied very intensively. In this work, we investigate the influence of a static external electric field on the secondary and tertiary structure formation of the V3 loop of the HIV-1 envelope glycoprotein gp120. Based on extensive molecular dynamics (MD) simulations, the conformational dynamics of the system were modeled applying a recently developed generalized Markov state modeling method termed Generalized Peron Cluster Analysis (G-PCCA) from [Reuter et al. (2018). JCTC, 14(7), 3579-3594. <https://doi.org/10.1021/acs.jctc.8b00079>]. G-PCCA enables the unsupervised and automatic coarse graining of both reversible and nonreversible molecular kinetics. Using G-PCCA the dominant conformational dynamics of the system were learned for different strengths of the electric field.

BP 12.32 Tue 14:00 Poster B2

Computer simulations of SAS-6 assembly on surfaces — ●DENNIS WÖRTHMÜLLER^{1,2} and ULRICH SCHWARZ^{1,2} — ¹Institute for Theoretical Physics, Heidelberg — ²Bioquant, Heidelberg

The scaffold protein SAS-6 self-assembles into a 9-fold ring that forms the structural basis for centrioles and thus is essential for many important cellular processes, including cell division and the genesis of cilia and flagella. Recently the self-assembly of SAS-6 has been studied by high-speed AFM on mica surfaces (Niervergelt et al., Nature Nanotechnology 13:696-701, 2018). Motivated by this experimental study, we have developed a 2D Brownian dynamics simulation model to identify possible assembly pathways, including malformed structures. Our main finding is that strong fluctuations, which are suppressed by the interaction with the surface, lead to malformed structures. Fluctuations also result in a distribution of ring sizes that favors 8-rings over 10-rings.

BP 12.33 Tue 14:00 Poster B2

Range Expansions in a Stochastic Metapopulation Model — ●DAVID MURAMATSU¹, ERWIN FREY¹, and MARIANNE BAUER² — ¹Ludwig-Maximilians-Universität München, Germany — ²Princeton University, USA

In range expansions, the colonization of a territory by an invading species, the front between invaded and new territory roughens due to stochastic fluctuations. To investigate the growth laws describing the front width of a given system, large sized systems have to be considered, since finite size effects may otherwise obscure the dynamics that govern the interface. Naive implementations of exact simulation algorithms like the Gillespie algorithm scale unfavorably in the system size such that the simulation of ensembles of large systems with complex interactions quickly becomes unfeasible. We address this problem by implementing a parallelized version of the Gillespie algorithm, which scales linearly in the system size, suited for lattice based systems that display local fast dynamics while having a low rate of particle exchange between lattice sites. We employ this algorithm to determine the growth law governing the front width of a system which has been inaccessible to previously used simulation methods.

BP 12.34 Tue 14:00 Poster B2

Fast discrete Cell Volume Tracking for Blood Flow Simulations using the Lattice Boltzmann Method — ●MORITZ LEHMANN, SEBASTIAN MÜLLER, and STEPHAN GEKLE — University of Bayreuth, Germany

The Lattice Boltzmann Method (LBM) is often used to simulate the movement of red blood cells through blood vessels via the immersed boundary method. However, the basic model does not include the different fluid viscosities of the inside of cells and the blood plasma, which also affect cell deformation. For taking into account multiple viscosity domains, we present a fast tracking algorithm that can determine whether any lattice point of LBM is located inside or outside an arbitrarily enclosed cell volume and we investigate how a viscosity change affects cell deformation.

BP 12.35 Tue 14:00 Poster B2

DMPC/cholesterol membranes at high hydrostatic pressure — ●GÖRAN SURMEIER, MICHAEL PAULUS, CHRISTIAN STERNEMANN, SUSANNE DOGAN, MIKE MORON, MARC MORON, and JULIA NASE — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

Phospholipid bilayers, which are the basic component of cell membranes, form various liquid-crystalline and gel-like phases depending on temperature, pressure, and their composition. A typical constituent that regulates the structure of cell membranes is cholesterol. Due to its rigid sterol rings, it affects the mobility and order of lipid tail groups. We conducted a small angle X-ray scattering (SAXS) and X-ray reflectivity (XRR) study on the structure of 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) model membranes containing cholesterol at high hydrostatic pressures. We were able to extract a detailed pressure- and cholesterol content-dependent phase diagram of multilamellar DMPC vesicles in the gel-like regime at 20 °C from SAXS. Additionally, XRR was used to obtain more in-depth information about the vertical membrane structure of solid-supported DMPC/cholesterol multilayers in an aqueous buffer solution. Combining both techniques enables to distinguish substrate-, pressure- and composition-induced effects. We observed that cholesterol strongly affects the compressibility of the membranes. At high concentrations, the spacing changes linearly over the whole pressure range, indicating that configurational

changes are suppressed. Experiments were performed at beamlines BL9 at DELTA (Dortmund, Germany) and ID31 at the ESRF (Grenoble, France).

BP 12.36 Tue 14:00 Poster B2

Effect of reactive oxygen and nitrogen species on lipid monolayers — ●FLORIAN GELLERT, HEIKO AHRENS, RENKO KENSBOCK, and CHRISTIANE A. HELM — Institute of Physics, University of Greifswald, 17489 Greifswald

Oxidative degeneration of lipids can lead to severe damages of the biological cell membrane. The phenomenon is initiated by reactive radicals, such as certain reactive oxygen/nitrogen species (ROS/ RNS). To investigate this behaviour, we use monolayers at the air/ water interface of unsaturated lipids as model membranes. Self-assembling- and phase transition behaviour of monolayers in a Langmuir-Blodgett trough are studied by isotherms. Domain formation is studied by video-speed Brewster angle microscopy. The reactive species are formed either by a low temperature plasma jet (kINPen) or are dissolved in the subphase at low concentrations. Thus, we address the question whether the ROS/ RNS attacks the unsaturated alkyl chains or the head group of the lipid.

BP 12.37 Tue 14:00 Poster B2

A Biomimetic Model to Probe Adhesion Induced Lipid Membrane Properties — ●PHILIPP PAULI and CORNELIA MONZEL — Experimental Medical Physics, Heinrich-Heine University Düsseldorf, 40225 Düsseldorf, Germany

Adhesion plays an important role in the biological functions of cells influencing signalling, cell migration, or the building of tissue. The basis of adhesion are the short range attractive forces induced by biological molecules like cadherins or integrins. Using giant unilamellar vesicles (GUV), it is possible to mimic the envelope of a cell - namely the plasma membrane - and to decipher physical mechanisms underlying cell adhesion. As biomimetic model system, GUVs lack the complex structures of cells and enable quantification of designated membrane properties.

Utilizing the biotin-neutravidin binding between a substrate and a vesicle, we investigate the adhesion strength relative to a variable number of adhesive bonds by calculating the contact angle between the surface and the vesicle. The contact angle information is measured via microinterferometry. Moreover, using a ternary mixture of lipids, we study the effect of adhesion on the formation of liquid domains using fluorescence microscopy. Thus, a model system is developed to probe how variable adhesive linker densities affect lipid organization in the membrane.

BP 12.38 Tue 14:00 Poster B2

Complexity of micelle formation as studied by a minimum particle-based model — ●SIMON RASCHKE and ANDREAS HEUER — Institute of Physical Chemistry, WWU Münster, Correnstr. 28/30 48149 Münster, Germany

The formation of self assembled structures such as micelles has been intensively studied and is well understood. The ability of a solution of amphiphilic molecules to develop micelles is depending on the concentration and characterized by the critical micelle concentration (cmc), above which micelle formation does occur. We developed a minimalistic coarse grained model for amphiphilic molecules in the continuum and simulated the time evolution via dynamic Monte Carlo simulations in the canonical (NVT) ensemble. This approach enables long timescales and allows studying of related processes. The model is also capable of simulating the frame-guided assembly process [1], which makes vesicle formation into a predefined frame possible and reliable below cmc. Equilibration in the cmc domain turns out to happen on very long timescales and the cluster formation is highly non trivial. We discuss the influences of local energies, curvature, frame-guides and disorder and their connection to the processes of cluster formation.

[1] Y. Dong, D. Liu, Angewandte Chemie International Edition 2014, 10, 53.

BP 12.39 Tue 14:00 Poster B2

The impact of antifoam agents on lipid membranes at the air-water-interface — ●MIKE MORON, MICHAEL PAULUS, JULIA NASE, SUSANNE DOGAN, and METIN TOLAN — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

The control of foam by means of antifoam agents is of great importance in a number of industrial and medical applications. For example, the

oral medication of simethicone is prescribed in the case of surfactant intoxication and also in order to dispose patients for colonoscopy. While the macroscopic behavior of liquid systems containing antifoam agents and lipids is well described, the behavior of antifoam agents on the molecular scale is not completely understood.

We present surface pressure-dependent in-situ X-ray reflectometry (XRR) experiments and a Brewster-angle microscopy (BAM) study on Langmuir monolayers consisting of different lipids and antifoam agents. Both, the XRR and BAM measurements were performed at the liquid-air interface.

A stearic acid monolayer served as a model for a foam lamella and the impact of an industrial used antifoam agent was analysed. Furthermore, a dipalmitoylphosphatidylcholine (DPPC) monolayer was prepared to mimic a cell membrane and the impact of the medical antifoam agent simethicone was studied. The measurements showed a strong effect on the lipid layers structure for low surface pressures of the lipid films. For high surface pressures the antifoam agents had little to nearly no effect on the lipid films.

BP 12.40 Tue 14:00 Poster B2

3D-Printed Microfluidic Chip to Study Protein Organization in a Lipid Bilayer — ●SEVDE PUZDA, RALF SEEMANN, and JEAN-BAPTISTE FLEURY — Saarland University, Saarbruecken, Germany

We developed a layout for a 3D microfluidic chip whose master can be fabricated by state of the art 3D-Printing. The microfluidic chip allows to form, in a quasi-automatic manner, a free-standing lipid bilayer. The bilayer is produced by contacting two water droplets in an oil phase, where lipids molecules have been dispensed. Interestingly, this method does not require any microfluidic pumps (volume, or pressure). The bilayer formation is demonstrated by electrophysiological measurements and optical investigations with a normal view direction onto the bilayer. Proteins are reconstitute in this bilayer, and their dynamical self-organization properties are study in-situ.

BP 12.41 Tue 14:00 Poster B2

Small-angle X-ray Scattering on Photo-switchable Lipid Membranes — ●MARTINA OBER¹, PATRICK URBAN¹, STEFANIE PRITZL¹, DAVID KONRAD², DIRK TRAUNER^{2,3}, THEOBALD LOHMÜLLER^{1,3}, and BERT NICKEL^{1,3} — ¹Department of Physics, and Center for Nano Science, Ludwig-Maximilians-Universität, Munich, Germany — ²Department of Chemistry and Center of Integrated Protein Science, Ludwig-Maximilians-University, Munich, Germany — ³Nanosystems Initiative Munich, Germany

Light-switchable lipids which are prepared by incorporation of a photo-sensitive azobenzene into a phosphatidylcholine (Azo-PC) enabled a novel approach to study and control the properties of membranes. Azo-PC undergoes a reversible photo-isomerisation of cis- and trans-state on irradiation with UV, respectively visible light, which is well understood on the molecular level. The photo-isomerisation induces a configurational change in the lipid which further affects the overall structure of an Azo-PC membrane. Here, we use small-angle x-ray scattering (SAXS) to perform structure analysis and phase behaviour studies of Azo-PC membranes in a physiological environment. Our research will help to extend the molecular control of photo-switchable lipids to a control of photo-switchable membranes in order to investigate membrane perforation, drug release, and membrane enzyme activity.

BP 12.42 Tue 14:00 Poster B2

Mechanical parameters of phospholipid multi-layers from off-specular x-ray scattering — ●MAX SCHEU, TIM SALLDITT, KILIAN FRANK, and KARLO KOMOROWSKI — Institut für Röntgenphysik, Göttingen

The structural analysis of phospholipid bilayers which exert a prominent role in different biological systems is of increasing importance for understanding processes such as membrane adhesion or fusion. In order to determine the continuum mechanical parameters namely compression and bending modulus of solid-supported phospholipid multi-layers different specular and off-specular x-ray scattering experiments were conducted. Via comparison to smectic elastic theory the results give insight to membrane dynamics as well as to potential pre-critical phenomena prior to the so-called stalk phase transition. We used a model with three free parameters, derived from membrane displacement correlation functions in the kinematic approximation of the scattering function, to describe stratified interfaces of membranes with correlated roughness. This model was used to simulate complete reciprocal space maps and extract the bending rigidity and the compression modulus from experimental data. In particular the structural changes

of lamellar phases of different phospholipids, promoted by change in relative humidity or ionic environment, are evaluated by measurement and modeling in direct vicinity of bragg peaks. These findings may help to ascertain further insight on interaction potentials of membranes as well as transmembrane cellular medication uptake.

BP 12.43 Tue 14:00 Poster B2

Study of the Structure and Kinetic of Photoswitchable Lipid Monolayers Influenced by Different Sugar Groups — ●SVENJA CAROLIN HÖVELMANN¹, JONAS ERIK WARIAS¹, ALEXANDER HEBEL¹, FRANZISKA REISE³, THISBE LINDHORST³, OLAF MAGNUS MAGNUSSEN¹, and BRIDGET MARY MURPHY^{1,2} — ¹Institut für Experimentelle und Angewandte Physik, University of Kiel, Germany — ²Ruprecht Haensel Laboratory, University of Kiel, Germany — ³Otto Diels-Institut für Organische Chemie, University of Kiel, Germany

The phospholipid membranes with their mechanical and dynamical properties have an important role in biological functions. To study these properties we use a model system of a Langmuir film of amphiphilic phospholipids with embedded photoswitchable molecules. These molecules are glycolipids containing an azobenzene photoswitch between the chain and the head group and are embedded in a monolayer of dipalmitoylphosphatidylcholine (DPPC). In order to investigate the influence of a different number of sugar groups attached to the molecules multiple molecules are prepared. Langmuir isotherms and X-ray reflectivity are used to study the structural differences between the molecules and the structural changes when illuminated as the orientation of the azobenzene-glycolipid switches reversibly between trans- and cis-conformation by illumination of UV and blue light. Differences between the molecules in terms of their switching behaviour and membrane conformations can be observed.

BP 12.44 Tue 14:00 Poster B2

Protein-radical interaction: structure analysis using atomic force microscopy — ●SANJAI KARANTH^{1,2}, UNA JANKE^{1,2}, and MICHAELA DELCEA^{1,2} — ¹Institute of Biochemistry, University of Greifswald, Greifswald, Germany — ²ZIK HIKE, University of Greifswald, Greifswald, Germany

Reactive nitrosative species (RNS) such as nitric oxide (NO.) released in the body attack the thiol groups of proteins altering their function (e.g. protein activation upon ligand binding)[1]. Here, we investigate in a biomimetic system the interaction of RNS with integrin α IIb β 3 (a α IIb β 3)- a transmembrane protein present on blood platelets and responsible for thrombotic activity. α IIb β 3 protein was reconstituted into nanodiscs which generate planar lipid bilayers which stabilize the protein. Using atomic force microscopy (AFM) imaging, we were able to distinguish the different states of protein (i.e. open/active and closed/bent state). Radical attack on the nanodiscs was performed and structural analysis was carried out using AFM imaging and single molecule force spectroscopy (SMFS). Nanodiscs prove to be a reliable membrane system to study biophysical properties of transmembrane proteins.

[1] Mor-Cohen, R. (2016). Disulfide bonds as regulators of integrin function in thrombosis and hemostasis. *Antioxidants & redox signaling*, 24(1), 16-31.

BP 12.45 Tue 14:00 Poster B2

Limiting shapes of confined lipid vesicles — ●BOR KAVČIČ¹, AI SAKASHITA^{2,3}, HIROSHI NOGUCHI³, and PRIMOŽ ZIHERL^{4,5} — ¹IST Austria, Klosterneuburg, Austria — ²Ochanomizu University, Tokyo, Japan — ³University of Tokyo, Tokyo, Japan — ⁴University of Ljubljana, Ljubljana, Slovenia — ⁵Jožef Stefan Institute, Ljubljana, Slovenia

We theoretically study the shapes of lipid vesicles confined to a spherical cavity, elaborating a framework based on the so-called limiting shapes constructed from geometrically simple structural elements such as double-membrane walls and edges. Partly inspired by numerical results, the proposed non-compartmentalized and compartmentalized limiting shapes are arranged in the bilayer-couple phase diagram which is then compared to its free-vesicle counterpart. We also compute the area-difference-elasticity phase diagram of the limiting shapes and we use it to interpret shape transitions experimentally observed in vesicles confined within another vesicle. The limiting-shape framework may be generalized to theoretically investigate the structure of certain cell organelles such as the mitochondrion.

BP 12.46 Tue 14:00 Poster B2

Influencing liposome structure by terpenoids: a TEM anal-

ysis — •BERNHARD KALTSCHMIDT, INGA ENNEN, DANIELA RAMERMANN, and ANDREAS HÜTTEN — Thin Films & Physics of Nanostructures, University of Bielefeld, Bielefeld, Germany

Today, multiresistant bacteria are more and more common in hospitals. Therefore the development of novel treatments is mandatory. Terpenoids are plant substances with antimicrobial activity. A new approach is to use the antibacterial properties of terpenoids as therapeutics. Since most terpenoids are insoluble in water, here we dissolved them in EtOH and used liposomes as carriers. Liposomes are nanoscale spherical vesicles, which were produced with an extruder and then analysed by Cryo transmission electron microscopy (Cryo-TEM). Different approaches were tested to determine the best imaging parameters. As terpenoids 1,8 cineol, campher, menthol and thymol of pharmaceutical grade were used. Cryo-TEM revealed a gradient of multi-lamellar liposomes to unilamellar liposomes. The highest antibacterial activity could be shown by thymol.

BP 12.47 Tue 14:00 Poster B2

Subsampling impact on the inferred properties of cortical networks — •MEHRDAD HASANPOUR^{1,2}, PAOLO MASSORBIO³, and ANNA LEVINA^{1,2} — ¹University of Tübingen, Germany — ²MPI for Biological Cybernetics, Germany — ³University of Genova, Genova, Italy

Uncovering the topological properties of the brain network is essential for understanding brain function. Typically network structure is inferred from observations of a tiny fraction of the system, resulting in a severe subsampling of the whole network. How this inevitable subsampling influences the inferred network properties, such as the widely used small-world index, remains mostly unknown. The small-world index is defined as a clustering coefficient divided by diameter. For random, small-world, and scale-free networks we demonstrate analytically and numerically that the subsampling preserves the clustering coefficient. However, the diameter is strongly influenced by the subsampling, biasing the inference of small-worldness in subsampled networks. Our primary goal is to understand how to correct for such bias rigorously. Brain networks have a highly complex structure that is not captured by simple random networks we consider in theoretical studies. For a more realistic comparison, we investigate functional networks extracted from the High-Density Multi-Electrode Array recordings from cortical cultures using transfer entropy. The extracted network contains 4096 nodes, allowing for a further subsampling. We demonstrate that already the thresholding procedure used for extraction of the binary network is strongly influenced by subsampling.

BP 12.48 Tue 14:00 Poster B2

Influence of nanostructured polymer surfaces on neuronal development — •FRANO MILOS¹, ANDREEA BELU¹, DIRK MAYER¹, MARIA ROSA ANTONGNAZZA², VANESSA MAYBECK¹, and ANDREAS OFFENHÄUSSER¹ — ¹Institute of Complex Systems ICS-8, Forschungszentrum Jülich GmbH, Jülich, Germany — ²Center for Nano Science and Technology @Polimi, Istituto Italiano di Tecnologia, Milano, Italy

The complexity of the extracellular matrix consists of micro- and nanoscale structures that influence neuronal development, differentiation, and neuritogenesis through contact guidance. Therefore, the ability to manipulate neuronal growth has great implications for both neuronal repair and the potential design of implantable biomedical devices. We employ precisely designed nanostructured polymers to investigate the effects of surface topography on growth and guidance of primary cortical neurons using time-lapse fluorescent microscopy. Recently, we demonstrated that nanoscale pillars accelerate axon establishment and change the periodicity of the axon growth dynamics resulting in longer axons aligned to the underlying topography. These results demonstrate that axon growth can be modulated and guided by the dimensions of physical cues on the surface. Axon growth cones sense their environment through complex signaling pathways that modulate cytoskeletal dynamics and induce growth in a specific direction. Therefore, we aim to investigate F-actin dynamics and mechanosensing in relation to surface topography during different stages of development to elucidate the mechanisms underlying the topography-induced responses.

BP 12.49 Tue 14:00 Poster B2

Spike Termination in Networks of Bistable Neurons — •MUHAMMET UZUNTARLA¹, JOAQUIN J. TORRES², ALI CALIM¹, and ERNEST BARRETO³ — ¹Department of Biomedical Engineering, Bulent Ecevit University, Turkey — ²Department of Electromagnetism and Physics of the Matter, University of Granada, Spain —

³Department of Physics and Astronomy, George Mason University, USA

In neural systems, synchronization is widely considered to be responsible for the origin of oscillatory brain rhythms. Findings from experimental and theoretical studies suggest that it results from interplay between intrinsic properties of individual neurons, synaptic interaction dynamics and topological features. An interesting synchronization-induced emergent behavior is termination of ongoing population activity. We observe and study this phenomenon whereby neural activity spontaneously ceases. Here, we investigate the behavior of three types of networks composed of bistable HH neurons with a scale-free topology, involving either electrical or chemical synapses that are either excitatory or inhibitory. We find that periodic synchronous population activity emerges in all three networks, and strongly synchronized population spiking events lead to complete cessation of activity in excitatory networks, but not in gap junction or inhibitory networks. We identify the underlying mechanism responsible for this phenomenon by examining the particular shape of excitatory postsynaptic currents. We also examine the effects of the synaptic time constant, coupling strength, and channel noise on the occurrence of the phenomenon.

BP 12.50 Tue 14:00 Poster B2

Taming the bias when estimating correlations from spike recordings — JENS WILTING¹, JOHANNES ZIERENBERG¹, •LEONHARD LEPPIN^{1,2}, and VIOLA PRIESEMANN¹ — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Georg-August-Universität Göttingen, Germany

What can we infer about a dynamical system if we can only observe a very small part of it? The problem of subsampling is common to the study of many systems. It is particularly severe in neuroscience, because electrophysiological recordings of spiking activity can only assess a small fraction of all neurons simultaneously. This subsampling has hindered characterizing even most basic properties of collective spiking in cortical networks. We proved that whenever a population is subsampled, the observed spike count cross-correlation between the populations can be strongly underestimated. The same holds for the autocorrelation strength of subsampled activity of a single population. These limitations hinder the correct inference of the underlying network dynamics. To overcome the systematic bias, we derived a novel estimator, which can infer properties of activity propagation even under strong subsampling. In this framework, the dynamical state is characterized by the average number of spikes triggered causally by a single spike in a neuron. Our generalization of the estimator to many populations now enables us to infer afferent contributions, recurrent propagation within a population, and reciprocal propagation between populations, and thereby enables us to contribute to identifying functional connections between brain areas.

BP 12.51 Tue 14:00 Poster B2

Tailored dynamic range using an ensemble of networks — •JOHANNES ZIERENBERG¹, JENS WILTING¹, VIOLA PRIESEMANN¹, and ANNA LEVINA² — ¹Max Planck Institute for Dynamics and Self-Organization — ²Tübingen University

The dynamic range quantifies the range of inputs that a neural network can discriminate. It is maximized at a non-equilibrium phase transition. However, besides the actual size of the dynamic range, it is crucial that the interval of discriminable inputs covers the relevant inputs. We show analytically for a generic spiking model that – while the dynamic range indeed is maximal at criticality – the discriminable intervals are virtually indistinguishable from each other in the vicinity of the phase transition. We identify the constrained discriminable interval to be a result of *coalescence* (the simultaneous activation of the same unit from multiple sources). In our model, we can compensate coalescence by implementing adaptive synaptic weights and thereby obtain specific discriminable intervals that can be tuned by changing the distance to criticality. This enables us to optimally address particular tasks by constructing tailored ensembles of coalescence-compensated networks, e.g., discriminating very broad or bimodal input distributions, with implications for machine learning approaches such as reservoir computing networks.

BP 12.52 Tue 14:00 Poster B2

Signatures of criticality in efficient coding networks — •SHERVIN SAFAVI^{1,2}, MATTHEW CHALK³, NIKOS LOGOTHETIS¹, and ANNA LEVINA^{1,2} — ¹MPI for Biological Cybernetics — ²University of Tübingen — ³Institut de la Vision, Sorbonne Université

Theoretical and experimental evidence brought forward a hypothesis that the brain operates close to a critical state. Numerous studies investigated neural models that can attain various distances to criticality depending on a control parameter and quantified information processing capabilities as a function of closeness to criticality. However, quantifying these capabilities in a general sense is not sufficient to assure usefulness of criticality for the brain. Therefore, we introduce a complementary approach. We study a network that is optimized for a task relevant for the brain. Then, we investigate whether we observe the scale-free neuronal avalanches exclusively in the optimized network. More specifically, we used a network of leaky integrate-and-fire neurons with parameters optimized for efficient coding. Previously, it was shown that performance of such networks varies non-monotonically with the noise amplitude. We discovered, that only in the network with optimal noise level the avalanche size distribution follows a power-law and with too low or too high noise, the network appears either supercritical or sub-critical, respectively. We demonstrate that scale-free distribution of neuronal avalanches might be a consequence of optimal efficient coding in spiking neural networks. This result has important implications, as it shows how two influential, and previously disparate fields - efficient coding, and criticality - might be intimately related.

BP 12.53 Tue 14:00 Poster B2

Evidence of quantum consciousness in evoked zero-spin echoes — ●CHRISTIAN KERSKENS¹ and DAVID LOPEZ^{1,2} — ¹Trinity College Institute Neuroscience, Trinity College Dublin — ²Faculty of Psychology, University of Warsaw, Warsaw, Poland

That consciousness could have its' basis in quantum computing has been speculated for many years. Unfortunately, unitary quantum gates, the main ingredient of quantum computing, are not compatible with irreversible biological systems which are effectively non-unitary. This is in line with experiments which so far haven't connected consciousness to quantum computing. Here, we used magnetic resonance imaging (MRI) to study long-range quantum coherence in the human brain. We were surprised to find that the cardiac pressure pulse evoked zero-spin echoes (ZSEs) in brain parenchyma. The ZSE signals, which are thought to be generated by long-range intermolecular zero-quantum coherence (iZQC), were much higher than expected. In contrast, single quantum coherence (SQC) imaging, which is also indirectly related to iZQC, was not affected. These findings suggest that we observed a non-classical effect originated from a small subdomain of the parenchyma. This evoked quantum effect was directly connected to consciousness as only sporadic ZSE signals were detected during sleep while a loss of the evoked quantum effect would probably always result in unconsciousness because the cardiac pressure pulse is necessary for consciousness. Our findings are unexpected but in line with recent biological research.

BP 12.54 Tue 14:00 Poster B2

Topological reinforcement as a principle of modularity emergence in brain networks — ●FABRIZIO DAMICELLI¹, CLAUS-CHRISTIAN HILGETAG^{1,3}, MARC-THORSTEN HÜTT², and ARNAUD MESSE¹ — ¹Institute of Computational Neuroscience, University Medical Center Hamburg-Eppendorf, Hamburg University, Germany — ²Department of Life Science and Chemistry, Jacobs University Bremen, Germany — ³Department of Health Sciences, Boston University, USA

The self-organization of modular structure in brain networks is mechanistically poorly understood. We propose a simple plasticity model based on a fundamental principle, the Topological Reinforcement (TR), which promotes connections between nodes with high neighborhood similarity. This mechanism systematically evolves synthetic random networks toward a modular architecture by enhancing initial weak "proto-modules". Moreover, we show that this topological selection principle can also be implemented in biological neural networks evolving in a Hebbian fashion, where what "fires together, wires together" and, under proper conditions, the results were consistent between both scenarios, i.e., TR and Hebbian rule. We propose the selective reinforcement of topological overlap as a fundamental principle guiding the emergence of modular structure in brain networks. This bridges the gap between previous pure generative and activity based models of modularity emergence in brain networks, offering a common underlying principle at the topological level.

BP 12.55 Tue 14:00 Poster B2

Taming Stochastic, Nonlinear Rate Neurons With Field Theory — ●JONAS STAPMANN^{1,2}, TOBIAS KÜHN¹, DAVID DAHMEN¹,

CARSTEN HONERKAMP², and MORITZ HELIAS^{1,3} — ¹Institute of Neuroscience and Medicine (INM-6), Forschungszentrum Juelich, Germany — ²Institute for Theoretical Solid State Physics, RWTH Aachen, Germany — ³Department of Physics, Faculty 1, RWTH Aachen, Germany

Many phenomena observed in biological neural networks can only be explained by assuming nonlinear interactions. Due to effects like synaptic failure and channel noise, neuronal dynamics is also inherently stochastic. The investigation of the interaction of both of these properties is challenging because due to the nonlinearity, correlations of higher order influence those of lower order.

To cope with this problem, the dynamics of a self-interacting stochastic rate neuron is reformulated in the language of field theory by means of the Martin, Siggia, Rose, de Dominicis and Janssen formalism. The loop-wise fluctuation expansion of the corresponding effective action then incorporates corrections to the mean dynamics and time-dependent statistics due to fluctuations in the presence of nonlinear neuronal gain. From this, we derive a deterministic non-Markovian equation of motion of the mean value which illustrates that the interaction of nonlinearity and stochasticity introduces memory into the system.

BP 12.56 Tue 14:00 Poster B2

Estimating autocorrelation times of subsampled autoregressive processes under non-stationary parameters — ●JORGE DE HEUVEL, JENS WILTING, VIOLA PRIESEMANN, JOHANNES ZIERENBERG, and PAUL SPITZNER — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland

Collective cortical dynamics are often approximated by linear autoregressive models. Only recent methodological advances enable us to infer network autocorrelation times even under subsampling, assuming stationarity. However, cortical dynamics are likely subject to non-stationary input, which can lead to a severe overestimation of the network autocorrelation time. Here, we present a novel approach for the subsampling-invariant estimation of network autocorrelation even under non-stationary input. A trial based experimental setup is applied, where the external input is time-dependent but similar over each trial. Our estimator is verified on both numerical data and experimental recordings.

BP 12.57 Tue 14:00 Poster B2

Synchronization of cilia — ●BENJAMIN M. FRIEDRICH — cfaed, TU Dresden, Dresden, Germany

I will present a historical overview on synchronization of cilia and flagella, featuring key experiments in the field. Two mechanisms, (i) synchronization by direct hydrodynamic interactions and by (ii) mechanical self-stabilization in self-propelled swimmers will be addressed. I will review the minimal model of rotating spheres of Vilfan and Jülicher, which has been influential in the field. This model highlights how synchronization depends on broken parity-time symmetry. Recently, this theoretical model has been realized experimentally using colloidal particles driven by optical tweezers.

BP 12.58 Tue 14:00 Poster B2

Reconstitution of cilia-like beating — ●VEIKKO F. GEYER — Technische Universität Dresden, B CUBE - Center for Molecular Bioengineering, Dresden, Germany

I will present a historical overview on the study and reconstitution of bending oscillations in filament bundles and cilia-like beating, featuring key experiments and major challenges in the field.

To study ciliary beating, two approaches have been used: (i) the top-down (study of the dynamics of ciliary fragments) and (ii) the bottom-up (combining ciliary components - filaments, motors, cross-linkers) approach.

I will review the known requirements for bending oscillations in a minimal motor-filament system and discuss how those requirements have been tested experimentally by different approaches and by different groups.

BP 12.59 Tue 14:00 Poster B2

Interaction of superparamagnetic iron oxide nanoparticles and transferrin — ●ULRIKE MARTENS¹, ALI ABOU-HASSAN², and MIHAELA DELCEA¹ — ¹Institute for Biochemistry/ZIK HIKE, Greifswald University, Germany — ²Laboratoire PHENIX, Sorbonne Université, Paris, France

Recent research demonstrated that nanoparticles (NPs) can enhance or suppress the immune response by binding to proteins of the blood

stream. One important blood protein is transferrin which is composed of two distinct domains each containing an iron binding site. Its main role is to deliver iron to all biological tissues. By applying various biophysical techniques we investigated the interactions of superparamagnetic iron oxide nanoparticles (SPIONs) including maghemite $\gamma\text{-Fe}_2\text{O}_3$ and magnetite Fe_3O_4 with different coatings (e.g. citrate, chitosan) with transferrin. SPIONs present many advantages related to their magnetic properties, including magnetic manipulation and separation. The tools used allowed the characterization of the functionalized NP surface and the identification of structural changes of the proteins (e.g. circular dichroism spectroscopy) upon interaction with nanoparticles. In particular, dynamic light scattering measurements as well as SDS-PAGE revealed the corona formation of our model protein transferrin on the NPs, while transferrin also acted as a stabilizing agent of the colloidal suspension as verified by zeta potential measurements. In addition, the influence of the NPs on the iron binding site of transferrin in comparison to the binding to iron-free transferrin (apotransferrin) was studied via UV-Vis spectroscopy and urea PAGE.

BP 12.60 Tue 14:00 Poster B2

Principal component analysis of constrained molecular dynamics simulations — ●MATTHIAS POST, STEFFEN WOLF, and GERHARD STOCK — Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, Freiburg, Germany

Describing the structure and dynamics of biomolecular systems via conventional unbiased molecular dynamics simulations becomes impractical, if their states are separated by high energy barriers such that conformational changes of interest do not occur in reasonable computer time. One way to overcome this problem is to pull these systems with a constant force ensuring this conformational change. While data from constrained molecular dynamics simulations do not allow for a direct estimate of the free energy from their biased probability distribution, they can be readily reweighed via Jarzynski's identity to do so. Using this approach, we apply principal component analysis on these non-equilibrium data to construct a multi-dimensional free energy landscape able to distinguish between different reaction pathways. We compare unbiased and constrained data on deca-alanine, a well-established model problem of testing biased simulations and understanding fundamental mechanisms of protein folding.

BP 12.61 Tue 14:00 Poster B2

Identification of metastable conformational states of protein dynamics — ●DANIEL NAGEL — Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, 79104 Freiburg, Germany

Well-defined microstates, describing metastable conformational states, are the key to generate a Markov state model of protein dynamics. Taking a dimensional-reduced trajectory, these can be found by a recently proposed density-based geometrical clustering algorithm by Sittel et al., which is self-consistent in its data-based input parameters and computationally efficient. While for simple geometrical clustering methods such as k -means it was necessary to rely on a large number of microstates to properly discretize barriers and subsequently use dynamic clustering techniques to reduce the large set of microstates to a manageable number of macrostates, density-based clustering by design cuts at the energy barriers producing directly a reasonable number of microstates. Even though the latter algorithm performs much better, projection artifacts in the transition regions artificially shorten the estimated lifetimes. A simple corrective is to use dynamical boundary corrections, namely dynamical coring which requires staying for a minimum time after a state transition in the new state for the transition to be counted. This method increases metastability and Markovianity significantly by identifying misclassified interstate fluctuations as intrastate fluctuations. To illustrate the simplicity and performance of the workflow, two well-established biomolecular systems (alanine dipeptide and villin headpiece) are examined.

BP 12.62 Tue 14:00 Poster B2

Optimizing PDMS Stamp Transfer Preparation of MoS_2 -Nanopores for DNA Translocation Experiments with Optical Tweezers — ●JULIAN CREMER¹, INGA ENNEN², SEBASTIAN KNUST¹, MARTINA VIEFHUES¹, and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience, Bielefeld University, Germany — ²Thin Films & Physics of Nanostructures, Bielefeld University, Germany

To better understand the translocation of biological molecules through nanopores we measure the forces acting on λ -DNA during a translocation through solid-state nanopores with Optical Tweezers. For high

sensitivity, we milled pores smaller than 10 nm with a transmission electron microscope (TEM) in freestanding MoS_2 -monolayers with a thickness of 0.67 nm.

The defect-free MoS_2 -monolayers are produced by a simple but efficient viscoelastic PDMS stamp transfer technique. Since the contact with PDMS causes minute but nevertheless relevant residues on the MoS_2 we investigated the removal of these residues particularly with regard to enable nanopore experiments. Thus, we performed high-resolution TEM as well as atomic force microscopy (AFM) measurements to optimize the preparation. These include pretreatments of the PDMS e. g. UV-ozone cleaning as well as variations of the PDMS stamp thicknesses and steps after the transfer like annealing or plasma treatment.

In this work we present first results towards the preparation of free-standing residue-free MoS_2 -nanopores and controlled translocation experiments.

BP 12.63 Tue 14:00 Poster B2

Protein interactions studied by single molecule force spectroscopy — ●ANNELIE KLEIN^{1,2}, INA BUCHHOLZ^{1,2}, FELIX NAGEL^{1,2}, and MIHAELA DELCEA^{1,2} — ¹Biochemistry Institute, University of Greifswald, Felix-Hausdorff-Str. 4, 17487 Greifswald, Germany — ²ZIK HIKE, University of Greifswald, Fleischmannstr. 42, 17489 Greifswald, Germany

Endogenous proteins (i.e. self-proteins) which undergo mutations or post-translational modifications under stress conditions (e.g. pH, salt, drugs) may suffer alterations of their function often leading to autoimmune diseases. For example, the soluble non-blood protein serine protease inhibitor Kazal type 1 (SPINK1) is associated with chronic pancreatitis. The mechanism of this disease is not well understood. Here, we investigate the interaction of wild type and mutant SPINK1 with trypsin by single molecule force spectroscopy (SMFS). SPINK1 is a trypsin inhibitor in the pancreas and its mutation N34S is associated with hereditary chronic pancreatitis. In a biological trypsin inhibition assay we showed that wild type and mutant have the same inhibitory activity. However, the sensitive SMFS technique revealed a clear difference in the binding of trypsin to wild type SPINK1 (~94 pN) and to mutated N34S (~45 pN), respectively. Our results indicate that N34S mutation affects SPINK1 inhibitory efficiency, which could lead to chronic pancreatitis.

BP 12.64 Tue 14:00 Poster B2

Characterization of Magnetic Field Generating Tips for Spatio-Temporally Controlled Manipulation of Magnetic Nanoparticles — ●MOHAMMAD R. SAFARI and CORNELIA MONZEL — Experimental Medical Physics, Heinrich-Heine University Düsseldorf, 40225 Düsseldorf, Germany

The manipulation of magnetic nanoparticles is a powerful approach to probe and actuate biological functions in living systems and bears high potential for future medical applications. In comparison to complementary approaches involving chemical and electrical field manipulation, magnetic fields bear the advantage of applying a remote and spatio-temporally defined stimulus, which is nondestructive in the context of a biological sample. In view of realizing the manipulation of single cell functions, we here utilize micrometer magnetic tips to take advantage of their high spatial flexibility, variability in shape, and hence the possibility to dynamically tune magnetic fields and forces. We combine experimental magnetic nanoparticle tracking with in vitro attraction assays and finite element modeling, in order to obtain a comprehensive understanding of the magnetic forces applied (~10fN). Via systematic characterization of a library of different magnetic tips, we assess their suitability for nanoparticle manipulation approaches on submicrometer scales.

BP 12.65 Tue 14:00 Poster B2

AFM-based Single-Molecule Force Spectroscopy on the Streptavidin:Biotin Interaction — ●STEFFEN M. SEDLAK¹, LEONARD C. SCHENDEL¹, KATHERINE R. ERLICH¹, ACHIM LÖF¹, RAFAEL C. BERNARDI², MAGNUS S. BAUER¹, CARLEEN KLUGER¹, and HERMANN E. GAUB¹ — ¹Department of Physics and Center for NanoScience, LMU Munich, Germany — ²University of Illinois at Urbana-Champaign, Urbana, IL, USA

The high-affinity interaction of the small molecule biotin with the tetrameric protein streptavidin (SA) is a widely applied tool for detection, labeling and immobilization of molecules. We study single biotin:SA interactions under force using AFM-based single-molecule force-spectroscopy (SMFS) and steered Molecular Dynamics (sMD)

simulations. Probing monovalent SA in various specific tethering geometries, we investigated how the mechanical stability of the biotin:SA interaction depends on the force loading geometry and revealed the underlying molecular mechanism. We made use of the different unbinding forces to realize a protein-based bottom-up nanoscale assembly of single fluorescent molecules by single-molecule cut-and-paste; a unique approach that enables spatially controlled arrangements of diverse molecules into a single ensemble. We also studied SA of different valencies and distinguished unbinding forces of biotin from different SA subunits in AFM-based SMFS. sMD allowed to understand the force-propagation pathways through the SA tetramer. Identifying a long-lived tethering geometry, we can reliably measure single molecules at comparably high constant forces for many hours in magnetic tweezers.

BP 12.66 Tue 14:00 Poster B2

Narrow escape: How long does it take for a camel to go through the eye of a needle? — •ELISABETH MEISER¹, SUSANNE FENZ¹, REZA MOHAMMADI², and NICOLAS VOGEL² — ¹University of Würzburg, Biocenter: Cell and Developmental Biology, Würzburg, Germany — ²Friedrich-Alexander University Erlangen-Nürnberg, Institute of Particle Technology, Erlangen, Germany

The narrow escape problem (NEP) is a common problem in biology and biophysics. It deals with Brownian particles confined to a given domain with reflecting borders and only a small escape window. The mean first passage time of the particle can be calculated analytically for diffusion in two and three dimensions in several geometries. We aim to systematically test the solution of the NEP in two dimensions with micro-patterned planar model membranes. Micro-patterned membranes were produced by a lithography-based method to achieve patterned glass followed by vesicle fusion. Two lithography methods were tested: UV- and colloid-lithography. UV-lithography relies on a UV-cross-linkable resist to produce a pattern of hydrophilic and hydrophobic regions on the substrate by selective illumination. Colloid-lithography is alternative approach to prepare particular small membrane patches (d=1µm). It exploits the shadowing effect of polymeric microspheres whilst coating the substrate with a thin layer of gold to achieve a structured gold film. After appropriate functionalization of the gold, membranes will only form on the bare glass. We will present our first results on membrane patterning and diffusion in solid supported lipid bilayers on the single-molecule level.

BP 12.67 Tue 14:00 Poster B2

Microfluidic rock-like reactors to study the synthesis of the first nucleotides — •THOMAS MATREUX¹, MAXIMILIAN WEINGART¹, VICTOR SOJO¹, DAVID LAPPE¹, SAIDUL ISLAM², MATT POWNER², CHRISTOF B. MAST¹, and DIETER BRAUN¹ — ¹Systems Biophysics, Ludwig-Maximilian University of Munich (LMU) — ²Department of Chemistry, University College London (UCL)

The emergence of the first biomolecules is one of the most intriguing questions in the origins of life field. While synthesis pathways of nucleotides, amino acids and lipids were widely addressed in the last decade [1], their feasibility under geologically plausible boundary conditions is still unclear. How do laboratory experiments transfer to a realistic, prebiotic scenario with catalytic rock surfaces and thermal non-equilibrium boundary conditions and without clearly separated pipetting steps?

To address these questions, we have developed a microfluidic setup that allows for controlled, but prebiotically plausible sequential mixing by the presence of porous geo-material and provides an uninterrupted flow to produce activated nucleotides [1]. Microfluidic structures are made from FEP, which lets us focus on the interactions with the added synthetic rock. The reaction chambers are sandwiched between highly heat conducting sapphire plates ensuring complete thermal control including possible thermal gradients. This new experimental approach offers a variety of new reaction schemes by connecting prebiotic chemistry with geoscience and non-equilibrium physics.

[1] Sutherland Nature doi.org/10.1038/nature08013 (2009)

BP 12.68 Tue 14:00 Poster B2

Correlated Single Molecule Twist and Fluorescence Measurements on CRISPR-Cas Systems — •PIERRE ALDAG¹, JULIENE MADARIAGA², INGA SONGAILIENE³, VIRGINIUS SIKSNYS³, and RALF SEIDEL¹ — ¹Peter Debye Institute for Soft Matter Physics, University of Leipzig — ²Centro Nacional de Biotecnología (CSIC), Madrid — ³Institute of Biotechnology, Vilnius University

CRISPR-Cas systems are RNA-guided ribonucleoprotein (RNP) complexes with nuclease activity that provide prokaryotes with an adaptive

defense mechanism against foreign nucleic acids. The RNP complex recognizes complementary target sites by base-pairing its RNA component with one of the strands of the target DNA while displacing the other one forming a so-called R-loop structure. Considering the vast potential of CRISPR-Cas systems in gene editing technology, it is crucial to fully understand the mechanism behind the targeting process by these enzymes. Here, we employed a combined magnetic tweezers and total internal reflection fluorescence microscopy setup to carry out correlated single-molecule force and fluorescence spectroscopy measurements. The magnetic tweezers allow us to probe the R-loop formation of the CRISPR system. Using fluorescently-labelled Cascade complexes we are able to additionally follow association and dissociation events prior to the actual R-loop formation. These measurements reveal information about the timescales of the target search as well as about the efficiencies of the search under varying torque conditions. This leads to a better understanding of the target recognition mechanisms by CRISPR-Cas enzymes.

BP 12.69 Tue 14:00 Poster B2

Understanding the Sequence-Structure-Mechanics Relationship of Coiled Coil Dimers under Shear — MELIS GOKTAS, CHUANFU LUO, PATRICIA LOPEZ-GARCIA, ISABELL TUNN, RUBY M. A. SULLAN, ANA E. BERGUES-PUPO, ANA VILA VERDE, REINHARD LIPOWSKY, and •KERSTIN G. BLANK — Max Planck Institute of Colloids and Interfaces, Potsdam Golm Science Park, 14424 Potsdam, Germany

Coiled coils (CCs) are superhelical motifs found in many cytoskeleton and extracellular matrix proteins, suggesting that they possess mechanical function in Nature. Despite their wide abundance, surprisingly little is known about their molecular, mechanistic response to forces. With the goal of shedding light on their sequence-structure-mechanics relationship, we have characterized a series of CC heterodimers with AFM-based single molecule force spectroscopy (SMFS) and Molecular Dynamics simulations. The SMFS experiments show that CCs with a length of 3-5 heptads rupture at forces between 20-55 pN, when mechanically loaded in 'shear' geometry. Simulations show an initial rise in the force, followed by a force plateau and ultimately chain separation. During the plateau phase, the individual helices uncoil and recoil, with recoiling being more frequent at lower pulling speeds. Modifications that stabilize the individual helices are thus expected to increase the mechanical stability of CCs. These results aid the design of CC-based molecular force sensors and material building blocks.

BP 12.70 Tue 14:00 Poster B2

Simultaneous Force and Fluorescence Spectroscopy inside Zero-Mode Waveguides — •LEONARD C. SCHENDEL, STEFFEN M. SEDLAK, MAGNUS S. BAUER, and HERMANN E. GAUB — Department of Physics and Center for NanoScience, LMU Munich, Germany

In the past years, Zero-Mode Waveguides (ZMWs) have emerged to a powerful application in modern life science. They provide subdiffraction detection volumes in single-molecule fluorescence measurements and hence experimental performance at physiological concentrations of fluorescently labeled biomolecules.

Here, single-molecule force spectroscopy using an atomic force microscope and ZMWs are combined in order to investigate force-activation pathways of enzymes. For this purpose, high concentrations are dictated by experimental conditions and requirements, this being high Michaelis-Menten constants of enzymes and the limited time span of keeping the protein's binding pocket open/accessible.

The implementation of a covalent site-specific chemistry together with an optical non-invasive cantilever localization routine shows the ability to probe monovalent streptavidin in an automated fashion. We mechanically remove a bound biotin and are able to simultaneously observe reoccupation of the vacant site by fluorescently labeled biotin. In the future, this improved methodology will be applied to investigate enzymes upon possible force-activation mechanisms.

BP 12.71 Tue 14:00 Poster B2

Influence of Ligand Binding on the Mechanical Stability of a Single Protein Revealed by AFM-based Force Spectroscopy — •PHILIPP R. MÜLLER, STEFFEN M. SEDLAK, LEONARD C. SCHENDEL, JONAS C. FISCHER, MAGNUS S. BAUER, CARLEEN KLUGER, and HERMANN E. GAUB — Department of Physics and Center for NanoScience, LMU Munich, Germany

AFM-based force spectroscopy enables a large number of measurements of individual proteins. Covalent and site-specific immobilization

strategies are key for consistent and reproducible force spectroscopy data. Fingerprint domains that exhibit a characteristic unfolding pattern serve as internal force reference and to reliably identify single-molecule interactions.

Streptavidin (SA) is a tetrameric protein that is frequently used in force spectroscopy experiments and binds biotin, as well as desthiobiotin and Strep-tag II with high affinity.

Here, we investigate the effect of ligand binding on the mechanical stability of a single SA subunit. In a tetrameric SA, we tether one of the four SA subunits by its C- and N-terminus and unfold it in the presence and absence of different ligands. Furthermore, combining functional and non-functional SA subunits, which cannot bind any ligands, we are able to create SA of different valencies in a controlled way. Using these SA variants, we analyze the influence of different ligands, binding to the tethered or the neighboring subunit, on the mechanical stability of the molecule. Unfolding patterns and rupture forces depend on the type of ligand employed.

BP 12.72 Tue 14:00 Poster B2

Comparing the Mechanical Strengths of the Interaction of Biotin with Avidin-like proteins by AFM-based Single Molecule Force Spectroscopy — •JONAS C. FISCHER, STEFFEN M. SEDLAK, LEONARD C. SCHENDEL, PHILIPP R. MÜLLER, MAGNUS S. BAUER, CARLEEN KLUGER, and HERMANN E. GAUB — Department of Physics and Center for NanoScience, LMU Munich, Germany

Avidin-like proteins are a widely applied tool in nano- and biotechnology for immobilization, labeling and detection of molecules.

Here, we investigate the interaction of the tetrameric proteins streptavidin, traptavidin and streptactin with the small molecule biotin by AFM-based Single-Molecule Force Spectroscopy. Site-specific and covalent immobilization of different receptor molecules on the same surface enables stable and parallel long-term measurements of unbinding events. By the use of fingerprint domains providing characteristic unfolding patterns true single-molecule interactions are identified.

Both traptavidin and streptactin differ from wild-type streptavidin from *Streptomyces avidinii* only by three amino acids. The unbinding force of biotin from streptavidin is strongly dependent on tethering geometry. The rupture forces for the C-terminal anchoring is about two times higher as for N-terminal attachment. While traptavidin behaves in a similar manner, the rupture forces for streptactin differ: We observe a loading rate dependent transition from a low force binding to a high force binding state.

BP 12.73 Tue 14:00 Poster B2

A classification scheme for clustering and identification of DNA events through a nanopore — •ÁNGEL DÍAZ CARRAL¹, CHANDRA SHEKAR SARAP¹, KE LIU², ALEKSANDRA RADENOVIC², and MARIA FYTA¹ — ¹Institute for Computational Physics, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — ²Institute of Biotechnology, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

DNA molecules can electrophoretically be driven through a nanoscale opening in a material giving rise to measurable electronic current blockades important for DNA sensing. In this work, we propose a methodological approach to interpret nanopore events based on experimental ionic current data of DNA homopolymers through molybdenum-disulphide nanopores. Experimental ionic traces are used to train an unsupervised Machine Learning model for identifying molecular events related to different conformations of DNA molecules threading the nanopore. We have tested different features for the classification of the translocation events, and conclude on the efficiency of using the current blockade height for classification. This allows us to indeed distinguish folded over unfolded DNA events through the pore. We discuss the impact of such a scheme in sensing the identity of DNA with a nanopore.

BP 12.74 Tue 14:00 Poster B2

Topological insulator and semiconductor beads as micro-oscillators induced by laser beam — •WARLEY H. CAMPOS^{1,2}, TIAGO A. MOURA¹, JAKSON M. FONSECA¹, JOAQUIM B. S. MENDES¹, MÁRCIO S. ROCHA¹, and WINDER A. MOURA-MELO¹ — ¹Departamento de Física, Universidade Federal de Viçosa, Viçosa 36570-900, Brazil — ²Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz 55128, Germany

The optical tweezers (OT) is a powerful technique used to trap microscopic objects with light. It became an essential tool for high accuracy measurements in areas such as biological and soft matter physics. We

perform the first experimental studies upon the optical trapping of topological insulator (TI) [Bi₂Te₃ and Bi₂Se₃] and Germanium (Ge) microparticles under a Gaussian laser beam OT. For such materials gradient and radiometric forces compete, generating oscillatory dynamics perpendicular to the optical axis. We describe the oscillations with an effective model that captures the forces acting on the particle, amplitude of oscillation, periodicity and their dependence on particle size. Ge beads oscillate in a preferential direction determined by the polarization of the laser beam, this was not observed for neither of the TI materials. Our results open an avenue for dynamical measurements with unprecedented simplicity and purely optical control. Among the possible applications for the near future, stand out the optical rheology of soft matter interfaces and biological membranes, as well as dynamical force measurements in macromolecules and biopolymers.

BP 12.75 Tue 14:00 Poster B2

Planar Antennas for Biosensing and Diagnostics — •NAVID SOLTANI^{1,2}, NEMANJA MARKSEVIC^{1,2}, AVIJIT KUMAR DAS^{2,3}, SERGEY DRUZHININ^{2,4}, HEIKO IHMELS^{2,3}, HOLGER SCHÖNHERR^{2,4}, and MARIO AGIO^{1,2} — ¹Laboratory of Nano-Optics — ²Research Center of Micro and Nanochemistry and Engineering (Cμ) — ³Organic Chemistry II — ⁴Laboratory of Physical Chemistry I, University of Siegen, Siegen, Germany

Molecular fluorescence plays an important role in biosensing and diagnostics. However, dye molecules in conventional biochips exhibit radiation patterns such that even with high numerical aperture (NA) objectives a large fraction of the emitted photons is lost. Here, we investigate the implementation of a biosensor based on planar antennas [1], which change the radiation pattern of a dipole emitter and increase the photon collection efficiency by orders of magnitude without requiring high NA objectives. We focus on specific biological relevant molecules [2], interfaces [3] and bioassays to investigate the physical limit of detection down to the single-molecule level and to study the interaction of organic dyes and DNA molecules in nanostructured environments.

[1] S. Checcucci, P. Lombardi, S. Rizvi, F. Sgrignuoli, N. Gruhler, F. B. C. Dieleman, F. S. Cataliotti, W.H. P. Pernice, M. Agio and C. Toninelli, *Light: Science & Applications* 6, 16245 (2017) [2] P. M. Pithan, D. Decker, S. I. Druzhinin, H. Ihmels, H. Schönherr, Y. Voß, *RSC Advances*, 7, 10660 (2017). [3] N. Hain, D. Wesner, S. I. Druzhinin, H. Schönherr, *Langmuir*, 32, 11155 (2016).

BP 12.76 Tue 14:00 Poster B2

Competition between mutant and wild-type E. coli cells during carbon starvation — •ZARA GOUGH¹, FELIX FLESCHHUT¹, ELENA BISELLI¹, HAMID SEYED-ALLAEI¹, SEVERIN SCHINK^{1,2}, and ULRICH GERLAND¹ — ¹Technical University of Munich, Physics Department, James-Frank-Str 1, 85748 Garching, Germany — ²Harvard Medical School, Department of Systems Biology, 200 Longwood Ave, Boston 02115 MA, USA

Surviving nutrient limitation is an important part of the microbial life cycle. Recently, it was shown that survival of carbon starved *E. coli* is quantitatively characterized by two parameters that set the exponential death rate of the population: maintenance rate and recycling yield. Following this exponential death, *E. coli* enter a long-term phase exhibiting cycles of death and regrowth. Mutant subpopulations have been observed to thrive during regrowth cycles, eventually overtaking wild type cells. We investigate how maintenance rate and recycling yield change in mutants harvested during this phase and how these cells compete with wild type cells in order to dominate the entire population, despite exhibiting traits of poorer fitness, such as slower growth rate and faster death rate, compared to wild type cells grown in identical conditions. Our work will extend our quantitative understanding of bacterial physiology in environments where, due to lack of nutrients, population competition is crucial for survival.

BP 12.77 Tue 14:00 Poster B2

A mathematical model for an inducible CRISPR-dCas9 based switch in yeast — ANJA HOFMANN² and •JOHANNES FALK¹ — ¹Technische Universität Darmstadt, Institut für Festkörperphysik, Germany — ²Technische Universität Darmstadt, Clemens-Schöpf-Institut, Germany

The robust and precise on and off switching of one or more genes of interest, followed by expression or repression is essential for many biological circuits as well as for industrial applications. However, many regulated systems published to date influence the viability of the host cell, show high basal expression or enable only the overexpression of

the target gene without the possibility of fine regulation. By combining the advantages of well-established systems, namely the scaffold RNA CRISPR/dCas9 platform, and LexA-ER-AD as heterologous transcription factor it is possible to overcome these limitations. On our poster, we compare experimental data with a minimal model that only captures the most basic processes but is still capable of covering all important results of the experiment. Our research hence helps to gain a better understanding of the underlying principles and the functioning of the inducible CRISPR/dCas9 system.

BP 12.78 Tue 14:00 Poster B2

How to generate a long-range signalling gradient based on short-range molecular interactions? — ●JOHANNA DICKMANN^{1,2}, STEFFEN WERNER¹, JOCHEN RINK², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Animal bodies show a fascinating degree of organisation as testified by their complex body plans. In the context of embryonic development, signalling gradients (spatially graded profiles of signalling intensity) emerged as key concepts of body plan patterning. They have been explained by a substance diffusing away from a local source and being degraded. In case of regeneration, new tissue has to be patterned on adult length scales. It is debatable if a diffusion-based mechanism is fast enough to explain gradient formation on adult length scales. Flatworms are masters of regeneration, re-growing a perfectly patterned body from arbitrary amputation fragments at an adult length of up to 2 cm. Their main body axis - as for most animals - is patterned by a Wnt signalling gradient. In addition to a local Wnt source, they show spatially graded Wnt expression. Based on these observations, we hypothesise that additional Wnt sources are generated in response to signalling, organised by a local, signalling-independent source. We formalise the suggested mechanism in a physical model using differential equations, analyse the model both analytically and numerically, and test it experimentally by interfering with the gradient. This way, we hope to unravel a novel mechanism for long-range gradient formation.

BP 12.79 Tue 14:00 Poster B2

Understanding the lifespan of worm dauer by modeling its metabolic pathway — ●XINGYU ZHANG¹, DAMLA KAPTAN², SIDER PENKOV², VAMSHIDAR GADE², BHARATH RAGHURAMAN², WOBERTA GALLI³, EDMUND KOCH³, ANDREJ SHEVCHENKO², TEYMURAS KURZCHALIA², and VASILY ZABURDAEV¹ — ¹FAU Erlangen-Nürnberg, Germany — ²MPI-CBG, Germany — ³TU Dresden, Germany

Understanding a lifespan of an organism, which is governed by multiple

mechanisms, is an intrinsically complex problem. Here, we focus on *C. elegans* dauer larvae, the stage of an organism development where the mechanisms of survival are dominant. Recently, we discovered that dauer of *C. elegans* can intake and metabolize external ethanol as a carbon source, somewhat contradicting the conventional picture of dauer worms as almost an isolated system. Interestingly, the lifespan of dauer increases when small amounts of ethanol are supplied, but starts to decrease when ethanol concentration becomes higher. To understand the mechanism of how the lifespan of dauer is related to the supplied ethanol, we developed a theoretical model based on the known metabolic pathway of *C. elegans* dauer accounting for the ethanol utilization. The model considers the lack of energy resources and the accumulation of toxic compounds from the metabolic activity as two factors that can potentially limit the lifespan of dauer. Results of the model show a qualitative agreement of the lifespan when compared to experimental data including dauers with various mutations in the metabolic pathway.

BP 12.80 Tue 14:00 Poster B2

Load distribution among the main structures of a passively flexed lumbar spine — FALK MÖRL¹, SYN SCHMITT², ●JULIA MARIA RIEDE², and MICHAEL GÜNTHER² — ¹Biomechanics & Ergonomics, FSA mbH Erfurt, Germany — ²Biomechanics and Biorobotics, SimTech, Universität Stuttgart, Germany

Mechanical loads may induce degeneration of spinal structures. It is still unknown how the load during spine motion is distributed among the spine's main structures: muscles, vertebrae and their connecting joints, ligaments and intervertebral discs. Currently there exists no measurement method to capture the function of all spinal structures at the same time. Therefore, computer simulations are the method of choice to overcome the need of in vivo measurements. Still, the model with its initial conditions has to reproduce the biophysics of the human spine.

To get a good prediction for the load distribution of spinal structures we therefore combined experimental with simulation methods. On the simulation side we have a valid forward dynamics multibody model of the human spine. Hence we obtain valid simulation results that can subsequently be compared to the experimental results. On the experimental side stands a precise and objective measurement of human lumbar spine flexion torque. Both the experiment and the simulation were laid-out for a passive spine, i.e. no muscle activation, in the lumbar region. This allows for a detailed investigation of load distribution ensuring reasonable basic conditions for a passive human spine.