# Biological Physics Division
# Fachverband Biologische Physik (BP)

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## Overview of Invited Talks and Sessions

(Lecture Rooms: HÜL 386 and ZEU 250; Posters P1 and P3)

### Plenary Talks related to BP

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|---|---|---|---|---|
| PV XI | Wed | 14:00–14:45 | HSZ 01 | **Motions in the molecular machinery powering life** — •Gerhard Hummer |
| PV XVII | Thu | 14:00–14:45 | HSZ 02 | **Optical Antennas for Enhanced Light-Matter Interactions** — •Lukas Novotny |
| PV XVIII | Fri | 8:30– 9:15 | HSZ 01 | **Optical Tweezers: Gene Regulation, Studied One Molecule at a Time** — •Steven Block |

### Invited and Topical Talks

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| BP 1.1 | Mon | 9:30–10:00 | HÜL 386 | **What determines the path of kinesin motors along the microtubules?** — •Zeynep Ökten |
| BP 2.7 | Mon | 11:15–11:45 | ZEU 250 | **Single molecule torque and twist measurements probe the key players of the central dogma** — •Jan Lipfert |
| BP 4.1 | Mon | 15:00–15:30 | HÜL 386 | **Role of membrane elasticity in clathrin-mediated endocytosis** — Sandrine Morlot, Saleem Mohammed, Nicolas Chiaruttini, Valentina Galli, Marius Klein, Luìs Dinis, Martin Lenz, Giovanni Cappello, •Aurélien Roux |
| BP 5.7 | Mon | 16:30–17:00 | ZEU 250 | **Particle-based stochastic computer simulations of biological systems** — •Ulrich Schwarz |
| BP 20.1 | Tue | 13:00–13:30 | HÜL 386 | **Catch bond interaction between glycosaminoglycans and cell surface sulfatase Sulf1** — Alexander Harder, Ann-Kristin Moeller, Fabian Milz, Phillipp Neuhaus, Volker Walhorn, Thomas Dierks, •Dario Anselmetti |
| BP 20.6 | Tue | 14:45–15:15 | HÜL 386 | **Synthetic mechanobiology: Dissecting and rewiring force-based signaling** — •Sanjay Kumar |
| BP 23.1 | Wed | 9:30–10:00 | HÜL 386 | **Intermediate filaments - mechanical building blocks and dynamic elements of the cell** — •Sarah Köster |
| BP 24.1 | Wed | 9:30–10:00 | ZEU 250 | **Collaboration between biomolecules: A physical analysis** — •Ulrich Gerland |
| BP 24.5 | Wed | 10:45–11:15 | ZEU 250 | **Gene expression in embryos: from single molecules to network dynamics** — •Thomas Gregor |
| BP 27.1 | Wed | 14:00–14:30 | ZEU 250 | **Legged locomotion. - From biology to mechanics and return.** — •Reinhard Blickhan |
| BP 28.1 | Wed | 15:00–15:30 | HÜL 386 | **Single Molecule Mechanics of Proteins** — •Matthias Rief |
| BP 31.1 | Wed | 17:00–17:30 | ZEU 250 | **Active torque generation by the actomyosin cortex** — •Stephan Grill |
| BP 33.1 | Thu | 9:30–10:00 | HÜL 386 | **Self-Focusing of the Ran Gradient in Mitosis: Signaling, Mechanics, and Spindle Size** — •Daniel Needleman, Doogie Oh |
| BP 38.1 | Thu | 15:00–15:30 | HÜL 386 | **Analyzing integrin's force transduction using novel biosensors** — •Carsten Grashoff |

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| BP 43.1 | Fri | 9:30–10:00 | ZEU 250 | **The Dynamics of Neuronal Circuits** — •Fred Wolf |

## Invited talks of the joint symposium SYMS

See SYMS for the full program of the symposium.

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| SYMS 1.1 | Wed | 9:30–10:00 | HSZ 02 | **Imaging and manipulation of single functional molecules on surfaces** — •Leonhard Grill |
| SYMS 1.2 | Wed | 10:00–10:30 | HSZ 02 | **Adiabatic quantum motors** — •Felix von Oppen |
| SYMS 1.3 | Wed | 10:30–11:00 | HSZ 02 | **Operation of molecular devices and machines on surfaces** — •Saw Wai Hla |
| SYMS 1.4 | Wed | 11:15–11:45 | HSZ 02 | **Driving and Controlling Molecular Surface Rotors with a Terahertz Electric Field** — •Raymond Dean Astumian |
| SYMS 1.5 | Wed | 11:45–12:15 | HSZ 02 | **Unidirectional motion by inelastic electron tunneling** — •Karl-Heinz Ernst |

## Invited talks of the joint symposium SYCP

See SYCP for the full program of the symposium.

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| SYCP 1.1 | Thu | 9:30–10:00 | HSZ 02 | **Why do polymer collapse and polymer topology frustrate each other** — •Alexander Y. Grosberg |
| SYCP 1.2 | Thu | 10:00–10:30 | HSZ 02 | **Nanoscopy of nuclear Genome Structure** — •Christoph Cremer |
| SYCP 1.3 | Thu | 10:30–11:00 | HSZ 02 | **Blood Clotting Inspired Polymer Physics** — •Alfredo Alexander-Katz |
| SYCP 1.4 | Thu | 11:15–11:45 | HSZ 02 | **Modeling dynamic spatial genome organization in yeast** — •Christophe Zimmer |
| SYCP 1.5 | Thu | 11:45–12:15 | HSZ 02 | **Ring polymers in the melt state: the physics of crumpling** — •Ralf Everaers, Angelo Rosa |

## Invited talks of the joint symposium SYGP

See SYGP for the full program of the symposium.

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| SYGP 1.1 | Thu | 15:00–15:30 | HSZ 02 | **Noisy invasions: large fluctuations in stochastic invasion models** — •Baruch Meerson |
| SYGP 1.2 | Thu | 15:30–16:00 | HSZ 02 | **Fractal clustering of inertial particles in random velocity fields** — •Bernhard Mehlig, Kristian Gustavsson |
| SYGP 1.3 | Thu | 16:00–16:30 | HSZ 02 | **Stochastic population dynamics on rugged fitness landscapes** — •Joachim Krug |
| SYGP 1.4 | Thu | 16:45–17:15 | HSZ 02 | **Modeling cancer as a stochastic process** — •Tibor Antal |
| SYGP 1.5 | Thu | 17:15–17:45 | HSZ 02 | **Von Neumann's growth model: from statistical mechanics to cell metabolism** — •Andrea De Martino |

## Sessions

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|---|---|---|---|---|
| BP 1.1–1.12 | Mon | 9:30–13:00 | HÜL 386 | **Molecular Motors** |
| BP 2.1–2.12 | Mon | 9:30–13:00 | ZEU 250 | **DNA/RNA and related enzymes** |
| BP 3.1–3.4 | Mon | 11:00–12:40 | CHE 89 | **Symposium SKM Dissertation-Prize 2014** |
| BP 4.1–4.7 | Mon | 15:00–17:00 | HÜL 386 | **Membranes and Vesicles I** |
| BP 5.1–5.7 | Mon | 15:00–17:00 | ZEU 250 | **Protein structure and dynamics I** |
| BP 6.1–6.12 | Mon | 17:30–19:30 | P3 | **Posters: Membranes and vesicles** |
| BP 7.1–7.48 | Mon | 17:30–19:30 | P3 | **Posters: Cell adhesion, mechanics and migration** |
| BP 8.1–8.10 | Mon | 17:30–19:30 | P3 | **Posters: Active cell and tissue mechanics** |
| BP 9.1–9.6 | Mon | 17:30–19:30 | P3 | **Posters: Biotechnology and bioengineering** |
| BP 10.1–10.10 | Tue | 9:30–12:30 | P1 | **Posters: Molecular Motors** |
| BP 11.1–11.15 | Tue | 9:30–12:30 | P1 | **Posters: Cytoskeleton** |
| BP 12.1–12.13 | Tue | 9:30–12:30 | P1 | **Posters: Imaging** |
| BP 13.1–13.8 | Tue | 9:30–12:30 | P1 | **Posters: DNA/RNA and related enzymes** |
| BP 14.1–14.19 | Tue | 9:30–12:30 | P1 | **Posters: Protein Structure and dynamics** |

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| BP 15.1–15.3 | Tue | 9:30–12:30 | P1 | **Posters: Systems biology and neurosciences** |
| BP 16.1–16.38 | Tue | 9:30–12:30 | P1 | **Poster - Glasses / Stat. Phys. Bio. / Networks (joint DY/BP/CPP/SOE)** |
| BP 17.1–17.11 | Tue | 9:30–12:30 | ZEU 146 | **Microswimmers (joint DY/BP)** |
| BP 18.1–18.7 | Tue | 9:30–11:30 | ZEU 118 | **Complex Fluids and Soft Matter (joint DY/CPP/BP)** |
| BP 19.1–19.5 | Tue | 9:30–11:30 | HÜL 186 | **Focus Session: Dynamical Patterns in Neural Systems: From Brain Function to Dysfunction (joint DY/BP)** |
| BP 20.1–20.9 | Tue | 13:00–16:00 | HÜL 386 | **Cell adhesion, mechanics and migration I** |
| BP 21.1–21.8 | Tue | 14:00–16:00 | ZEU 250 | **Membranes and Vesicles II** |
| BP 22.1–22.4 | Tue | 15:00–16:00 | GÖR 226 | **Networks, From Topology to Dynamics I (joint SOE/DY/BP)** |
| BP 23.1–23.12 | Wed | 9:30–13:00 | HÜL 386 | **Cytoskeleton (joint BP/CPP)** |
| BP 24.1–24.5 | Wed | 9:30–11:15 | ZEU 250 | **Systems biology** |
| BP 25.1–25.9 | Wed | 9:30–12:00 | ZEU 160 | **Statistical Physics in Biological Systems (joint DY/BP)** |
| BP 26.1–26.7 | Wed | 11:45–13:30 | ZEU 250 | **Multi-cellular systems and Physics of Cancer** |
| BP 27.1–27.8 | Wed | 14:00–16:30 | ZEU 250 | **Modelling of non-linear dynamics in biological movement (focus session, joint BP/DY)** |
| BP 28.1–28.12 | Wed | 15:00–18:30 | HÜL 386 | **Protein structure and dynamics II** |
| BP 29.1–29.14 | Wed | 15:00–18:45 | ZEU 118 | **Networks – Statistics and Dynamics (joint DY/BP/SOE)** |
| BP 30.1–30.10 | Wed | 15:00–18:15 | ZEU 222 | **Biomaterials and Biopolymers I (joint CPP/BP)** |
| BP 31.1–31.5 | Wed | 17:00–18:30 | ZEU 250 | **Cell adhesion, mechanics and migration II** |
| BP 32 | Wed | 19:00–20:00 | HÜL 386 | **BP Mitgliederversammlung** |
| BP 33.1–33.9 | Thu | 9:30–12:30 | HÜL 386 | **Active cell and tissue mechanics (focus session) I** |
| BP 34.1–34.8 | Thu | 9:30–11:45 | ZEU 250 | **Imaging** |
| BP 35.1–35.5 | Thu | 9:30–12:15 | HSZ 02 | **The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (Symposium SYCP, joint CPP/BP/DY)** |
| BP 36.1–36.5 | Thu | 11:00–12:15 | GÖR 226 | **Evolutionary Game Theory and Economic Models (joint SOE/BP/DY)** |
| BP 37.1–37.3 | Thu | 12:15–13:00 | GÖR 226 | **Networks, From Topology to Dynamics II (joint SOE/DY/BP)** |
| BP 38.1–38.8 | Thu | 15:00–17:30 | HÜL 386 | **Active cell and tissue mechanics (focus session) II** |
| BP 39.1–39.8 | Thu | 15:00–17:30 | ZEU 250 | **The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (accompanying session, joint CPP/BP/DY)** |
| BP 40.1–40.5 | Thu | 15:00–17:45 | HSZ 02 | **Stochastic Dynamics of Growth Processes in Biological and Social Systems (Symposium SYGP, joint DY/BP/SOE)** |
| BP 41.1–41.13 | Thu | 15:00–18:45 | ZEU 222 | **Biomaterials and Biopolymers II (joint CPP/BP)** |
| BP 42.1–42.9 | Fri | 9:30–12:00 | HÜL 386 | **Biotechnology and bioengineering** |
| BP 43.1–43.8 | Fri | 9:30–11:45 | ZEU 250 | **Neurosciences** |
| BP 44.1–44.11 | Fri | 10:00–12:45 | GÖR 226 | **Stochastic Dynamics of Growth Processes in Biological and Social Systems (accompanying session, joint DY/BP/SOE)** |

## Annual General Meeting of the Biological Physics Division

Wednesday 19:00–20:00 HÜL 386

- Award of the EPL poster prizes for biological physics
- Report of the current speakers
- Lessons learned and spring meeting Berlin 2015
- Miscellaneous

# BP 1: Molecular Motors

Time: Monday 9:30–13:00 Location: HÜL 386

**Topical Talk** BP 1.1 Mon 9:30 HÜL 386

**What determines the path of kinesin motors along the microtubules?** — •Zeynep Ökten — TU München, Germany

In long-range transport of cargo, prototypical kinesin-1 steps along a single protofilament on the microtubule, an astonishing behavior given the number of theoretically available binding sites on adjacent protofilaments. Using a laser trap assay, we analyzed the trajectories of several representatives from the kinesin-2 class on freely suspended microtubules. In stark contrast to kinesin-1, these motors display a wide range of left-handed spiraling around microtubules and thus generate torque during cargo transport. We provide direct evidence that kinesin*s neck region determines the torque generating properties. Disrupting the stability of the neck by inserting flexible peptide stretches resulted in pronounced left-handed spiraling. Mimicking neck stability by crosslinking significantly reduced the spiraling of the motor up to the point of protofilament tracking.

BP 1.2 Mon 10:00 HÜL 386

**Microtubule rotations reveal the 3D stepping trajectories of motor proteins on microtubule lattices** — •Aniruddha Mitra[1], Felix Ruhnow[1], and Stefan Diez[1,2] — [1]B CUBE, Dresden, Germany — [2]MPI-CBG, Dresden, Germany

Microtubules consist of about 13 protofilaments which act as tracks for motor proteins. It is interesting to know, whether processive motors step strictly along one of these tracks or whether they are able to switch between the tracks. We recently performed in vitro gliding motility assays on surfaces coated with kinesin-1 and kinesin-8 motor proteins and measured the rotations of microtubules around their longitudinal axis using quantum dots in combination with fluorescence-interference contrast (FLIC) microscopy and 2D nanometer tracking. We found that the cargo carrying motor kinesin-1 follows a single protofilament, while the highly processive microtubule-depolymerizing motor kinesin-8, does switch tracks with a bias towards the left. Because the attached quantum dots might interfere with the microtubule rotations, we recently devised a novel quantum-dot free method to obtain microtubule rotation data.

BP 1.3 Mon 10:15 HÜL 386

**The kinesin-8, Kip3, frequently switches microtubule protofilaments in a biased random walk** — •Michael Bugiel[1], Elisa Böhl[1], and Erik Schäffer[2] — [1]Nanomechanics Group, Biotechnology Center, TU Dresden, Tatzberg 47/49, 01307 Dresden, Germany — [2]Zentrum für Molekularbiologie der Pflanzen (ZMBP), University of Tübingen, Auf der Morgenstelle 32, 72076 Tübingen, Germany

The budding yeast Kinesin-8 Kip3 is a highly processive motor protein that walks to the end of cytoskeletal microtubules and shortens them in a collective manner. Microtubules usually consist of 12 to 15 circularly-arranged tubulin polymer chains, called protofilaments. Left-handed rotations of microtubules in Kip3 gliding assays indicate sideward motion of Kip3 perpendicular to the microtubule axis, i.e. a switching between single protofilaments. Here, we used high-resolution optical tweezers in a force feedback mode to track the path of single Kip3 motors by applying alternating sideward loads. Our studies show that Kip3 steps sideward in both directions, but follows the load on average with a preference towards the left. Based on statistical data analysis and comparison with simulations, we propose a diffusive sideward motion of Kip3 on the microtubule lattice. This diffusive switching mechanism may enable Kip3 to bypass obstacles and reach the microtubule end for length regulation.

BP 1.4 Mon 10:30 HÜL 386

**Teams of molecular motors in optical traps from a theoretical perspective** — •Florian Berger, Corina Keller, Stefan Klumpp, and Reinhard Lipowsky1 — Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

Intracellular transport of cargos is achieved by the cooperative action of molecular motors, which pull the cargo along cytoskeletal filaments. A lot of single molecule studies together with theoretical considerations have contributed to develop a common understanding how single kinesin motor respond to an external force. However, it is far from obvious, how an external load force influence the dynamics of a small team of molecular motors. Starting from the single molecule properties, we introduce a theoretical framework for cooperative transport and study the response of a motor team to a constant force (force-feedback trap) and a time dependent force (stationary trap). Within in our simple description, we discuss the basic differences of these two measurement techniques and point out the implications for transport in a soft crowded environment.

BP 1.5 Mon 10:45 HÜL 386

**Length regulation of microtubules: the effect of limited resources** — •Matthias Rank, Louis Reese, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Length regulation of microtubules is strongly associated with the motion and action of molecular motors as kinesin-8 Kip3p. This processive motor has been shown to depolymerise microtubules; its activity thus competes with spontaneous tubulin polymerisation. We describe the kinesin motion in terms of the totally asymetric simple exclusion process (TASEP) with modified dynamic rules at the terminal site. In particular—mimicking situations in real cells—we investigate the effect of limited resources on the dynamics. We find rich phase behaviour which differs fundamentally from the case of an infinite reservoir. We supplement our mean-field theory with Monte Carlo simulations to obtain a complete theoretical picture of the process.

BP 1.6 Mon 11:00 HÜL 386

**Direct measurement of the pressure generated by a 1D protein gas confined within microtubule overlaps** — •Annemarie Lüdecke[1,2], Marcus Braun[1,2], Zdenek Lansky[1,2], Michael Schlierf[1], Pieter Rein ten Wolde[3], Marcel E. Janson[4], and Stefan Diez[1,2] — [1]B CUBE, TU Dresden, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]AMOLF, Amsterdam, Netherlands — [4]Laboratory of Cell Biology, Wageningen University, Wageningen, Netherlands

The integrity of the mitotic spindle during anaphase is facilitated by antiparallel microtubule-microtubule overlaps in the spindle midzone. Within these overlaps, motor proteins (e.g. kinesin-5, kinesin-14) as well as passive, non-enzymatic microtubule crosslinkers (e.g. from the MAP65 family) localize and influence the mechanical stability of the overlaps. Here, we show in vitro that the diffusible microtubule crosslinker Ase1, a member of the MAP65 family, can slow down and halt the shortening of microtubule-microtubule overlaps driven by the kinesin-14 Ncd. Using mathematical modeling we show that Ase1 confined in a microtubule overlap behaves like a 1D gas upon compression, i.e. producing an entropic force opposing the compression. Direct measurement of the entropic force by optical tweezers yielded values in the pN-range, comparable to the forces produced by motor proteins present in the spindle midzone. We hypothesize that entropic pressure may be a general mechanism of force production in biological systems.

**15 min. break**

BP 1.7 Mon 11:30 HÜL 386

**Stochastic dynamics of small ensembles of non-processive molecular motors: The parallel cluster model** — •Thorsten Erdmann[1,2], Philipp J. Albert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [2]BioQuant, Heidelberg University, Heidelberg, Germany

Forces in the actin cytoskeleton are generated by small groups of non-processive myosin II motors. For such small groups comprising few tens of myosin II molecules, stochastic effects are highly relevant. Using a three-state crossbridge model with the assumptions of fast power-stroke kinetics and equal load sharing between motors in equivalent states, the stochastic reaction network is reduced to a one-step master equation for binding and unbinding dynamics (parallel cluster model) together with rules for ensemble movement. For constant external load, ensemble dynamics is determined by the catch bond character of myosin II, leading to an increase of the fraction of bound motors under load and firm attachment of small ensembles. This adaptation to load results in a concave force-velocity relation described by a Hill relation. When working against an external linear spring, myosin II ensembles

adjust themselves to an isometric state with constant average position and load. Ensemble dynamics is now determined by the distribution of motors over different bound states. Above a critical spring stiffness, myosin II can no longer perform the power stroke. This stalls ensemble movement but slow unbinding from the pre-power-stroke state protects the ensembles against detachment. [Reference: T. Erdmann, P.J. Albert & U.S. Schwarz, J. Chem. Phys. 139, 175104 (2013).]

BP 1.8 Mon 11:45 HÜL 386

**Dynamical Phenomena in Coupled Muscle Myosins** — •Lennart Hilbert, Zsombor Balassy, Shivaram Cumarasamy, Anne-Marie Lauzon, and Michael C. Mackey — McGill University, Montréal, Québec, Canada

The length ($l$) of muscle myosin filaments in smooth muscle cells is distributed following $exp(-l/L_0)$, $L_0 = 0.116 - 0.182\,\mu m$ [Liu et al., J Physiol, 2013]. The kinetics of skeletal muscle myosin groups working on a commonly propelled actin filament qualitatively change at $L_1^c \approx 0.3\,\mu m$ and $L_2^c \approx 1.0\,\mu m$ lengths of interaction between a myosin-coated surface and myosin-propelled actin filaments ($L$, motility assay) [Hilbert et al., Biophys J, 2013]. In this study, motility assays of smooth muscle myosin showed the same kinetic regimes for increasing $L$ as seen for skeletal muscle myosin: (1) actin arrest to surface, (2) alternating arrest and forward sliding (autocorrelation time $0.3\,s$), (3) continuous forward sliding; transition lengths $L_1^c \approx 0.27\,\mu m$ and $L_2^c \approx 0.75\,\mu m$. The regimes were reproduced by a mathematical model of $N = 5$ to 100 myosin binding sites ($N \propto L$) on individual actin filaments interacting with surface-fixed myosins. Binding site kinetics were mechanically coupled via actin, and dependent on $L$, a stable focus (arrest) and a limit cycle (sliding) existed that entrained global behavior. The dynamic phenomena and resulting $L$-dependent statistics from our actin sliding experiments were captured by a reduced mathematical model with two fast variables (exhibiting limit cycle or stable focus) and one slow variable (switching between cycle and focus).

BP 1.9 Mon 12:00 HÜL 386

**Single-molecule studies of RNA polymerase I elongation** — •Ana Lisica[1], Marcus Jahnel[1], Christoph Engel[2], Patrick Cramer[2], and Stephan W. Grill[1] — [1]MPI-CBG and MPI-PKS, Dresden, Germany — [2]Gene Centre Munich, LMU, Munich, Germany

Eukaryotic RNA polymerases (Pol I, Pol II and Pol III) have a highly conserved core and active center region. This implies that the mechanism of RNA polymerization is similar in all three polymerases. Additionally, Pol I and Pol III have specific surface subunits. Furthermore, the strength of the intrinsic activity of transcript cleavage differs highly: Pol I and Pol III possess a strong RNA cleavage mechanism, while Pol II has a weak one and needs a transcription factor (TFIIS) to cleave the RNA. To observe fine differences in transcription dynamics that stem from structural differences between these machines, we are using high-resolution dual-trap optical tweezers to analyze the mechanochemical details of the Pol I elongation in comparison to Pol II. Here we present the first single-molecule optical tweezers traces of Pol I transcribing a bare DNA template. A comparison with the Pol II dynamics revealed that Pol I is faster, with significantly higher overall and pause-free velocities, it pauses less often than Pol II, exhibits shorter pauses and can transcribe against higher opposing forces. Surprisingly, we find that the intrinsic transcript cleavage ability of Pol I is functional only with backtracked RNAs shorter than about 18 nt. Together, our results contribute to the understanding of unique micromechanical function and cellular role of this essential enzyme.

BP 1.10 Mon 12:15 HÜL 386

**Myosin II Activity Softens Cells in Suspension** — •Chii Jou Chan[1,2], Andrew Ekpenyong[1,2], Jochen Guck[1,2], and Franziska Lautenschläger[1,3] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge, United Kingdom — [2]Biotechnology Center, Technische Universität Dresden, Dresden, Germany — [3]Department of Physics, Saarland University, Saarbrücken, Germany

The cytoskeleton of cells is crucial for many cellular functions that require shape change or force generation, which is enacted by actin in concert with the motor protein myosin. While studies investigating the contribution of myosin-activity on the mechanical properties of cells have been performed on cells attached to a substrate, we investigated mechanical properties of cells in suspension using an optical stretcher. Both naturally suspended cells and naturally attached cells were treated with myosin inhibitors (Blebbistatin, Y-27632). We find that all cells, once in suspension, stiffen when myosin activity is inhibited and vice versa This is exactly opposite to what has been reported for cells attached to a substrate, which stiffen via pre-stress by myosin activity. Possible reasons for this difference and likely molecular mechanisms will be discussed. Our findings shed new light on the role of myosin II in the control of cell mechanical properties when cells are not attached to flat, rigid surfaces.

BP 1.11 Mon 12:30 HÜL 386

**Linking single-motor dynamics to ciliary ultrastructure using single-molecule super-resolution microscopy in Caenorhabditis elegans.** — •Felix Oswald[1], Bram Prevo[1], Pierre Mangeol[1], Jonathan Scholey[2], and Erwin Peterman[1] — [1]VU University Amsterdam, Amsterdam, Netherlands — [2]University of California, Davis, Davis, United States of America

Cilia are finger-like protrusions that are present in most eukaryotic cells fulfilling crucial motility and sensory functions. Their shape and structural integrity is determined by microtubules and a variety of other structural components such as transition fibers and Y-shaped links. In Caenorhabditis elegans two kinesin-2-family motors, kinesin-II and OSM-3, are responsible for building and maintenance of the chemosensory cilia. It is known that both kinesins are active on the microtubule doublets and that OSM-3 alone maintains the microtubule singlets. It is not known, however, how other structural features influence their dynamics. In order to address this question we use single transgenes encoding for fluorescently labeled kinesins in combination with single-particle tracking PALM (sptPALM). By localizing single-motor proteins deep inside the living organism we are able to build super-resolution roadmaps that reveal ultrastructural details. This allows us to relate the rich single-motor dynamics to ciliary subdomains and their specific structural features. Our findings are the outset to understand the influence of ciliary ultrastructure on motor dynamics.

BP 1.12 Mon 12:45 HÜL 386

**Dynein, microtubule and cargo: a ménage à trois** — •Nenad Pavin[1], Vaishnavi Ananthanarayanan[2], and Iva Tolic-Norrelykke[2] — [1]Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

To exert forces, motor proteins bind with one end to cytoskeletal filaments, such as microtubules and actin, and with the other end to the cell cortex, a vesicle or another motor. A general question is how motors search for sites in the cell where both motor ends can bind to their respective binding partners. In the case of nuclear movements in meiotic prophase, we identify the steps of the dynein binding process: from the cytoplasm to the microtubule and from the microtubule to cortical anchors. We found that dyneins on the microtubule move either in a diffusive or directed manner, with the switch from diffusion to directed movement occurring upon binding of dynein to cortical anchors. We explain theoretically how this dual behavior of dynein, together with the two steps of binding, enables dyneins to self-organize into a spatial pattern needed for them to generate large collective forces.

Ananthanarayanan, Schattat, Vogel, Krull, Pavin, Tolic-Norrelykke, Cell 2013.

# BP 2: DNA/RNA and related enzymes

Time: Monday 9:30–13:00 Location: ZEU 250

BP 2.1 Mon 9:30 ZEU 250

**Thermal disequilibrium causes natural selection of replicating DNA** — •Moritz Kreysing[1,2], Lorenz Keil[1], Simon Lanzmich[1], Christof Mast[1], Stephan Krampf[1], and Dieter Braun[1] — [1]Systems Biophysics, LMU Munich, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics

Here we report on experimental findings that a mere temperature gradient across a sub-millimeter sized compartment can be used to filter bio-molecules from dilute solutions. Because the characteristics of this thermophoretically based filter are strongly non-linear with regard to polymer length, the through-flow system is able to accumulate exclusively long polymers, as firstly shown here by the length selective fractionation of solute DNA strands. Exploiting convectively driven temperature cycles [1], the trapped DNA is additionally able to replicate in a PCR type manner. As we demonstrate, the combination of length selective accumulation and replication renders this compartment a niche in which heterogeneous populations of DNA strands are subject to a selection pressure in favor of molecular complexity, a so far unresolved prerequisite to the onset of Darwinian evolution [2].

References: 1) C. Mast and D. Braun, PRL, 104:188102 (2010), 2) D. Mills, L. Peterson, S. Spiegelman, PNAS, 58:217 (1967)

BP 2.2 Mon 9:45 ZEU 250

**Neutral Evolution of Duplicated DNA: An Evolutionary Stick-Breaking Process Causes Scale-Invariant Behavior** — Florian Massip[1,2] and •Peter F. Arndt[2] — [1]INRA, Jouy-en-Josas, France — [2]Max Planck Institute for Molecular Genetics, Berlin, Germany

Recently, an enrichment of identical matching sequences has been found in many eukaryotic genomes. Their length distribution exhibits a power law tail raising the question of what evolutionary mechanism or functional constraints would be able to shape this distribution. Here we introduce a simple and evolutionarily neutral model, which involves only point mutations and segmental duplications, and produces the same statistical features as observed for genomic data. Further, we extend a mathematical model for random stick breaking to analytically show that the exponent of the power law tail is -3 and universal as it does not depend on the microscopic details of the model.

BP 2.3 Mon 10:00 ZEU 250

**Insights into the thermodynamic profile of "mutated" Cytosine rich DNA strands: A theoretical study** — •Vasileios Tatsis and Andreas Heuer — Institut für Physikalische Chemie, Münster, Germany

Cytosine rich DNA sequences form four stranded structures (i-motif) under acidic conditions. The i-motif is an intercalated structure formed by association in a head to tail orientation of two parallel duplexes whose strands are held together by hemiprotonated Cytosine·Cytosine(+) pairs. Our theoretical work examines how point defects in the central strands and variations of the Cytosine sequences' length affect the thermodynamical stability of the i-motif structure. We employ the fully atomistic Molecular Dynamics method with an explicit solvent model. We use as an initial structure for the "mutations" a single stranded deprotonated DNA i-motif. Furthermore, in order to enhance the conformational sampling and to compute the thermodynamic stability of the new "mutated" i-motif structures, we use the Metadynamics and the Steered Molecular Dynamics techniques. The output from this theoretical study is compared with experimental results derived from CD-experiments.

BP 2.4 Mon 10:15 ZEU 250

**Extreme polymerization and aggregation of DNA/RNA in thermal traps** — •Christof Mast[1], Severin Schink[2], Moritz Kreysing[1], Urlich Gerland[2], and Dieter Braun[1] — [1]Systems Biophysics, Physics Department, Center for Nanoscience, LMU Munich, Germany — [2]Arnold-Sommerfeld-Center for Theoretical Physics and Center for Nanoscience, LMU Munich, Germany

Biopolymers like RNA, DNA and proteins are the fundamental actors in all life on earth. It is however unclear, how the first long RNA polymers with enzymatic activity could arise in a prebiotic scenario: Even in millimolar concentrations, ribonucleic acids only polymerize to short strands with a length of 20 bases. We demonstrate how a simple thermal gradient in a hydrothermal pore-like geometry is able to trap longer polymers exponentially better than shorter polymers. Polymerization leads to even longer polymers due to the increased total mass in the trapping center. Polymerization and thermal trapping are mutually self-enhancing. This process is described by an experimentally supported theory of trapped polymerization. Theoretical extrapolation to RNA-world conditions shows that a pore height of 5 cm and a temperature difference of 10 K are sufficient to form RNA polymers longer than the shortest RNA based replicator. Thermal traps also support the sequence specific formation of large aggregates made by the reversible polymerization of sticky-ended dsDNA. The melting temperature of the aggregates and the sticky ends match. No aggregates were found with non-polymerizing dsDNA pieces or without thermal trapping which therefore acts as a highly sequence selective process.

BP 2.5 Mon 10:30 ZEU 250

**Complex RNA folding kinetics revealed by single molecule FRET and hidden Markov models** — •Bettina Keller[1], Andrei Kobitski[2], G. Ulrich Nienhaus[2], and Frank Noé[3] — [1]Freie Universität Berlin, Institut für Chemie, Takustr. 3, 14195 — [2]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [3]Freie Universität Berlin, Institut für Mathematik, Arnimallee 6, 14195

We have developed a hidden Markov model and optimization procedure for photon-based single-molecule FRET data, which takes into account the trace-dependent background intensities. This analysis technique reveals an unprecedented amount of detail in the folding kinetics of the Diels-Alderase ribozyme. Depending on the Mg2+ concentration, 7 to 9 states can be distinguished, including putative native, near-native and misfolded states. Some states exist only at either low or high Mg2+ concentrations, while other states exhibit little sensitivity to Mg2+. There is a general tendency for structures to become more compact upon the addition of Mg2+. A hierarchy of timescales was found, including dynamics of 10 ms or faster, likely due to tertiary structure fluctuations, and slow dynamics on the seconds timescale, presumably associated with significant changes in secondary structure. The folding pathways proceed through a series of intermediate secondary structures. There exist both, compact pathways and more complex ones in which structures show tertiary unfolding, then secondary refolding, and subsequently tertiary refolding.

BP 2.6 Mon 10:45 ZEU 250

***In situ* release of DNA from artificial gene carriers** — •Natalja Strelnikova[1], Adriana Toma[1], Rolf Dootz[2], and Thomas Pfohl[1] — [1]University of Basel, Department of Chemistry, Switzerland — [2]Max Planck Institute for Dynamics and Self Organization, Göttingen, Germany

In chromosomes DNA exists in a highly organized state, wrapped around histones, forming a composite material called chromatin. Decondensation of DNA plays an essential role in gene expression. DNA must be unpacked for transcription, arousing interest in the understanding of underlying interaction mechanisms of DNA decompaction. Our goal is to discover the real-time dynamics of the release of DNA from artificial gene carriers (dendrimer PAMAM 6/DNA). We employ a newly developed soft lithography-based microfluidics reaction device in combination with a lab source X-ray instrument. Using SAXS and SAXD (small angle X-ray scattering and diffraction), we can study the nanostructural evolution of the involved processes. We observe the dynamics of DNA release from the gene carrier using heparin as an anionic competitor. Here, negatively charged heparin competes with phosphate groups of DNA to interact with positively charged amines of PAMAM 6. The impact of the heparin and the salt concentrations as well as the pH on the disintegration of DNA/PAMAM 6 complexes can be analyzed in a temporal manner.

**15 min. break**

**Topical Talk** BP 2.7 Mon 11:15 ZEU 250

**Single molecule torque and twist measurements probe the key players of the central dogma** — •Jan Lipfert — Department of Physics and CeNS, University of Munich, Germany

Single-molecule manipulation techniques have provided unprecedented

insights into the structure, function, interactions, and mechanical properties of biological macromolecules. While many single-molecule manipulation techniques naturally operate in the space of (linear) extension and force, recently a number of techniques have been developed that enable measurements of rotation angle and torque. These new methods provide exciting opportunities to probe biological important macromolecules. In particular, the helical nature of double-stranded DNA and RNA intrinsically links key processes such as replication, transcription, and genome repair to rotational motion and the accumulation of torsional strain.

In my talk, I will briefly review novel magnetic tweezers assays that enable direct measurements of single molecule torque and twist, notably magnetic torque tweezers (MTT) and freely-orbiting magnetic tweezers (FOMT). Using these techniques, we have for the first time mapped out the complete force-torque phase diagram for double-stranded RNA, discovering some similarities but also striking differences to its better studied cousin, DNA. In addition, I will briefly describe results on Rad51-DNA filaments, a key intermediate in DNA repair, and applications of our novel magnetic tweezers techniques to probe nucleosome dynamics.

BP 2.8 Mon 11:45 ZEU 250

**Hybrid Single-Molecule-FRET-Magnetic Tweezers Probe Force-Dependent Conformational Space** — •Marko Swoboda, Maj Svea Grieb, Stephan Friebe, Steffen Hahn, and Michael Schlierf — B CUBE, TU Dresden, Arnoldstraße 18, 01307 Dresden, Germany

Single-molecule methods are often separated in force-based and fluorescence-based techniques. Single-molecule Förster resonance energy transfer (smFRET) has proven to be a powerful tool to probe distance changes on the nanometer scale. The technique therefore perfectly matches biomolecular dimensions but lacks the ability to manipulate molecules. Magnetic tweezers are a prime tool to study the mechanics of DNA and its interacting enzymes but their spatial resolution is limited to the direction of force and torque application.

Here, we demonstrate a hybrid instrument, combining smFRET and magnetic tweezers. This allows us to simultaneously probe conformational dynamics in a molecular system, using both force and distance information. We demonstrate the instrument's capabilities by studying the behavior of a fluorescently labeled DNA undergoing rapid conformational fluctuations.

BP 2.9 Mon 12:00 ZEU 250

**Probing the kinetics of a model helicase-nuclease with a temperature-controlled Magnetic Tweezers** — •Benjamin Gollnick[1], Carolina Carrasco[1], Francesca Zuttion[1], Neville S. Gilhooly[2], Mark S. Dillingham[2], and Fernando Moreno-Herrero[1] — [1]Centro Nacional de Biotecnología, CSIC, Darwin 3, Campus de Cantoblanco, 28049 Madrid, Spain — [2]School of Biochemistry, Medical Sciences Building, University of Bristol, University Walk, Bristol BS8 1TD, UK

Motor protein activities such as ATP hydrolysis and translocation are temperature-dependent; by studying their kinetics under different thermal conditions one can estimate the associated physicochemical parameters. Here, we present a temperature-controlled Magnetic Tweezers setup that allows us to perform single-molecule experiments at temperatures in solution of up to 40 °C with a precision of 0.1 °C. Using this instrument we have been able to compare the translocation activity of individual copies of the bacterial DNA helicase-nuclease complex AddAB - an enzyme involved in the initial steps of double-stranded DNA break repair by homologous recombination - at different thermal settings with results obtained from ensemble measurements. Interestingly, although the two complementary approaches give rise to a systematic difference between their corresponding velocities measured at each temperature, they yield almost identical estimates of the kinetic barrier of the translocation process, which turns out to be on the order of 21 kT and hence similar to activation energies observed for other translocating proteins.

BP 2.10 Mon 12:15 ZEU 250

**RNA folding dynamics studied with structure based models** — •Michael Faber and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces Potsdam-Golm Science Park; Am Mühlenberg 1 OT Golm; 14476 Potsdam; Germany

RNA molecules form well defined three-dimensional structures on physiologically relevant timescales which are crucial for their enzymatic activity. Already during transcription structured RNA can have regulatory functions. Key to RNA folding is the formation of intramolecular base pairs which is called the secondary structure. We have developed a structure-based model of RNA and use a kinetic Monte-Carlo method to study the dynamics of secondary structures. We apply our methods to the folding and unfolding of several RNA structures in the presence and absence of external load forces. To study the effect of transcription on folding we look at co-transcriptional folding of riboswitches.

BP 2.11 Mon 12:30 ZEU 250

**Kinetics of conformational fluctuations in DNA hairpin-loops in crowded fluids** — •Olivia Stiehl and Matthias Weiss — Experimentalphysik I, Universität Bayreuth, Germany

Biochemical reactions in crowded solutions are commonly anticipated to differ strongly from those in dilute solutions. Macromolecular crowding not only induces excluded-volume interactions with surrounding molecules but it has also been frequently reported to initiate anomalous diffusion (subdiffusion). Both facets are supposed to stabilize complex formation of reaction partners.

A typical biochemical reaction is the thermally driven opening and closing transition of DNA hairpin-loops. Using fluorescence correlation spectroscopy (FCS), we have revealed that crowding not only slows down the opening/closing kinetics but also increases the steady-state fraction of the closed state significantly [1]. Our results also show that subdiffusion leads to an even stronger shift of the two-state equilibirum towards the closed state in comparison to pure excluded-volume effects. For that reason, we conclude that biochemical reactions are sensitive to both, excluded-volume interactions and changes of the diffusive behavior of the reactants.

Preliminary UV-absorption data also support the notion that the simplification of a two state model is no more justified in crowded solutions as soon as the DNA strand exceeds a certain length.

[1] O. Stiehl, K. Weidner-Hertrampf and M. Weiss: Kinetics of conformational fluctuations in DNA hairpin-loops in crowded fluids. New J. Phys. 15 (2013) 113010.

BP 2.12 Mon 12:45 ZEU 250

**The car–parking model solves the random completion problem of DNA replication** — •Jens Karschau[1,2], Peter J. Gillespie[3], J. Julian Blow[3], and Alessandro P. S. de Moura[1] — [1]University of Aberdeen, Aberdeen, U.K. — [2]MPI PKS, Dresden, Germany — [3]University of Dundee, Dundee, U.K.

Eukaryotic cells have a large yet fixed amount of replication starting points — origins of replication — whose distance amongst them gives the time to synthesise a DNA segment, and the largest distance ultimately dictates when the last remaining segment is fully synthesised so that a cell is ready to divide.

A naive assumption would be to have origins equally separated from each other to partition the DNA into small segments, so to have minimal replication time. In a model for proteins finding origin positions randomly we show how these origin positions are taken as a result from the spatial requirement for proteins to bind stably at random positions. This explains experimental data of protein-DNA adsorption kinetics showing saturation over time. In a second step, this leads to a problem in statistical physics known as the car-parking problem. A model akin to this successfully explains the criteria to have small segments, because during protein adsorption it is more likely for origin-forming proteins to land in large empty regions on DNA. With our model we solve a long-standing conundrum: how to have optimal origin spacing when adsorption occurs at random sites, i.e. the random completion problem. Its solution directly emerges from physical principles of our adsorption model.

# BP 3: Symposium SKM Dissertation-Prize 2014

Time: Monday 11:00–12:40 Location: CHE 89

**Invited Talk** BP 3.1 Mon 11:00 CHE 89

**Interplay of ordering behavior and optical properties in organic semiconductor blends** — •Katharina Broch — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Binary mixtures of organic semiconductors (OSCs) have recently become an important field of research due to their potential applications in opto-electronic devices. In these systems, the mixing (intermixing vs. phase separation) and ordering behavior is crucial, since it affects the optical and electronic properties. Investigating binary mixtures of the three prototypical OSCs pentacene (PEN), perfluoropentacene (PFP) and diindenoperlyene (DIP) in all possible combinations, allows to study systematically the influence of the competing effects of favorable intermolecular interactions and steric incompatibility on film structure and optical properties. The focus of the talk will be on the optical spectra determined post-growth, for which the impact of intermolecular interactions, including charge transfer [1], and of differences in mixing and ordering behavior on the spectral shape and peak positions will be discussed [2]. In particular, for PEN:DIP an anisotropic ordering behavior, comparable to that observed in some liquid crystals, is found, which is fundamentally new for OSCs [3] and which opens possibilites for a targeted tuning of intermolecular interactions in blends. [1] K. Broch et al., Phys. Rev. B, 83 (2011), [2] K. Broch et al., J. Phys. Chem. C, 117 (2013), [3] A. Aufderheide et al., Phys. Rev. Lett., 109 (2012).

**Invited Talk** BP 3.2 Mon 11:25 CHE 89

**Fingerprints of Geometry and Topology on Low Dimensional Mesoscopic Systems** — •Jan Carl Budich — Department of Physics, Stockholm University, SE-106 91 Stockholm, Sweden

Triggered by the discovery of the quantum spin Hall effect in two dimensional time reversal symmetric insulators, the impact of topology on the physics of Bloch bands has been systematically studied in recent years culminating in the formulation of a periodic table of topological insulators. We demonstrate the close analogy between geometric phases occurring in quantum systems that adiabatically depend on time via external control parameters and the formal description of topological insulators. While geometric phases may have immediate observable consequences, the experimental implications of the intrinsic topological features of band structures can be much more subtle. As for the mentioned quantum spin Hall state, the salient experimental signature of bulk topology is the necessity of metallic edge states characterized by the locking of spin and momentum. This peculiar constraint leads to novel quantum transport effects relating to the field of spintronics. We discuss how these phenomena are influenced by the presence of electronic correlations and by a finite bias voltage driving the edge channels out of thermal equilibrium, respectively.

**Invited Talk** BP 3.3 Mon 11:50 CHE 89

**Spin injection into GaAs - the spin solar cell and spin photodiode** — •Bernhard Endres, Mariusz Ciorga, Maximilian Schmid, Martin Utz, Dominique Bougeard, Dieter Weiss, Christian Back, and Günther Bayreuther — Universität Regensburg

Efficient spin injection into semiconductors is a prerequisite for the realization of spintronic devices which primarily make use of the electron spin orientation for data storage and information processing. In III-V semiconductors, a sizable spin polarization can be created by illumination, requiring circularly polarized light at a well-defined wavelength. In contrast, we demonstrate the spin solar cell effect as a new and efficient method for optical spin generation without these restrictions [1]. A laser beam is used to create electron-hole pairs in a (Ga,Mn)As\n-GaAs p-n-junction and to detect the spin accumulation via the magneto-optic Kerr effect (T=15 K). The photo-voltage causes electrons to tunnel across the narrow barrier from the n-GaAs into the (Ga,Mn)As. Since tunneling into (Ga,Mn)As is spin-dependent, spin-polarized electrons accumulate in the n-GaAs. A second working mode, the spin photodiode effect, is realized by applying a negative voltage to the (Ga,Mn)As contact which drives optically excited spins of reverse polarity from the (Ga,Mn)As conduction band into the GaAs layer. This new approach to convert light of arbitrary polarization into spin current is expected to work at room temperature and allows adaptation to different ferromagnets like Fe on mainstream semiconductors like Si.

[1] B. Endres et al., Nature Commun. 4, 2068 (2013).

**Invited Talk** BP 3.4 Mon 12:15 CHE 89

**Unraveling the impact of subsurface and surface properties of a material on biological adhesion - a multi-scale approach** — •Peter Loskill[1], Hendrik Hähl[1], Markus Bischoff[2], Kellar Autumn[3], Mathias Herrmann[2], and Karin Jacobs[1] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany — [2]Institute of Medical Microbiology and Hygiene, Saarland University, 66421 Homburg/Saar, Germany — [3]Department of Biology, Lewis & Clark College, Portland, OR 97219, USA

Understanding the adhesion of biological objects to inorganic surfaces is an important research objective in physics and the life sciences. To characterize biological adhesion, most studies describe a substrate solely by its surface properties; the composition of the material beneath the surface is frequently overlooked. That way, long-range van der Waals (vdW) interactions are disregarded. This work reveals that biological objects of all scales - nanoscopic proteins, microscopic bacteria, and macroscopic geckos - are influenced by nanoscale differences in the interface potential. By using tailored silicon wafers with a variable silicon oxide layer thickness, the vdW part of the interface potential is tuned independently from the surface properties. By modifying the wafers with silane monolayers, the surface chemistry can be varied separately as well. On these model substrates, adsorption and adhesion experiments were performed. Protein adsorption was investigated by in situ X-ray reflectometry, bacterial adhesion was explored via AFM force spectroscopy with bacterial probes, and gecko adhesion was characterized using a mechanical testing platform.

# BP 4: Membranes and Vesicles I

Time: Monday 15:00–17:00 Location: HÜL 386

**Invited Talk** BP 4.1 Mon 15:00 HÜL 386

**Role of membrane elasticity in clathrin-mediated endocytosis** — Sandrine Morlot[1], Saleem Mohammed[1], Nicolas Chiaruttini[1], Valentina Galli[1], Marius Klein[3], Luìs Dinis[4], Martin Lenz[5], Giovanni Cappello[3], and •Aurélien Roux[1,2] — [1]Biochemistry Department, University of Geneva, CH-1211 Geneva, Switzerland — [2]Swiss National Centre for Competence in Research Programme Chemical Biology, CH-1211 Geneva, Switzerland — [3]Institut Curie, Centre de Recherche; CNRS, UMR 168, Physico-Chimie Curie; Université Pierre et Marie Curie, F-75248 Paris, France — [4]Departamento de Fìsica Atòmica, Molecular y Nuclear, Facultad de Ciencas Fìsicas, Universidad Complutense de Madrid, ES-28040, Madrid, Spain — [5]James Franck Institute, University of Chicago, IL-60637 Chicago, U.S.A.

In Clathrin-mediated endocytosis, Clathrin assembles into a soccerball-like structure at the plasma membrane that was proposed to deform the membrane by scaffolding. However, controversies in the community have appeared on the exact role of Clathrin: does its polymerization force is sufficient to curve the membrane, or deformation by other means (protein insertion) is required? We studied the formation of Clathrin buds from Giant Unilamellar Vesicles, and found that the pits can be flattened when membrane tension is increased. This suggested that the Clathrin polymerization force could be counteracted by membrane tension, which we further proved by directly measuring Clathrin polymerization force: by pulling a membrane tube out of a GUV aspirated in a micropipette, we can measure the force required to hold the tube through an optical tweezer system. When Clathrin is added, it polymerizes onto the GUV predominantly, and the force drops. From these measurements, we can deduce that the polymerization strength of Clathrin is in the range of a few hundred micronewtons per meter. This value confirms that clathrin polymerization can be counteracted efficiently by membrane tension. To finalize endocytosis, the clathrin-bud needs to be separated from the plasma membrane. Membrane fission requires the constriction and breakage of a transient neck, splitting one membrane compartment into two. The GTPase Dynamin forms a helical coat that constricts membrane necks of Clathrin-coated pits to promote their fission. Dynamin constriction is necessary but not sufficient, questioning the minimal requirements for fission. Here we show that fission occurs at the edge of the Dynamin coat, where it is connected to the uncoated membrane. At this location, the specific shape of the membrane increases locally its elastic energy, facilitating fission by reducing its energy barrier. We predict that fission kinetics should depend on tension, bending rigidity and the Dynamin constriction torque. We verify that fission times depend on membrane tension in controlled conditions in vitro and in Clathrin-mediated endocytosis in vivo. By numerically estimating the energy barrier from the increased elastic energy, and measuring the Dynamin torque, we show that: 1- Dynamin torque, about 1nN.nm, is huge but necessary to achieve constriction, and 2- Dynamin work sufficiently reduces the energy barrier to promote spontaneous fission.

BP 4.2 Mon 15:30 HÜL 386

**Measuring local viscosities near membranes of living cells with photonic force microscopy** — •Felix Jünger and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

The diffusive motion of a particle in the vicinity of a boundary surface is relevant from a biological point of view, since the viscous drag $\gamma$ changes significantly with the distance to the interface, e.g. a cell membrane. In our work we use photonic force microscopy (PFM) to investigate how $\gamma$ changes when an optically trapped 1$\mu$m polystyrene bead approaches the plasma membrane of different biological cells. The bead's temporal fluctuations are tracked interferometrically in three dimensions with nanometer precision and on a microsecond time scale. The autocorrelation of the bead's motion reveals the friction coefficient $\gamma$(d) as a function of bead-membrane distance d.

We find a simple exponential decay for $\gamma$(d) with a hydrodynamic decay length $\Lambda$(d) that fits well to the obtained experimental data. We investigated different cell types (J774, HT29, MDCK) and a giant unilamellar vesicle (GUV). We find that all values $\Lambda$(d) measured at biological membranes are significantly longer than those of a rigid glass coverslip, giving rise to the conclusion that the deformable shape of the membrane influences the hydrodynamic interaction.

BP 4.3 Mon 15:45 HÜL 386

**Artificial DNA Membrane Nanopores** — •Kerstin Göpfrich[1], Jonathan Burns[2], Vivek Thacker[1], Thomas Zettl[1], Silvia Hernandez-Ainsa[1], Eugen Stulz[3], Stefan Howorka[2], and Ulrich Keyser[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Department of Chemistry, University College London, UK — [3]Department of Chemistry, University of Southampton, UK

Membrane nanopores are essential components of biological and artificial cells. Our group has shown that we can create artificial nanopores using DNA origami self-assembly (N.A.W. Bell, *Nanoletters*, 2012; S.M. Hernandez-Ainsa, *ACS nano*, 2013) and anchor them in lipid membranes (J. Burns, K. Göpfrich, *Angewandte Chemie*, 2013).
Insertion of negatively charged DNA pores into a hydrophobic membrane is achieved by attaching functional hydrophobic groups in strategic positions on the DNA nanopores. Pore formation in lipid vesicles is studied for different nanopore designs and hydrophobic modifications via fluorescent imaging (V.V. Thacker, *Applied physics letters*, 2012). Single-channel current recordings of our artificial DNA nanopores are performed using a high-throughput lipid nanobilayer system that has recently been introduced by our group (K. Göpfrich, *Langmuir*, 2013; J.L. Gornall, *Nano letters*, 2011). Pore architecture and functionality of our DNA nanopores can be easily adapted, opening the pathway to design novel membrane channels.

BP 4.4 Mon 16:00 HÜL 386

**Nanometer-resolved radio-frequency absorption and heating in bio-membranes** — •Stephan Gekle[1] and Roland Netz[2] — [1]Physikalisches Institut, Universität Bayreuth — [2]Fachbereich Physik, Freie Universität Berlin

Radio-frequency (RF) electromagnetic fields are readily absorbed in biological matter and lead to dielectric heating. To understand how RF radiation possibly influences biological function, a quantitative description of dielectric absorption and heating at nanometer resolution beyond the usual effective medium approach is crucial.

We report an exemplary multi-scale theoretical study for biomembranes that combines i) atomistic simulations for the spatially resolved absorption spectrum at a single planar DPPC lipid bilayer immersed in water, ii) calculation of the electric field distribution in planar and spherical cell models, and iii) prediction of the nanometer resolved temperature profiles under steady RF radiation.

For a spherical cell model, we find a strongly enhanced RF absorption on an equatorial ring, which gives rise to temperature gradients inside a single cell under radiation.

BP 4.5 Mon 16:15 HÜL 386

**Induced phagocytic particle uptake into a giant unilamellar vesicle using optical tweezers** — Andreas Meinel, Benjamin Tränkle, and •Alexander Rohrbach — University of Freiburg, Georges-Köhler-Allee 102, 79110 Freiburg

Phagocytosis, the uptake and ingestion of solid particles into living cells, is a central mechanism of our immune system. Due to the complexity of the uptake mechanism, the different forces involved in this process are only partly understood. Therefore the usage of a Giant Unilamellar Vesicle (GUV) as the simplest biomimetic model for a cell allows to investigate the influence of the lipid membrane on the energetics of the uptake process. Here, we use a photonic force microscope (PFM) to approach an optically trapped 1 um latex bead to a immobilized GUV to finally insert the particle into the GUV. By analysing the mean displacement and the position fluctuations of the trapped particle during the uptake process in 3D with nanometre precision, we are able to record force and energy profiles, as well as changes in the viscous drag and the stiffness. The measured energy profiles, which are compared to a Helfrich energy model for local and global deformation, show a good coincidence with the theoretical results.

BP 4.6 Mon 16:30 HÜL 386

**Cooperative wrapping of nanoparticles by membrane tubes** — •Michael Raatz, Thomas R. Weikl, and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Department of Theory and Bio-Systems, Potsdam, Germany.

The bioactivity of nanoparticles crucially depends on their ability to cross biomembranes. Recent simulations indicate the cooperative wrapping and internalization of spherical nanoparticles in tubular membrane structures. We systematically investigated the energy gain of this cooperative wrapping by minimizing the energies of the rotationally symmetric shapes of the membrane tubes and of membrane segments wrapping single particles. We found that the energy gain for the cooperative wrapping of nanoparticles in membrane tubes relative to their individual wrapping as single particles strongly depends on the ratio $\rho/R$ of the particle radius R and the range $\rho$ of the particle-membrane adhesion potential. For a potential range of the order of one nanometer, the cooperative wrapping in tubes is highly favorable for particles with a radius of tens of nanometers and intermediate adhesion energies, but not for particles that are significantly larger.

BP 4.7 Mon 16:45 HÜL 386

**On the dynamic properties of giant unilamellar vesicles under flow - towards a model for shear force transduction in cells** — •Bernhard Sebastian, Tobias Favero, and Petra Dittrich — ETH Zürich, Schweiz

We present a novel method for the study of external shear force transduction through vesicle membranes and their effect on the dynamics of the enclosed lumen in 3D using defocusing fluorescence microscopy.

Blood cells and endothelial cells are frequently exposed to mechanical strain induced by external flow, hence shear stress. External forces are transferred to the intracellular lumen through a process called mechanotransduction. We used giant unilamellar vesicles (GUVs) as a model system to investigate the effects of shear force induced mechanotransduction on the dynamics of the vesicle membrane as well as inside the lumen. Vesicles were trapped on a microfluidic chip. Fluorescent beads enclosed inside GUVs were used as flow tracer particles. A novel 3D tracking program allowed for visualization of the bead movement and its analysis in three dimensions at high spatial resolution using conventional fluorescence wide-field microscopy.

We observed bead movement along the GUV membrane in a bihemispheric pattern including rare crossing events between the hemispheres, independent of external flow speed. Detailed analysis of the bead trajectories revealed regions of high and low velocity that spatially depend on the magnitude of external flow. Flow in the GUV membrane was found to differ from that inside the lumen.

## BP 5: Protein structure and dynamics I

Time: Monday 15:00–17:00 Location: ZEU 250

BP 5.1 Mon 15:00 ZEU 250

**Rapid force spectroscopy** — •Jakob Tómas Bullerjahn, Sebastian Sturm, and Klaus Kroy — Universität Leipzig, Institut für theoretische Physik, 04103 Leipzig, Germany

Dynamic force spectroscopy, the examination of intermolecular binding affinities and kinetics through single-molecule manipulation techniques, is a valuable complement to more traditional means of structural investigation. In contrast to scattering techniques or classical microscopy, it allows the experimentalist to gauge the dynamic and plastic behavior of a given material by directly probing the underlying free energy landscape, on a molecular scale. However, in spite of the strong forces required to do so, established theories of force spectroscopy still build on Kramers' quasistatic theory. Originally devised for the usually slow process of spontaneous unbinding, it is set to break down at high loading rates. We extend these theories to fast loading rates by explicitly resolving the nonequilibrium internal bond dynamics. Our analytical results turn out to hold almost universally, for fast and slow loading alike, breaking down only within a narrow parameter range close to a well-defined critical loading rate. Their large range of applicability moreover renders them an ideal companion to Bayesian methods of data analysis. Yielding highly competitive results, even without precise *a priori* knowledge of the underlying energy landscape, our generic analytical theory suggests itself as a unified framework for analyzing and comparing force spectroscopy data from a wide range of experiments and simulations.

BP 5.2 Mon 15:15 ZEU 250

**Influence of Antifreeze Proteins on Local Water Structure Dynamics in Presence of Osmolytes** — •Anand Narayanan Krishnamoorthy[1] and Jens Smiatek[2] — [1]Institute of Computational Physics, Stuttgart, Germany — [2]Institute of Computational Physics, Stuttgart, Germany

Antifreeze proteins are synthesized by various organisms to enable their cells to survive low temperature environments like in the polar regions. These proteins produce a difference between the melting and freezing points of the solutions termed as thermal hysteresis. The main objective of this study is to examine the dynamics of water molecules and hydrogen bonds at the protein-water interface of antifreeze protein using atomistic molecular dynamics simulations. For this work a prototype of AFP (antifreeze protein) from antarctic notothenioids (Ala-Ala-Thr repeats) and a mutant which is not antifreeze active were generated and compared. The hydration dynamics results reveal that the retarded water dynamics in the AFP compared to its mutant could be a possible reason for the antifreeze activity. A considerable change of the hydration dynamics was additionally observed for the AFP in presence of osmolytes. The mechanism of the interaction was investigated by analyzing the preferential binding parameter derived from Kirkwood-Buff integrals.

BP 5.3 Mon 15:30 ZEU 250

**Electrochromic shift calculations exhibit the light-activation mechanism of BLUF photoreceptors** — •Florimond Collette, Marcel Schmidt am Busch, and Thomas Renger — Institut für Theoretische Physik, Johannes Kepler Universität Linz, Altenberger Strasse 69, 4040 Linz, Austria

The photoreceptor family named BLUF, short for 'sensors of blue-light using flavin adenine dinucleotide (FAD)', is involved in a variety of important physiological reactions like phototaxis, photosynthetic gene regulation and virulence. Upon illumination with blue light, the photoreceptor switches into a light-adapted signaling state, with a measurable 10 to 15 nm redshift of the absorption maximum. The spectroscopic shift is explained by an alteration in the hydrogen-bonding pattern surrounding the chromophore [1]. Two opposite molecular models exist. One model is supported by the majority of crystallographic studies [2], whereas the second is favored by most spectroscopical works [3]. Within the framework of a quantum chemical/electrostatic calculation scheme, we estimated absorption shifts of the flavin chromophore for a series of site-directed mutants and different BLUF proteins. Our calculations accurately reproduce a series of spectroscopic data and provide compelling evidence for the model supported by the majority of crystallographic studies [4].

[1] S. Masuda, *Plant Cell Physiol.* **54**, 171 (2013).
[2] S. Anderson *et al.*, *Biochemistry* **44**, 7998 (2005).
[3] A. Jung *et al.*, *Proc. Natl. Acad. Sci. USA* **102**, 12350 (2005).
[4] F. Collette *et al.*, submitted.

BP 5.4 Mon 15:45 ZEU 250

**Observation of the size and shape of the initial crystallites involved in crystallisation of the model protein lysozyme** — •Raimund J. Heigl[1], Andreas Ostermann[2], Jörg Stellbrink[3], Aurel Radulescu[1], Dieter Richter[3], and Tobias E. Schrader[1] — [1]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Lichtenbergstr.1, 85747 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Lichtenbergstr.1, 85747 Garching, Germany — [3]Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Lysozyme serves as a model protein for the study of protein crystallisation. Yet, the size and shape of the first crystallites leading to the formation of macroscopic crystals is not known. Especially for the method of neutron protein crystallography large crystals need to be grown. Here, good understanding of the evolution of crystal growth would be advantageous. We have found crystallisation conditions of hen egg white lysozyme in $D_2O$ which lead to the growth of a fair number of crystals. Preliminary data has been recorded on the small angle neutron scattering (SANS) instrument KWS-2 at the MLZ. It shows a decrease at an intermediate q-range between 0.01 $Å^{-1}$ and 0.02 $Å^{-1}$ and an increase at smaller q-values indicating the growth of small crystallites. Dynamic light scattering measurements point to a

size distribution of three different hydrodynamic radii. One around 5 nm does not change much with time whereas the middle sized radius rapidly increases.

BP 5.5 Mon 16:00 ZEU 250

**Correlation between Supercoiling and Conformational Motions of the Bacterial Flagellar Filament** — •Andreas Stadler[1], Tobias Unruh[2], Keiichi Namba[3], Fadel Samatey[4], and Giuseppe Zaccai[5] — [1]FZ Jülich, ICS-1 & JCNS-1, 52428 Jülich — [2]Univ. Erlangen-Nürnberg — [3]Osaka University, Osaka, Japan — [4]Institute of Science and Technology, Okinawa, Japan — [5]Institut Laue-Langevin, Grenoble, France

The bacterial flagellar filament is a very large macromolecular assembly of a single protein flagellin. Various supercoiled states of the filament exist, which are formed by two structurally different conformations of flagellin in different ratios.

We investigated the correlation between supercoiling of the protofilaments and molecular dynamics in the flagellar filament using quasielastic and elastic incoherent neutron scattering in the picosecond and nanosecond time scales. Thermal fluctuations in the straight left- and right-handed (L- and R-type) filaments were measured and compared to the wild-type filament. Amplitudes of motion in the picosecond time scale were found to be similar in the different conformational states. Mean square displacements and protein resilience in the 0.1 nanosecond time scale demonstrate that the L-type state is more flexible and less resilient than the R-type, while the wild-type state lies in between. Our results provide strong support that supercoiling of the protofilaments in the flagellar filament is determined by the strength of molecular forces in and between the flagellin subunits.

BP 5.6 Mon 16:15 ZEU 250

**Revealing Rad51 and 53BP1 distribution in HeLa cell nuclei after low and high LET irradiation** — •Judith Reindl[1], Guido A. Drexler[2], Stefanie Girst[1], Christoph Greubel[1], Christian Siebenwirth[1], Sophie Drexler[2], Anna A. Friedl[2], and Günther Dollinger[1] — [1]Universität der Bundeswehr, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany — [2]Ludwig-Maximilians-Universität München, 80336 München, Germany

53BP1 and Rad51 are prominent representatives for two DNA damage repair compartments, the flanking chromatin and the single-stranded DNA (ssDNA) compartment. The correlation between these two repair proteins is revealed by super high resolution STED microscopy with respect to the damage distribution inside a cell nucleus. Ionizing radiation creates double-strand breaks (DSB) of high local density and different complexity with respect to its LET (Linear Energy Transfer). Therefore low LET proton and high LET carbon ion irradiation at the irradiation facility SNAKE are used to generate different damage distributions inside cell nuclei. It is possible to image and analyse the ionizing radiation induced foci (IRIF) in their fine structure and visualize the mutual exclusion of the two damage repair compartments in one cell nucleus by analysing the correlation of Rad51 and 53BP1. Therefore a newly designed analysis program is used, which examines the local correlation of two signalling channels. The presented experimental findings clearly support the two compartment model which could be demonstrated for the first time in one cell for Rad51 and 53BP1.

**Topical Talk** BP 5.7 Mon 16:30 ZEU 250

**Particle-based stochastic computer simulations of biological systems** — •Ulrich Schwarz — Heidelberg University, Heidelberg, Germany

Evolution is a tinkerer and biological systems have evolved because they work, not because they are beautiful or optimal. Although some biological systems show striking examples of pattern formation, self-assembly or control circuits that occur in a similar manner in physical or engineered systems, very often these aspects are strongly intertwined in biological systems. From the modelling point of view, particle-based stochastic computer simulations are a very fruitful approach to investigate these different aspects of biological systems in one unifying framework. We will first discuss this point for the Min-proteins, which have been shown to develop beautiful spatio-temporal oscillations patterns in reconstitution assays, but which are also related to bacterial regulation. We will then discuss self-assembly of viral capsids, which in some cases might be regulated by event-driven switches in capsomere reactivity. In both cases, particle-based stochastic computer simulations have been successfully used to investigate the detailed dynamics leading to the final state.

## BP 6: Posters: Membranes and vesicles

Time: Monday 17:30–19:30 Location: P3

BP 6.1 Mon 17:30 P3

**Modeling vesicular transport in Chromaffin cells** — •Daungruthai Jarukanont — university of Kassel, Kassel, Germany

In cell communications, the transport of vesicles is essential for storage and release of chemical messenger molecules. Here, we demonstrate that the statistical analysis of electrophysiological measurements viewed as a time series of spikes permits to determine the equation of motion governing vesicle transport. We perform amperometric measurements of Chromaffin cells for inter-release events interval analysis. Histogram of most recording follow Inverse-Gaussian distribution which can be connected to Brownian motion of particles with a drift term. Therefore we model the vesicles as diffusive particles with external force in membrane direction. Their motion follow over-damped Langevin equation with constant drift velocity, and their density evolve by the corresponding Fokker-Planck equation. The simulations are able to reproduce our and others published experiments in good agreement.

BP 6.2 Mon 17:30 P3

**Lipid bilayers on microporous substrates** — •Theresa Kaufeld[1], Claudia Steinem[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut - Biophysik, Georg-August Univesität Göttingen — [2]Institut für organische und biomolekulare Chemie, Georg-August Universität Göttingen

We have designed microporous substrates with individually addressable arrays of micrometer-sized apertures for a combination of electrical experiments and fluorescence microscopy, which are also suitable for other techniques such as mechanical manipulation of lipid bilayers. An integrated electrode facilitates access for microscope objectives. We characterized the substrates in terms of surface roughness and pore geometry by SEM and AFM. We then used impedance spectroscopy to characterize the substrate electrically with and without the integrated electrode and measured a resistance in the kilo-Ohm range, which is clearly distinguishable from the Giga-Ohm seal we found with pore-spanning lipid bilayers. Solvent-free lipid bilayers were formed by GUV spreading and imaged with fluorescence microscopy. Electric experiments using alamethicin as a test ion channel showed single-channel resolution.

BP 6.3 Mon 17:30 P3

**$\alpha$-Synuclein insertion into supported lipid bilayer as seen by in situ X-ray reflectivity** — •Hendrik Hähl[1], Isabelle Möller[1], Irena Kiesel[2], Dorinel Verdes[1], Christian Sternemann[2], and Stefan Seeger[1] — [1]Institute of Physical Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich — [2]Fakultät Physik/DELTA, TU Dortmund, D-44221 Dortmund

$\alpha$-Synuclein ($\alpha$S) is a small 140 residues protein, which is unstructured in its cytosolic form and folds into $\alpha$-helices upon insertion into the cell membrane. The protein is closely related to the Parkinson disease (PD) via the appearance of aggregates in neuronal cells, which consist mainly of missfolded $\alpha$S. Yet, neither the normal function of $\alpha$S nor its role in the pathogenesis of the disease is fully understood. Both seems to be associated with the interaction with the membrane. In its membrane bound form the protein may cause disruption or permeabilization of the membrane. Especially variants appearing in early-onset forms of PD show an increased propensity to membrane destabilization. Here, we applied in situ X-ray reflectivity at high beam energy to monitor the structural changes of supported lipid bilayers upon inclusion of $\alpha$S and thus aim at a better understanding of the membrane interaction of $\alpha$S. By comparison with the evolution of a blank bilayer, the wild type form as well as the highly toxic variant E57K were found

to intrude deeply into the lipid head groups of the bilayer. Moreover, an observed decrease in the bilayer's thickness due to the protein insertion shows the protein's ability to force a remodeling of the membrane.

BP 6.4 Mon 17:30 P3

**Hydration repulsion between membranes and polar surfaces: simulation approaches versus continuum theories** — •Matej Kanduc[1], Alexander Schlaich[1], Emanuel Schneck[2], and Roland Netz[1] — [1]Free University Berlin, D-14195 Berlin, Germany — [2]Institut Laue-Langevin, Grenoble, France

A computer all-atom simulation approach for the study of the hydration repulsion between lipid membranes and polar surfaces is presented. We show the main results on repulsive hydration pressures, interaction thermodynamics, and interaction mechanisms. We have a close look at the influence of the experimental boundary conditions on the repulsion mechanisms due to the unfavorable overlap of interfacial water layers. To this end, we analyze several water order parameters in simulations of interacting polar surfaces and compare the results to the predictions of continuum theories.

BP 6.5 Mon 17:30 P3

**Coarse-grained simulations of membranes interacting with amyloid fibril forming peptides** — •André Kesser and Friederike Schmid — Johannes Gutenberg-Universität Mainz, Mainz

We are developing a generic coarse-grained model to investigate nucleation of amyloid peptides in the presence of lipid membranes. To this end, we combine a simple lipid membrane model developed in our group with a peptide model proposed by S. Auer and coworkers, which is derived from the popular tube model. Both peptides and lipids are represented by linear stiff chains connected by beads, with additional angular potentials, non-bonded Lennard-Jones type interactions and (in the case of peptides) additional hydrogen bonds. Currently we are building a c++ based Software to investigate these models by Monte Carlo and Molecular Dynamics simulations. We describe the model and present first results.

BP 6.6 Mon 17:30 P3

**Infrared mapping of membrane proteins with 30 nm lateral resolution** — Iban Amenabar[1], •Elmar Hassan Hubrich[2], Joachim Heberle[2], and Rainer Hillenbrand[1] — [1]CIC nanoGUNE Consolider, 20018 Donostia-San Sebastián, Spain — [2]Experimental Molecular Biophysics, Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany

Infrared spectroscopy is a common technique to study proteins. However, the diffraction limit prevents resolution on the nanometer scale. Using Fourier transform infrared nanospectroscopy (nano-FTIR), we were able to measure membrane proteins with a lateral resolution of 30 nm.

Nano-FTIR combines scattering-type scanning near-field optical microscopy (s-SNOM) and Fourier transform infrared spectroscopy (FTIR). A metalized tip of an atomic force microscope (AFM) is illuminated with a broadband infrared laser and the backscattered light is analyzed by a Fourier transform infrared spectrometer.

BP 6.7 Mon 17:30 P3

**Time-resolved electron tomography reveals how the plasma membrane is reshaped during endocytosis** — •Martin Schorb[1], Wanda Kukulski[1,2], Marko Kaksonen[2], and John AG Briggs[1,2] — [1]Structural and Computational Biology Unit, EMBL, Meyerhofstr. 1, 69117 Heidelberg — [2]Cell biology and Biophysics Unit, EMBL, Meyerhofstr. 1, 69117 Heidelberg

Endocytosis is a highly dynamic process that requires a precise temporal and spatial orchestration of multi-component protein modules in order to collect cargo, invaginate the plasma membrane and eventually form an endocytic transport vesicle. Using different pairs of endocytic proteins tagged with GFP and RFP, which act at different stages during endocytosis, we were able to label specific timepoints during the process. By then applying a correlative fluorescence and electron tomography (ET) method, we located specific intermediate stages in 211 individual endocytic budding events, and reconstructed them in 3D. This dataset provides description of plasma membrane (PM) morphology during the transitions from a plane membrane to tubular invagination, through formation of a constricted neck followed by scission of a vesicle. At each timepoint the presence or absence of key protein players is known. This represents a comprehensive, spatiotemporal description of the plasma membrane topology during endocytosis. A multi-parameter analysis of the membrane profile shapes provides quantitative information about how protein modules of the endocytic machinery coordinate the changes in membrane morphology required for vesicle budding in vivo.

BP 6.8 Mon 17:30 P3

**Investigation of DPPC-Membranes in the gel phase and its phase transition in Molecular Dynamics Simulations** — •Bartosz Kowalik[1], Alexander Schlaich[1], Emanuel Schneck[2], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut Laue-Langevin, 6 Rue Jules Horowitz, 38000 Grenoble, France

Membranes in gel phases and melting transitions to the liquid phase have become a topic of increasing interest recently. Experiments and computer simulations have revealed sharp phase transitions in many physical quantities, which still are not completely understood. In our work, we investigate such a membrane consisting of dipalmitoylphosphatidylcholine (DPPC) that forms a lipid bilayer in an aqueous surrounding. We perform Molecular Dynamics Simulations, which allow us to look into atomistic detail of such systems.

We examine in detail the thermodynamic phase transition. Also, we investigate the differences in structure, energy and order parameters, especially we present a framework to derive the bending rigidities of membranes from Molecular Dynamics Simulations.

BP 6.9 Mon 17:30 P3

**The role of ions in the Hydration Interaction between polar surfaces** — •Alexander Schlaich[1], Matej Kanduc[1], Emanuel Schneck[2], and Roland R. Netz[1] — [1]Fachereich Physik, Freie Universität Berlin, Arnimalle 14, 14195 Berlin — [2]Institut Laue-Langevin, 6 Rue Jules Horowitz, 38000 Grenoble, France

Atomistic computer simulations are an essential tool for the study of the hydration repulsion between biological membranes, which becomes the dominating force at nanometer separations, giving rise to membrane stability. However, the study of interaction pressures, interaction thermodynamics, and interaction mechanisms with computer simulations still is a challenging task as the correct chemical potential of water needs to be accounted for.

We present atomistic simulations of simple polar surfaces in water and analyze the influence of ions present in the water slab at prescribed chemical potential, using Thermodynamic Extrapolation, a technique which has become available only recently. At physiological conditions ions play an important role both for structural and physiological behavior of membranes. We also present their influence on dielectric properties of the water confined between the surfaces and check the applicability of continuum theory on the observed effects.

BP 6.10 Mon 17:30 P3

**Environmental effects on diffusion in the Trypanosome membrane** — Marius Glogger, Andreas Hartel, Markus Engstler, and •Susanne Fenz — University of Würzburg, Biocenter: Zoology I, Würzburg, Germany

Trypanosomes (T. brucei) are the pathogen of sleeping sickness. They exhibit a surface coat of identical variable surface glycoproteins (VSGs) as protection against the innate immune response of the host. This coat is extremely dense, but also highly dynamic. This ambivalent character is in the focus of our research interest. Here, we will present our insights on the effect of the environmental parameters, ambient medium and lipid matrix, on VSG dynamics as measured by Fluorescence Recovery after Photobleaching (FRAP). In order to perform FRAP on endogenously highly motile trypanosomes they have to be immobilized, e.g. embedded in gelatin gels. To probe whether this condition biases the measurements we performed control experiments in model membranes. Surprisingly, neither the absolute diffusion coefficient nor the mobile fraction was affected. We hypothesize that a low viscosity layer of buffer at the trypanosome-gelatine interface served as a lubricant. Thus, it ensured that the observable diffusion was still dominated by frictional dissipation within the membrane and with neighboring variant and invariant membrane proteins. VSGs are anchored to the cell membrane via a glycosylphosphatidylinositol (GPI) moiety. In a second set of experiments we will characterize the fluidity of the lipid matrix both in the inner and outer membrane leaflet and thus define the framework for a holistic interpretation of VSG dynamics.

BP 6.11 Mon 17:30 P3

**Strongly hydrogen bonded water in the hydrophobic tail of**

**lipid bilayers** — •Marie Tritschel and Stephan Gekle — Biofluid Simulation and Modeling, Universität Bayreuth

Recent vibrational sum frequency experiments [1] detected strongly hydrogen bonded water molecules at lipid interfaces which were tentatively attributed to hydrogen bonds between water molecules and the phosphate group. However, similar features were also detected in lipids without a phosphate group such as DPTAP.

Using molecular dynamics simulation we show that in addition to water phosphate bonds there exists a sizeable amount of water molecules strongly hydrogen bonded to the carbonyl group in the hydrophobic tail of DPPC. The interaction energy of these bonds is approximately twice as high as in bulk water. Since similar carbonyl groups are also present in DPTAP this may explain the experimental observations.

Finally, we show that the interaction energy of a hydrogen bond is similar when the second binding partner is either water or an atom from a neighbouring lipid, whereas it is higher when the water shares its two hydrogen bonds with the same lipid.

[1] M. Bonn, H. J. Bakker, A. Ghosh, S. Yamamoto, M. Sovago, and R. K. Campen; **132** *J. Am. Chem. Soc.* [2010], 14971

BP 6.12 Mon 17:30 P3

**Interaction of amphiphilic triblock copolymers with lipid bilayer membranes: Monte-Carlo simulations** — •Hauke Rabbel[1,2], Marco Werner[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden - Institute for Theoretical Physics

Amphiphilic ABA triblock copolymers show interesting behaviour in their interactions with lipid membranes. For example PEO-PPO-PEO, also known under the trademark Pluronics, have found applications in pharmaceutical contexts both as membrane sealents and permeabilizers. Despite their applications, the nature of the interaction with cellular membranes is not yet fully understood. Here we study the interactions of different types of ABA triblock copolymers with lipid bilayer membranes using the bond fluctuation model with explicit solvent[1,2]. We consider polymers with different A- and B-block lengths under variation of the relative hydrophobicities of the constituents. The results indicate that the surface active behaviour of ABA triblock copolymers adsorbed at lipid membranes can be understood by their hydrophilic-lipophilic balance, as supported by recent experimental observations[3]. Triblock copolymers with purely hydrophilic A-blocks and a well chosen hydrophobicity of the B-blocks may find use as membrane-active agents, when fixed in a membrane spanning conformation.

[1] I.Carmesin and K.Kremer, Macromolecules 1988, 21, 2819-2823
[2] M. Werner, J.-U. Sommer, V.A. Baulin, Soft Matter 2012, 8, 11714
[3] Wang, Marks, Lee, Biomacromolecules 2012, 13, 2616-2623

## BP 7: Posters: Cell adhesion, mechanics and migration

Time: Monday 17:30–19:30 Location: P3

BP 7.1 Mon 17:30 P3

**Mechanical Response of MDCK II Cells to Porous Substrates** — •Matthias Büchsenschütz-Göbeler[1], Jan Rother[3], Andreas Janshoff[3], Walter Arnold[1,2], and Konrad Samwer[1] — [1]I. Physikalisches Institut, Universität Göttingen — [2]Department of Material Science and Materials Technology, Saarland University — [3]Institut für Physikalische Chemie, Universität Göttingen

A large number of cellular processes, such as proliferation, differentiation and motility involve adhesion and mechanical adaption of living cells to surfaces. Usually, cells are part of whole cellular networks and connected by an extracellular matrix (ECM). Thereby, elasticity, chemical composition and topography of the ECM affect cell motility and viscoelasticity by changing signal transduction pathways that in turn influence organization of cytoskeleton. The viscoelastic response of living MDCK II cells and adhesion to porous surface elasticity has been investigated by conventional nanoindentation and by a microrheological approach using a modified atomic force microscope. The structure of the cytoskeleton has been monitored by scanning electron microscopy and total internal reflection microscopy. The results show that cells grown on porous substrates are generally softer than cells grown on smooth substrates. With increasing pore size the stiffness of the cells decreases until a certain threshold size is reached. For larger pore sizes the stiffness is increasing again. In addition to this mechanical behavior a correlation with the cytoskeletal structures of the cells is observed.

Financial support by the DFG SFB 937 is thankfully acknowledged.

BP 7.2 Mon 17:30 P3

**Xenopus spindle size is set by the microtubule mass balance in an active liquid crystal** — •Johannes Baumgart[1], Simone B. Reber[2], Anthony A. Hyman[2], and Frank Julicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauer Str. 108, 01307 Dresden, Germany

The spindle apparatus consists mainly of microtubules and associated proteins. Correct spindle length is essential to reliably segregate chromosomes. Although we have extensive knowledge of microtubule dynamics, we still lack an understanding of how their collective properties give rise to a spindle with a defined size. We describe the spindle as an active liquid crystal because the individual rod-like microtubules turnover fast and are short compared to the overall spindle length. Furthermore, they slide and align by the activity of specific motors and crosslinkers. This allows us to determine spindle size by using mass balance of dynamic microtubules considering a constant spindle mass density. Spindle size then results from the balance of localized nucleation mediated by chromatin and global disassembly of microtubules.

This model implies a linear relationship between spindle length and microtubule growth velocity. This is indeed observed experimentally (Reber et al., Nat Cell Biol, 2013, 15, 1116–1122). In experiments, *Xenopus laevis* egg extract was used, which rules out size control due to external constrains and component limitations.

BP 7.3 Mon 17:30 P3

**A Novel Method for Traction Force Microscopy and first Applications** — •Benedikt Sabass[1,2] and Ulrich S. Schwarz[2] — [1]Princeton University — [2]University of Heidelberg

We present a new and simple method to measure three-dimensional forces exerted by cells on flat elastic substrates. Traction force microscopy is a well-established technique for two-dimensional mapping of forces. However, the reconstruction of three-dimensional surface forces has been hampered by the difficulty to obtain reliable measurements of the vertical deformation of the substrate. The new method avoids this problem and only requires a standard experimental setup with a confocal microscope. We explain the mathematical background of our approach and describe the experiment. Advantages and disadvantages of the method are exemplified with simulated data. Finally, we discuss measurements that demonstrate the presence of weak out-of-plane forces in the case of adhering fibroblasts.

BP 7.4 Mon 17:30 P3

**Mechanical and spectroscopic analysis of single erythrocytes using whole human blood samples** — •Michael Göllner, Adriana Toma, and Thomas Pfohl — Department of Chemistry, University of Basel, Switzerland

Containing a wealth of information, human blood is the most used sample for diagnostic purposes. Microfluidics, with its unique advantages in performing analytical functions, has been increasingly used for whole blood and cell-based analysis. Single-cell studies using optical tweezers involve complex and expensive instrumentation to manipulate erythrocytes, which might be detrimental for easy application in medical diagnostics. Moreover, optical trapping shows photodamage causing difficulties with long-term and step-by-step analysis under reversible reaction control.

We developed a microfluidic setup in combination with optical and confocal Raman microscopy for single-cell assays starting with whole blood samples, which permits diffusion-controlled variation of the external environment without the need of optical tweezers for immobilizing the erythrocytes. Mechanical as well as spectroscopic properties like membrane elasticity, shape deformations and the full oxygenation

cycle of individual erythrocytes under different osmolarities are investigated.

BP 7.5 Mon 17:30 P3

**Stress fibre organisation dynamics in adult stem cells** — •Carina Wollnik[1], Kwang-Rae Kim[2], Ina Schachtschneider[2], Carsten Gottschlich[2], Stephan Huckemann[2], and Florian Rehfeldt[1] — [1]Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — [2]Institute for Mathematical Stochastics, Georg-August-University, Göttingen, Germany

Human mesenchymal stem cells (hMSCs) from bone marrow differentiate into other cell types like nerve, bone, and muscle cells. Here mechanical cues can be as important as biochemical ones as demonstrated by Engler et al. [1]. They showed substrate stiffness guides hMSCs towards different lineages in the absence of additional biochemical stimuli. Stress fibres composed of actin filaments, binding- and crosslinking-proteins and myosin motor-proteins, generate and transmit forces within the cell and to the ECM. Blocked motor-proteins stop the cell differentiation process, so stress fibre activity seems crucial. Though the differentiation process takes up to weeks, early characteristic stress fibre reorganisation can be detected within the first 24 hours and used as an early morphological marker[2]. In our experiments we use live-cell imaging of RFP-Lifeact transfected hMSCs and trace the stress fibres with sophisticated filament tracking algorithms [3], which enable us to investigate the dynamics of stress fibre formation in early stages after seeding that leads to a non-monotonic dependence of stress fibre polarization on the Young's modulus of the underlying substrate. [1]Engler et. al., 2006 [2]Zemel and F. Rehfeldt et al., 2010 [3]Gottschlich et al., 2009

BP 7.6 Mon 17:30 P3

**T-cell response to ligand presentation in the form of nano-dot arrays** — •Fuwei Pi[1], Pierre Dillard[1,2], Anne Charrier[1], Laurent Limozin[2], and Kheya Sengupta[1] — [1]Aix-Marseille Université, CNRS, CINaM UMR 7325, Marseille, 13288, France — [2]Laboratoire Adhésion & Inflammation, Aix-Marseille Université / Inserm U1067 / CNRS UMR7333, Marseille, 13288, France

We developed a simple cost-effective benchtop protocol to functionalize glass or polydimethylsiloxane elastomers with an array of nanometric protein dots for cell adhesion studies [1]. The diameter of the dot was varied down to about 80 nm. The adhesion of T-lymphocytes (Jurkat) on substrates patterned with the ligand anti-CD3 was studied using a variety of imaging techniques. The adhesion area was quantified using reflection interference contrast microscopy (RICM). Total internal reflection fluorescence (TIRF) microscopy was used to explore the possible colocalization of T-cell receptor microclusters and the activating anti-CD3 dots. The impact on the structure of the actin cytoskeleton was imaged with TIRF and confocal microscopy. We report modulation of the cell surface topography, and actin organization.

[1] F. Pi, P. Dillard, L. Limozin, A. Charrier, K. Sengupta; NanoLett. 13 7 3372-3378 (2013).

BP 7.7 Mon 17:30 P3

**Regulation of Hematopoietic Stem Cell Adhesion by Nanometric Presentation of Niche Ligand Candidates** — •Alexandra Burk[1,2], Cornelia Monzel[2], Hiroshi Yoshikawa[3], Anthony Ho[4], and Motomu Tanaka[1,2,5] — [1]Institute for Toxicology and Genetics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Physical Chemistry of Biosystems, Institute of Physical Chemistry, Heidelberg University, Heidelberg, Germany — [3]Department of Chemistry, Saitama University, Saitama, Japan — [4]Clinic for Internal Medicine V, Heidelberg University, Heidelberg, Germany — [5]Institute for Integrated Cell-Material Sciences (WPI iCeMS), Kyoto University, Kyoto, Japan

A major challenge in understanding the mobilization/immobilization mechanisms of hematopoietic stem cells (HSC) is to characterize the complex interplays of HSC-niche interactions in bone marrow such as the receptor/ligand pairs N-cad/N-cad and CXCR4/SDF1$\alpha$. To quantify these interactions, we designed well defined niche models consisting of planar lipid membranes on solid substrates displaying recombinant N-cadherin and human SDF-1$\alpha$ at defined intermolecular distances (5 nm to 100 nm). For contact- and label-free imaging of HSC, micro-interferometry (RICM) and phase contrast imaging was applied. To evaluate the strength of cell adhesion, we developed a new technique utilizing pressure waves induced by a picosecond laser pulse for non-invasive HSC detachment. Moreover, time-lapse analysis of cellular motion resulted in characteristic mean square displacements and modes of motion depending on the underlying substrate.

BP 7.8 Mon 17:30 P3

**Cell mechanics and innate immunity link up during infections** — •Andrew Ekpenyong[1,3], Si Ming Man[2], Sarra Achouri[1], Gilbert Ng[1,3], Kate Hughes[2], Panagiotis Tourlomousis[2], John Wright[2], Pietro Cicuta[1], Clare Bryant[2], and Jochen Guck[1,3] — [1]Cavendish Lab., Dept. of Physics, Univ. of Cambridge, UK — [2]Dept. of Vet. Medicine, Univ. of Cambridge, UK — [3]Biotech. Center, Technische Universität Dresden, Germany.

Infections, in which pathogens invade and colonize host cells, constitute some of the most serious diseases faced by humans. Host cells use immune system proteins and other molecules to fight viral and bacterial invaders. The mechanisms by which these proteins enable cells to survive infections remain unclear. Moreover, during infections, some immune system proteins are known to alter the cytoskeleton, the structure that largely determines cellular mechanical properties. We therefore used an optical stretcher to measure the mechanical properties of primary immune cells (macrophages) during bacterial infection. We found that macrophages become stiffer upon infection. Remarkably, macrophages lacking the proteins, Caspase 1 and NLRC4, lost the stiffening response to infection. This *in vitro* result correlates with our *in vivo* data whereby mice lacking Caspase 1 and NLRC4 have more lesions, implying increased bacterial spread. Thus, the immune-protein-dependent increase in cell stiffness in response to bacterial infection seems to have a functional role in the system level fight against pathogens. We will discuss how this functional link between cell mechanics and innate immunity reduces the spread of infection.

BP 7.9 Mon 17:30 P3

**Correlation analysis of the role of TRPC6 channels in the regulation of CXCR2-mediated chemotaxis of murine neutrophils** — •Peter Dieterich[1], Otto Lindemann[2], and Albrecht Schwab[2] — [1]Institut für Physiologie, TU Dresden — [2]Institut für Physiologie II, Westfälische Wilhelms-Universität Münster

Cellular motility and the ability of cells to sense and react to changes of their environment are of fundamental importance for efficient immune response. Chemoattractants trigger receptor initiated signaling cascades including the activation of plasma membrane $Ca^{2+}$ channels of the transient receptor potential channel family (TRPC). Here we disentangle the influence of TRPC6 channels on cell migration paths of murine neutrophils during chemotaxis caused by spatially increasing concentrations of keratinocyte-derived cytokine KC. Wildtype neutrophils show directed motion and diffusion. Blocking of the KC-receptor CXCR2 with a specific inhibitor reduces directed motion to $\sim$ 25% compared to wildtype cells and simplifies velocity autocorrelations to an exponential decay. Knock-out of TRPC6 channels results in reduced directed motion to $\sim$ 20%. However, stronger temporal autocorrelations of the migration process are conserved. In addition, data are assessed with a generalized Langevin equation, allowing to separate the migration pattern into motor and navigation system and to quantify intrinsic correlation more precisely.

BP 7.10 Mon 17:30 P3

**Two barriers or not? Dynamic force spectrosopy on the integrin $\alpha 7\beta 1$ invasin complex** — Kristian Boye[1], •Agnieszka Ligezowska[2], Johannes A. Eble[3], Bernd Hoffmann[2], Beate Klösgen[1], and Rudolf Merkel[2] — [1]MEMPHYS Center for Biomembrane Physics, University of Southern Denmark, DK-5230 Odense M, Denmark — [2]Institute of Complex Systems 7: Biomechanics, Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Center for Molecular Medicine, Frankfurt University, D-60590 Frankfurt am Main, Germany

Dynamic force spectroscopy was applied to test the force driven dissociation of the specific bond between integrin $\alpha 7\beta 1$ and the bacterial protein invasin. Using biomembrane force probe, the single bonds were exposed to 14 different loading rates ranging from 18pN/s to 5.3nN/s. Plotting median yield forces, ranging from 8pN to 72pN, against the logarithm of the corresponding force loading rate revealed two linear regimes seemingly representing two energy barriers. Thermal fluctuations of the ultra-soft force transducer and the environment set a natural detection limit of the technique. The lowest rupture forces were unavoidably obscured by thermal fluctuations that might have led to an artificial shift towards higher forces. An in-depth data analysis including the detection limits showed that the second linear regime might be entirely due to the force shift effect. It is not necessarily rooted in the physical properties of the bond system. The bond disso-

ciation could be well described by traverse over a single barrier [1].

[1] K. Boye et al., Biophys J. 105, 1-10 (2013)

BP 7.11 Mon 17:30 P3

**Diffusion heterogeneities in cells during Mitosis** — •Nisha Pawar and Matthias Weiss — Experimental Physics-I University of Bayreuth, Bayreuth, Germany

The Cytoplasm of the eukaryotic cell is highly complex and dynamic in nature. In addition, it is highly structured on many length scales. There are random motions within crowded and heterogeneous cytoplasm via protein complexes and organelles. Therefore diffusion behavior in cytoplasm can be expected to show spatial variations and a dependence on the cell cycle. The formation of mitotic spindle during the metaphase is expected to add another layer of complexity to the diffusion behavior of protein in the cytoplasm. We have probed the diffusion behavior of protein in cytoplasm during interphase and metaphase by Fluorescence Correlation Spectroscopy (FCS). Our results indicate that protein mobility not only heterogeneous in each of these states but also apparent mobility pattern depends on the cell cycle.

BP 7.12 Mon 17:30 P3

**Distinct response of adherent cells to substrate elasticity and ligand affinity** — •Christina Müller and Tilo Pompe — Institute of Biochemistry, Universität Leipzig, Germany

Cell fate decisions are triggered by physicochemical cues from the microenvironment. The mechanical properties of tissue, like stiffness or viscosity, can severely influence cells in their signaling, a process commonly referred to as 'mechanotransduction'. In this context we want to elucidate the impact of substrate stiffness and molecular friction of non-covalently attached adhesion ligands on early cell adhesion. We monitored human endothelial cells (HUVEC) on tailored polyacrylamide hydrogel layers with a graded stiffness in the range of 1 kPa to 10 kPa and a maleic acid copolymer coating. Coatings of different hydrophobicity provide a graded affinity for non-covalently attached fibronectin ligands. We used time-resolved Traction Force Microscopy to monitor the force generation of cells respective to substrate stiffness and ligand affinity during the first two hours of cell adhesion. For characterization of the cell response we determined the maximum traction stress Tmax,net contractile moment Mnet and strain energy U. We found differences in the temporal regulation of the local forces at the adhesion sites and the global contractility of adherent cells. While ligand affinity limits the slope and maximum value of cell traction stress, the total cell contractility is affected by substrate stiffness. In parallel, we investigate intracellular signaling processes to correlate the force generation to the biochemical key players in the cell's response to mechanical substrate parameters.

BP 7.13 Mon 17:30 P3

**Influence of direct laser written three-dimensional topographies on osteoblast-like cells** — •Judith K. Hohmann[1] and Georg von Freymann[1,2] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern — [2]Fraunhofer Institute for Physical Measurement Techniques IPM, Department of Materials Characterization and Testing, Kaiserslautern

Biological cells react to various signals of their environment. While biochemical pathways have been investigated for decades, the influence of physical characteristics of the cellular environment has only been studied in the very recent past. Especially information on the interaction with three-dimensional structures is barely available, since common chemical and/or physical surface treatments (e.g. acid-etching, sand blasting) lead to randomly shaped surface topographies.

Our well-defined three-dimensional templates are fabricated by direct laser writing and coated with titanium dioxide via atomic layer deposition. This allows us to provide biocompatible substrates with nearly arbitrary micro structures.

We report on how geometric parameters influence viability parameters of osteoblast-like cells. We observe a significantly higher proliferation on particular topographies compared to unstructured surfaces. Additionally, an influence of structural parameters on the morphology and focal adhesion contacts of osteoblast-like cells is obtained and differentiation is verified via alkaline phosphatase staining. Our results might lead to novel dental implant surfaces which promote osseointegration.

BP 7.14 Mon 17:30 P3

**Temperature induced sudden loss of cell nuclei integrity** — •Enrico Warmt, Tobias Kiessling, Roland Stange, Anatol Fritsch, Mareike Zink, and Josef Käs — Universität Leipzig, Experimentelle Physik I, Germany

The DNA double helix, is one of the most stable proteins in a cell. However, despite the high temperature stability of DNA itself, we have found a sudden loss of cell nuclei integrity at relative moderate temperatures ranging from 45 to 55 degree Celsius. Suspended cells hold in an optical double beam trap were heated under controlled conditions and nuclear shape was monitored. At specific critical temperatures an irreversible sudden shape transition of the nuclei was observed. These temperature induced transitions differ in character of shape change for different cell lines. The high connectivity of the nuclei to the cytosol becomes visible when the initial shape transition of the nucleus propagates toward the plasma membrane.

BP 7.15 Mon 17:30 P3

**Cell Shape and Forces on Micropatterned Substrates Predicted by a Cellular Potts Model** — •Philipp J. Albert and Ulrich S. Schwarz — Institute of Theoretical Physics, University of Heidelberg

Micropatterned substrates are increasingly used to decrease the variability inherent to cell experiments and to quantitatively study the relation between cell shape and function. When combined with traction force microscopy on soft elastic substrates, micropatterns can be used to evaluate the average relation between cell shape and forces, independent of the exact organization of the adhesion contacts and the cytoskeleton in an individual experiment. However, a conceptually transparent and easy-to-implement modeling framework for this situation is still missing. Here we show that a two-dimensional cellular Potts model (CPM) can predict cell shape and forces on micropatterned substrates in good agreement with experimental results if the energy function of previous formulations of the CPM is modified to account for adhesive energies and local contour reinforcement by peripheral bundles. While these additional elements are required to describe shape and forces during periods of strong contraction, the CPM-part describes more dynamic situation, such as spreading over a pattern. Together, these elements result in a flexible and efficient framework to predict cell shape and forces on arbitrary adhesive geometries.

BP 7.16 Mon 17:30 P3

**A Geometrical Model for Malaria Parasite Migration in Structured Environments** — •Anna Battista[1], Janina Hellmann[2], Friedrich Frischknecht[2], and Ulrich Schwarz[1] — [1]ITP and Bioquant, Heidelberg University, Heidelberg, Germany — [2]Department of Infectious Diseases, University Clinics Heidelberg, Heidelberg, Germany

Plasmodium sporozoites are the form of the malaria parasite that is injected into the skin of the host during a mosquito bite. They migrate rapidly through the dermis searching for a blood capillary to penetrate. Sporozoites have a curved shape and this is essential for their migration patterns: they describe circles on a flat substrate, roughly helical trajectories in an unstructured 3D environment, and irregular trajectories with circular elements in the skin [1,2,3]. Experiments with micro-fabricated pillar arrays [1] have shown that obstacles can deflect sporozoite trajectories into complex motility patterns, suggesting that the irregular trajectories in the skin result mainly from physical interactions with the environment. We propose a model that combines the prominent geometrical features of the parasite with a detailed interaction scheme upon collision with obstacles. The model is able to reproduce trajectories in homogeneous pillar arrays as well as to predict curvature-dependent selection of pillars in heterogeneous arrays. This cannot be explained via a pure hard-core interaction, but requires a favourable contact with a pillar. References [1] S. Muenter, Cell Host & Microbe 6, 551-562 (2009). [2] R. Amino, Nature Medicine 12, 220-224 (2006). [3] J.K. Hellmann, Plos Pathogens 7, e1002080 (2011).

BP 7.17 Mon 17:30 P3

**Ultra-soft PDMS elastomers for cell mechanic investigation** — •Viktor Heinrichs, Sabine Dieluweit, Jörg Stellbrink, Rudolf Merkel, and Dieter Richter — Forschungszentrum Jülich GmbH

The elasticity of cell environment (e.g. extra cellular matrix) plays an important role in cell morphology and protein expression. Every tissue in the organism owns a specific elasticity; the cerebral tissue is the softest one and has an elasticity (Young's modulus) below 1 kPa. Therefore, an elastic and biocompatible model substrate with well-

defined and adjustable properties for cell mechanic investigation is required. Cross-linked polydimethylsiloxane (PDMS) is frequently used because PDMS is nontoxic, easy to handle and commercially available, although an elasticity of 1 kPa is difficult to achieve. The preparation of the PDMS substrates is carried out by hydrosilylation reaction with well-defined polymers and crosslinking agent in the presence of platinum catalyst. The stiffness of PDMS networks can be varied by polymer chain length, reaction time of hydrosylilation and stoichiometrie. Quantification of mechanical properties was carried out by strained controlled rheometer (ARES-G2, TA Instruments). Using ultra-low frequency measurements (down to $10^{-5}$ $s^{-1}$) its Young's modulus was clearly formed to be 1.8 kPa. Using this approach, we created new well defined PDMS elastomers to simulate the cell environment and in particular for research of cerebral tissue. [1] N. Hersch, B. Wolters, G. Dreissen, R. Springer, N. Kirchgeßner, R. Merkel, B. Hoffmann, *Biol. Open* **2013,** *2, 251-361.*

BP 7.18 Mon 17:30 P3

**Spiral actin-polymerization waves can generate amoeboidal cell crawling** — •Alexander Dreher[1], Igor Aranson[2], and Karsten Kruse[1] — [1]Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany — [2]Argonne National Laboratory, Materials Science Division, 9700 South Cass Avenue, Argonne, USA

Amoeboidal cell crawling on solid substrates is characterized by protrusions that apparently randomly appear along the cell periphery and drive the cell forward. It is well-established that the protrusions result from local polymerization of the actin cytoskeleton. However, it is currently unknown how the formation of protrusions is triggered and whether the appearance of subsequent protrusions is coordinated. Recently, spontaneous formation of polymerization waves was observed in the actin cytoskeleton, which have been proposed to orchestrate the cytoskeletal dynamics during cell crawling. Here we study the impact of cytoskeletal polymerization waves on cell migration using a phase-field approach. In addition to directionally moving states, we found states reminiscent of the amoeboidal cell crawling. In this framework, new protrusions are seen to emerge from a nucleation process generating spiral actin waves in the cell interior. Nucleation of new spirals does not require noise, but occurs in a state that is apparently displaying spatio-temporal chaos.

BP 7.19 Mon 17:30 P3

**Preparation of *in vitro* extracted, covalently crosslinked cell membrane.** — •Patrick Paul[1], Ulla Nolte[1], Tobias Paust[1], Reinhard Fässler[2], and Kay E. Gottschalk[1] — [1]Institute of Experimental Physics, Ulm University, Ulm, Germany — [2]Department of Molecular Medicine, Max Planck Institute of Biochemistry, Martinsried, Germany

The interaction of proteins with the intracellular side of cell membranes is important for a variety of cellular functions. We are mainly interested in cell adhesion and migration and therefore, in the interaction in between integrins, proteins of the integrin complex and f-actin. To study this interaction, we extract the cell membrane with the unroofing technique [1] and covalently crosslink substrate with cell membrane *in vitro* to stabilize the system. The cell membranes of adherent cells are prepared in such way, that the intracellular side is exposed.
Furthermore, we verify our sample preparation with the help of atomic force microscopy, fluorescence light microscopy and scanning electron microscopy.

Reference:
[1] John Heuser, The Production of 'Cell Cortices' for Light and Electron Microscopy, 2000, Munksgaard International Publishers, 545-552

BP 7.20 Mon 17:30 P3

**Growth Dynamics of Cellular Clusters on Elastic Substrates** — •Philipp Linke[1], Carina Wollnik[1], Sara Kaliman[2], Damir Vurnek[2], Ana-Sunčana Smith[2], and Florian Rehfeldt[1] — [1]3rd Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — [2]Institute for Theoretical Physics and Cluster of Excellence: Engineering of Advanced Materials, University Erlangen-Nürnberg, Germany

Cellular motility is an important factor in many processes like wound healing, tissue formation, and immune reactions. Cells adhere to their environment using focal adhesions and react to the stiffness of their surroundings. To study the response of a distinct cell type to different stiffness we use collagen-I coated polyacrylamide (PA) gels with well-controlled stiffness to mimic different environments.

MDCK II cells have proven to be very useful as model system for endothelial morphogenesis. When growing on a flat surface, these cells usually form a cluster monolayer after a short time. We found recently that soft matrices mimicking the native mechanical conditions of kidney also lead to three dimensional structures. The formation dynamics of these structures is controlled by cellular contractility and the balance of cell-cell and cell-matrix contacts. We use Lifeact-RFP to visualize actin filaments in living cells to elucidate the growth dynamics of clusters of MDCK II cells. We are using the open source software Micro Manager in combination with a motorized xy-stage and a heating and CO2 incubation system to do parallel live cell microscopy of several clusters in physiological conditions.

BP 7.21 Mon 17:30 P3

**Mechanical Properties of the Nucleus probed by Atomic Force Microscopy (AFM)** — •Susanne Karsch and Florian Rehfeldt — 3rd Institute of Physics - Biophysics, Georg-August University, Göttingen, Germany

The nucleus, especially the nuclear envelope, consisting of two lipid bilayer membranes and a protein network made up by lamins, creates a specific microenvironment for the genome. Due to multiple connections with the cellular cytoskeleton, the nucleus is also mechanically interacting with the intra- and extra-cellular environment and plays a role in the mechano-sensing machinery. Experiments showed that the nucleus is several times stiffer than the cytoplasmic region, but the fundamental mechanical properties determining shape and structure are still poorly understood. Elucidating these properties is of high importance as it may impact gene expression and could be related to certain diseases. Biochemical modifications of cytoskeletal components can give hints how the nucleus interacts with the surrounding and subsequently varies its shape and mechanics. We measure mechanical properties of nuclei in cells and isolated nuclei by AFM to dissect contributions of the cytoskeleton. These measurements are complemented by confocal and fluorescent imaging to analyze and correlate the structure with mechanical properties.

BP 7.22 Mon 17:30 P3

**Resolution Limits and Regularization in Traction Force Microscopy** — •Jérôme R. D. Soiné[1,2], Christoph A. Brand[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [2]Bioquant, Heidelberg University, Heidelberg, Germany

Regularization is a standard technique to achieve unique solutions for inverse problems that are ill-posed. One such problem is reconstructing cellular traction fields of adherent cells on planar elastic substrates, a method known as traction force microscopy (TFM). Regularization is based on the idea of suppressing noise effects. However, in TFM the choice of the regularization term and of the regularization strength may affect reconstruction results such as the spatial distribution of traction hot spots, traction magnitudes and feature sizes. We have conducted a systematic investigation of the effects of using different regularization schemes in TFM. In contrast to unconstrained TFM, we constrained cellular force transmission to specific locations identified from fluorescence microscopy data for proteins localizing to focal adhesions. We then correlated the properties of these focal adhesions with the traction forces reconstructed by different methods. This enabled us to give a systematic overview on how regularization influences the reconstruction of cellular traction fields and to provide theoretical tools to adjust regularization for various experimental environments. We also compare our results to model-based traction force microscopy (MB-TFM), a method in which biophysical models are used to further suppress the effect of noise and to extract more information.

BP 7.23 Mon 17:30 P3

**Migration behavior of human mesenchymal stem cells on biomimetic elastic substrates** — •Daniel Meyer and Florian Rehfeldt — 3rd Institute of Physics - Biophysics, Georg-August University, Göttingen, Germany

Cell motility and migration processes are vital during biological development but also homeostasis. They are essential in tissue regeneration, morphogenesis, but also in pathological mechanisms like tumor metastasis. While migration due to biochemical gradients (e.g. chemotaxis) is very well studied, the influence of other parameters of the microenvironment such as topography and stiffness are less understood.

Nowadays, it is a widely appreciated fact that the mechanical properties of the matrix are significant factors for cellular processes. Here,

we use polyacrylamide (PA) substrates with well-controlled Young*s moduli E and distinct biochemical composition of ECM ligands to mimic in vivo microenvironments and analyze the migration behavior of human mesenchymal stem cells (hMSC) by life cell microscopy.

BP 7.24 Mon 17:30 P3

**Tailoring the surface potential using Au nanoparticles and Au films deposition for bioelectronic applications** — •Kyrylo Greben, Pinggui Li, Dirk Mayer, and Roger Woerdenweber — Peter Gruenberg Institute-8, Forschungszentrum Juelich, Juelich, Deutschland

Generally the growth of films (inorganic as well as organic) on a substrate depends strongly on the properties of the carrier. This also holds for the case of bioelectronic applications, where biological material is immobilized on an inorganic electronic, e.g. a semiconductor device. Therefore it is essential to be able to characterize the interface and the surface (structural, chemical but also electronic properties) of the carrier (substrate or electronic) under conditions that are identical or at least comparable to the conditions used during deposition or immobilization.

In this work we use the streaming current technique to analyze the surface properties of bio-compatible planar silicon and borosilicate glass substrates with different percentage of surface coverage (0 to 100%) of Au. The Au deposition is achieved either by immobilization of different concentration of Au nanoparticles or standard evaporation techniques. The isoelectric point changes from pH 3.1 for Si to pH 3.76 for the completely covered substrate in a nonlinear way. Reference measurement and the data obtained for the completely covered surfaces are in good agreement with the literature and measurements on inert materials like polypropylene (IEP at pH 4) and platinum (IEP at pH 3.82).

BP 7.25 Mon 17:30 P3

**From cytoskeletal dynamics to collective cell migration - a Monte Carlo study** — •Florian Martin, Claus Metzner, Janina Lange, and Ben Fabry — Biophysics Group, University of Erlangen

The growth of flat cell colonies on planar substrates is a spatial and temporal multi-scale process. Macroscopically and on long time scales, experiments show an almost deterministic increase of the colony radius and an outward streaming motion of individual cells. On mesoscopic time scales, cells change their shape within the monolayer and divide. Cell dynamics at shorter time scales is dominated by local cytoskeletal remodelling events, generating fluctuating traction forces that act on focal adhesions and are transmitted through cell-cell contacts. We present a bottom-up simulation of colony growth in which each cell is represented by a set of focal adhesions, attached to a dynamic stress fiber network that creates long-time correlated force fluctuations. The ongoing turn over of focal adhesions eventually leads to shape changes and migration of individual cells. As the proliferating and spreading cells are competing for adhesion sites on the substrate, a radial streaming motion emerges on a macroscopic scale. Also in agreement with measurements, the mean squared displacement of cytoskeletal markers shows a gradual transition from sub- to superdiffusive behaviour.

BP 7.26 Mon 17:30 P3

**Dynamics of Cellular Force Generation** — •Mari Gorelashvili[1], Philipp Paulitschke[2], Eva Weig[3], and Doris Heinrich[1,4] — [1]Fraunhofer Institute for Silicate Research ISC, Neunerplatz 2, 97082 Würzburg, Germany — [2]Ludwig-Maximilians University Munich, Geschwister-Scholl-Platz 1, 80539 Munich, Germany — [3]University of Konstanz, Universitätsstraße 10, 78464 Konstanz, Germany — [4]Leiden University, LION, Leiden Institute of Physics, Niels Bohrweg 2, 2333 CA Leiden,The Netherlands

Force generation is one of the basic mechanisms involved in cell-environment interaction. Different biochemical as well as biophysical properties of cellular force exertion have been revealed during the last decade. Nevertheless, simultaneous investigation of these mechanisms during cell migration in 3D environments is less studied. Here, we present a novel method for the investigation of force generation by living cells during the mirgation in quasi 3D environments. The method combines highly precise cellular force measurement and quantitative analysis of cytoskeleton dynamics. Well-defined flexible nanowire arrays serve as force sensors. During cell migration in-between these nanowires cytoskeleton structures and force sensors are imaged simultaneously by spinning disc confocal microscopy. Advanced quantitative analysis algorithms enable determining the force and investigation of underlying cytoskeleton dynamics with high spatial and temporal resolution.

BP 7.27 Mon 17:30 P3

**Cell type specific mechano-sensitivity on elastic hydrogels** — •Galina Kudryasheva[1], Florian Rehfeldt[1], and Assaf Zemel[2] — [1]3rd Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — [2]Faculty of Dental Medicine, Hebrew University, Jerusalem, Israel

It is now widely accepted that the mechanical properties of cellular micro-environments are as important in the regulation and function of cellular processes as biochemical ones. Especially striking is the mechanically guided differentiation of mesenchymal stem cells (hMSCs) on elastic hydrogels. While the complex differentiation mechanisms take several days up to weeks to fully develop, the structure and dynamics of the acto-myosin fibers can be used as an early morphological marker and modelled using classical mechanics with an active spring model. Using fluorescence microscopy we analyze the cytoskeletal structure of cells cultured on elastic poly-acrylamide (PA) substrates with different Young's moduli E in the physiological range. Quantifying the stress fiber organization by an order parameter S gives insight into the mechano-sensing process and determines the mechanical susceptibility as well as an intrinsic pre-stress of the cell. We use this approach to analyze the mechanical cell-matrix interactions of hMSCS during their mechano-differentiation process and compare them with already committed cell types to gain more insight in the integration of mechanical signals to transcriptional changes.

BP 7.28 Mon 17:30 P3

**Migration, Force Generation and Mechanocsensing of Cells in Collagen Gels** — •Julian Steinwachs[1], Claus Metzner[1], Stefan Münster[1], Katarina Aifantis[2], Kai Skodzek[1], and Ben Fabry[1] — [1]Lehrstuhl für Physikalisch Medizinische Technik - Friedrich Alexander Universität Erlangen-Nürnberg — [2]Department of Civil Engineering and Engineering Mechanics - University of Arizona

Collagen gels are frequently used to study cell migration in a 3-D environment. Mechanical properties of collagen gels are governed by non-affine deformation of the fibrils, such as buckling and tautening, resulting at the macroscopic scale in strain stiffening under shear and a strong lateral contraction under stretch. It is currently unknown how these macroscopic properties play out at the scale of a migrating cell, and how this depends on cell geometry. We develop a non-linear elastic material model for collagen gels based on observations from confocal microscopy that fibrils can evade mechanical stress using their internal degrees of freedom. The tautening of fibrils results in a strong material stiffening against expanding forces. By this mechanism, even a soft collagen gel can sterically constrain a migrating cell. We compute cell traction forces from collagen fiber displacements during the migration of carcinoma cells through dilute and dense collagen gels. We find that cells exert highly localized forces that lead to long-ranging collagen displacements and little material stiffening. At the same time, the average traction force magnitude increases for denser collagen gels. This observation may explain why cells can migrate more efficiently in stiffer gels, despite their narrower pore diameter.

BP 7.29 Mon 17:30 P3

**Fabrication of patterned neuronal networks on multi electrode arrays** — •Norman Shepheard[1], Stefan Niehörster[1], Matthias Schürmann[2], Savio Fabretti[1], Barbara Kaltschmidt[2], Christian Kaltschmidt[2], and Andy Thomas[1,3] — [1]Fakultät für Physik, Universität Bielefeld — [2]Fakultät für Biologie, Universität Bielefeld — [3]Fachbereich Physik, Johannes Gutenberg Universität Mainz

The geometry of neuronal networks seems to be one of the key features to understand the brain functions. Difficulties to examine these networks are caused by the large amount of connections between neurons. A first step is analyzing networks with reduced complexity, for example in vitro neuronal networks with two or three connected neurons. We fabricated patterned adhesion films for neurons on commercial multi electrode arrays (MEAs). The adhesion film consist of three layers on top of the MEA surface which is made from silicon nitride. These layers are (3-aminopropyl)triethoxysilane (APTES), glutaraldehyde and as top layer poly-L-lysin (PLL) which is covalent bound [1]. Patterning is done by using the UV-lithographic 'lift-off' technique [1]. There are several demands to the geometry of the pattern, like the size of the grid, which has to match the distance between two neurons and which has to fit to the electrodes given by commercial MEAs. We successfully coated the pattern with neurons which is the final test. The

aim of the overall project is to compare the behavior of small in vitro neuronal networks and artificial networks build up of memristors.

[1] Yong Hee Kim et al.; J Neurosci Methods. 2011; 202(1):38-44

BP 7.30 Mon 17:30 P3

**Observing lateral waves on cells of controlled morphology** — •Julia Strübig, Erik Bernitt, and Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen, Germany

Much of the current research on cell motility focusses on the wave-like organization of actin and its effectors. In spreading fibroblasts, laterally moving waves can be observed directly before the cell changes from an isotropic to a polarized state. In order to achieve reproducible conditions we force cells into well-defined morphologies using microcontact printing of spherical fibronectin substrates. Using phase contrast microscopy we observe cells exhibiting persistent wave propagation around their circumference. We find different types of these lateral waves of which excitation mechanisms and consequences are widely unknown. Our system allows us to study wave phenomena on cells in a controlled and reproducible manner.

BP 7.31 Mon 17:30 P3

**A real time drug-assay on individual motile cells** — •Axel Hochstetter[1], Eric Stellamanns[2], Sravanti Uppaluri[2], Niko Heddergott[3], Markus Engstler[3], and Thomas Pfohl[1,2] — [1]Departement Chemie, Universität Basel, Basel, Switzerland — [2]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany — [3]Biozentrum, Universität Würzburg, Würzburg, Germany

The protozoan flagellates Trypanosoma are not only causative agents of the sleeping sickness and the Chagas' disease, but they are also a model system for cell motility. These unicellular parasites live in bodily fluids of their hosts, preferentially in the blood stream. Especially blood capillary vessels are a world of microscopic dimensions - a world at low Reynolds numbers - where our macroscopic strategies of self-propulsion just do not work. To counter this, Trypanosomes show off their fascinating and complex patterns of motility.

In order to analyse these patterns, we present a straightforward microfluidic device in which diffusion controlled concentration changes can easily be induced together with a versatile method to measure their impact on living and motile eukaryotic cells. By combining microfluidics with optical tweezers and the motile protozoan flagellate Trypanosoma brucei brucei we can directly assess how drugs and other chemicals influence cells and their motility.

Our results show that our assay can be used for a quick and easy test of the effect of almost any water-soluble drug on motile cells, even for protozoa which are normally difficult to permanently observe.

BP 7.32 Mon 17:30 P3

**Stochastic Resonance as underlying mechanism of growth cone chemotaxis** — •Wolfram Pönisch, Melanie Knorr, and Josef Käs — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik I, Physik der weichen Materie, Leipzig, Deutschland

Axon guidance is the manipulation of the growth direction of a protruding growth cone, the fan-like shaped tip of a neurons axon. Previous research postulated an important role of stochastic resonance, the amplification of a signal by noise, during axon turning.

In order to get reliable data from experiments it is necessary to create stable and reproducible chemical gradients. In this project two different setups were examined critically: the Ibidi $\mu$-Slide Chemotaxis chip and the classical micropipette assays. None of them were able to create gradients with the required quality for the examination of stochastic resonance.

Additionally an earlier developed numerical model was applied to simulate the edge fluctuations of the growth cone considering different concentration gradients. This model predicts the existence of an optimal noise level for the membrane fluctuations in order to induce turning of the in silico growth cone in a chemoattractant gradient.

BP 7.33 Mon 17:30 P3

**Orientational order and motility in active droplets** — •Diana Khoromskaia and Gareth Alexander — Centre for Complexity Science, University of Warwick, Coventry, UK

Spatially confined active matter exhibits fascinating collective behaviour, for instance internally generated flows in, and macroscopic self-propelled motion of active fluid droplets. Both seem to be associated with a particular long-range orientational order of the active particles in the droplet. Our aim is to understand which type of orientational order enables the transmission of local activity onto large scales and leads to directed movement of the drop. We consider a three dimensional drop of active matter that has a fixed, flat shape and is located on a plane surface. We impose different orientational fields with topological defects and calculate the resulting flow fields inside the drop analytically by solving the Stokes equation, which contains an active stress. For certain cases we show that an asymmetry in the imposed orientation field is inherited by the flow and enables motility in the case of appropriate boundary conditions at the contact surface.

One example of an active droplet is a cell extract, that is a solution of active cytoskeletal compartments confined by the cell membrane. Thus, understanding the interplay of orientational order and directed macroscopic movement could reveal new insights into the basic mechanisms of cell motility.

BP 7.34 Mon 17:30 P3

**The influence of substrate stiffness on integrin mediated cell properties** — •Maja Gulic[1], Thomas Kerst[1], Reinhard Fässler[2], and Kay-E. Gottschalk[1] — [1]Institute for Experimental Physics, Ulm, Germany — [2]Max Planck Institute of Biochemistry, Martinsried, Germany

Mechanical cues influence very basic cell properties like proliferation, cell shape or cell migration. Important components of the cell adhesion and migration machinery are the integrins, the actin cytoskeleton and messenger proteins. The analysis of the exact contribution of the individual components of this machinery to cellular properties is hampered by its complexity. Therefore, we reduced the complexity and examined mouse fibroblasts expressing only the fibronectin-binding integrins avb3 or a5b1 or a combination of the two.

To analyze the effect of integrin expression on cellular force generation, we used cell traction force microscopy. We fabricated polydimethylsiloxane (PDMS) micropost arrays via photolithography. We designed microposts with different height and diameter to vary the spring constant. Measuring the deflection of a micropost during adhesion of a cell made it possible to calculate the cellular force. We show differences between the cell types on the same array type as well as for the same cell type on different micropost forms. In addition we manipulated components of the force generation apparatus as well as the extracellular matrix with resulting differences in the cellular forces.

BP 7.35 Mon 17:30 P3

**Probing the potential landscape of a bacterial protein chain motor used for self-propulsion** — •Julian Roth, Matthias Koch, and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler- Allee 102, 79110 Freiburg, Germany

The locomotion of swimming bacteria is normally related to rotary motors as e.g. flagella motors. This study concentrates on the helical bacterium Spiroplasma melliferum, a plant pathogen which lacks a stiff cell wall in contrast to most other bacteria. It is able to deform itself intensively, a property that is used for propulsion by generating a pair of kinks propagating down the length of the cell body - thus representing a linear motor. Kinks are generated by a cytoskeletal ribbon made of the unique protein Fibril, whose subunits can change their length through conformational changes. However, the functional principle and the mechanics of the Fibril ribbon have not yet been completely understood. In order to advance the understanding of contraction and relaxation of the Fibril ribbon our experiments are supported by a model, which we developed to describe the switching of the subunits of this ribbon according to Kramers rate theory. To test the validity of the model, we fix the ends of the cell by attaching optically trapped beads and probe its response to different external forces and environmental conditions as e.g. the addition of drugs. Additionally, we use the recently developed object-adapted optical trapping and shape-tracking technique [1] to image and analyze the complex cell movement. [1] Koch, M. & A. Rohrbach (2012). Nature Photonics 6(10): 680-686

BP 7.36 Mon 17:30 P3

**Theory on active stress of a cortical cytoskeletal network** — •Tetsuya Hiraiwa — Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany

Active mechanics of a cortical cytoskeleton, which is a network consisting of actin filaments, myosin motor filaments and passive crosslinker proteins located underneath the cell membrane, plays crucial roles in dynamic cellular behaviors, such as cytokinesis and cell migration. In both a living cell and a reconstituted system, a cortical cytoskeleton

behaves as active contractile gel. To understand mechanical property of such an active cortical cytoskeletal gel, we have theoretically studied on their active stress from a microscopic point of view. In this poster, we present an essential mechanical model of a cortical cytoskeletal network, and share with you our results on its spontaneously yielded active stress. In particular, since a cortical cytoskeleton in a living cell shows hydrodynamic characteristics, we consider the non-rigid network, in which there are few amount of crosslinkers and/or the crosslinkers can undergo turnover. We found that this system shows the crossover between the extensile and contractile states in terms of stress at a finite amount of passive crosslinkers, and hence would like to emphasize the significance of passive crosslinker proteins for the present mechanism of active contractility.

BP 7.37 Mon 17:30 P3

**Modeling cytoskeletal polarization during confinement-induced persistent amoeboid motion** — •Oliver Nagel[1], Can Guven[2], Matthias Theves[1], Meghan Driscoll[2], Wolfgang Losert[2], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Germany — [2]Department of Physics, University of Maryland, MD, USA

We studied the quasi one-dimensional motion of Dictyostelium discoideum amoebae inside narrow microfluidic channels with a cross section of 10 x 20 micrometer. Most of the cells performed a quasi one-dimensional random walk under these conditions. However a subpopulation of cells showed a completely different type of motion. They persistently moved in one direction for a long time without reversing or stopping. We performed laser scanning confocal imaging of a transfected Dictyostelium cell line that expressed myosin II-GFP together with LimE-mRFP, a marker for filamentous actin. Our experiments showed, that the polarized structure of the cell cortex was different from those of polarized cells in the absence of confinement. To systematically analyze the dynamics of local protrusions and retractions of the membrane, we used a custom made software tool for cell shape analysis. Taking into account the observed distributions of actin and myosin II in the cell cortex, we developed a model, based on the biased excitable network model by Iglesias and Devreotes [1] to describe this behavior. Ref.: 1. P. Iglesias and P. Devreotes, Current Opinion in Cell Biology, 24 (2012), 245*253 <doi:10.1016/j.ceb.2011.11.009>.

BP 7.38 Mon 17:30 P3

**Controlling adhesion of *Acanthamoeba castellanii* by substrate stiffness** — •Sören Björn Gutekunst and Christine Selhuber-Unkel — Institute for Materials Science, Christian-Albrechts-University Kiel, Germany

Acanthamoebae are found worldwide and are most commonly present in water reservoirs such as lakes and swimming pools, but even in soil and dust. Some acanthamoeba species are human pathogenic and can cause severe infections, such as acanthamoeba keratitis, which is caused by *Acanthamoeba castellanii*. Acanthamoeba keratitis is an infection of the human eye that is mainly caused by insufficient contact lens care. If Acanthamoeba castellanii trophozoites adhere to a soft contact lens material, they are easily transferred to the eye. In order to investigate the influence of substrate stiffness on the adhesion of Acanthamoeba castellanii, we produced polyacrylamide substrates of different elasticity and quantified the motility, number and spreading area of adherent amoeba as a function of substrate stiffness. Our data indicate that Acanthamoeba castellanii adhesion is promoted on soft substrates, suggesting the presence of a mechanosensing mechanism.

BP 7.39 Mon 17:30 P3

**Microrheology study of integrin dependent mechanical properties of fibroblasts under shear stress** — •Fenneke KleinJan[1], Yoojin Lee[1], Reinhard Fässler[2], and Kay Gottschalk[1] — [1]Ulm University, Institute of Experimental Physics, Ulm, Germany — [2]Max-Planck Institute of Biochemistry, Department of Molecular Medicine, Martinsried, Germany

Physical forces are increasingly recognized as an important biological signal. The protein family of integrins are a key element in force sensing, functioning as a bidirectional force signalling protein. They link the cytoskeleton and the extracellular matrix, giving the cells the opportunity to respond to force by adapting the cytoskeletal filaments. However, how the different integrins cooperatively modulate the force response of the cytoskeleton is not understood.

To study the crosstalk between integrin avb3 and a5b1 we use mouse embryonic fibroblasts that express only the single integrin or a combination of both. We focused on the local mechanical properties of isolated cytoskeletal filaments using microrheology, studying both fibroblasts under static conditions and under influence of shear stress. Preliminary results show that the avb3 integrin is responsible for reinforcing the network. Cells expressing avb3 and avb3a5b1 integrins have a similar elastic modulus under static conditions and this modulus shows a comparable decrease when cells are exposed to shear stress.

BP 7.40 Mon 17:30 P3

**Cell adhesion under lateral confinement** — •Andreas Müller and Tilo Pompe — Universität Leipzig, Institute of Biochemistry, Johannisallee 21-23, 04109 Leipzig, Germany

The process of structuring of multicellular organisms into tissues and organs relies on the collective organization of cells into compartments. In this context, geometry plays a fundamental role in guiding cell adhesion and cellular behavior, in close relation to biochemical and biophysical characteristics of the extracellular matrix.

In order to better understand the impact of geometry on individual cells, we micropattern hydrogel substrates with adhesion ligands arranged in stripes. Cells grown on these micropatterns show distinct cytoskeletal morphologies, i.e. a bimodal distribution of actin stress fiber spacing depending on stripe width. As underlying regulating cues we hypothesize changes in interfacial energies of cells or intracellular forces. We use traction force microscopy and immunofluorescence staining to identify mechanical, biochemical and structural parameters relevant for cell adhesion under geometrical confinement. Biophysical and biochemical perturbations are used to distinguish regulating elements of intracellular signaling. Substrate stiffness, ligand affinity as well as intracellular force activation were modulated to test a broad range of possible mechanisms.

Next to stripe width, substrate stiffness could be shown to be an important parameter for actin fiber assembly and force generation on micropatterned substrates. With these studies we aim to demonstrate the relevance of geometry for cellular mechanical homeostasis.

BP 7.41 Mon 17:30 P3

**Alteration of rolling adhesion in aged monocytes** — •Samira Khalaji[1], Kay-E Gottschalk[1], Lisa Zondler[2], Veselin Grozdanov[2], and Karin Danzer[2] — [1]Institut für experimentelle Physik, 89081 Ulm, Germany — [2]Institut für Neurologie , 89081 Ulm, Germany

Cells alter adhesion to the cells or extracellular matrix during tissue remodeling, morphogenesis, and other responses to the environmental signals. Adhesion of blood monocytes was measured by setting up flow experiments using unidirectional laminar flow and low shear stress (0.59-1 dyn/cm2). Cells were isolated from young adult (20-40 years) and older adult (+40 years) donors and cultured 24 hours with/without Lipopolysaccharide (LPS) before running the flow experiments. Number of rolling and firmly adhesive cells to the substrate during the time point of 7-10 minutes was quantified using live cell imaging, plotted and compared in respect to the age.

BP 7.42 Mon 17:30 P3

**Analytical analysis of cell deformation by hydrodynamic forces in microfluidic flow channels** — •Alexander Mietke[1], Elisabeth Fischer-Friedrich[2], Salvatore Girardo[1], Philipp Rosendahl[1], Stefan Golfier[1], Oliver Otto[1], and Jochen Guck[1] — [1]Biotechnology Center, TU Dresden, Tatzberg 47/49, 01307 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany

The mechanical response of cells or tissue to external loadings has gained significant interest during the last decades. A thorough theoretical understanding of the hydrodynamic forces acting on micron-sized objects is an essential prerequisite to probe and determine their mechanical properties. Here we present an analytic formalism to calculate the stresses and ensuing deformations of a spherical viscoelastic object being flowed through a microfluidic channel. Instead of performing full numerical simulations, we describe how a few simplifying assumptions can lead to a comprehensive analytical understanding of the system. This includes the different hydrodynamic stress components and the resulting deformations of the object. Our theory gives direct information about the scaling of shape measures depending on the experimental conditions and the mechanical properties of the object. Computations to determine and visualise flow fields and object deformations can be performed within a second. Finally, we demonstrate that our model is in agreement with experimental data. This analysis forms an important stepping stone for the further development of emerging high-throughput microfluidic cell mechanical phenotyping

approaches.

BP 7.43 Mon 17:30 P3

**Competition for space during bacterial colonisation of a surface** — •Diarmuid Lloyd and Rosalind Allen — SUPA, School of Physics and Astronomy, University of Edinburgh, Edinburgh, UK

In the natural environment, bacterial populations often form densely packed self-assembled structures in cavities or on surfaces. Understanding how cells compete for space in these communities is essential if we are to translate our understanding of population dynamics and evolution in well-mixed communities to these real-life situations.

We have used fluorescence microscopy to study the competition for space between thousands of bacterial cells as they colonize a two-dimensional agarose surface. For each individual progenitor cell, we quantify the likelihood that their descendants will out-perform their neighbours for local space, under a range of environmental conditions, and how this affected the patterns of genetic segregation within the resulting surface community.

We find that for low-density populations cells which start growing earlier tend to out-compete their neighbours regardless of geometry. In contrast, for high-density populations, neighbour geometry may become significant.

BP 7.44 Mon 17:30 P3

**Volume and morphological changes in single erythrocytes at high hydrostatic pressure** — •Alfons Schulte[1], Sang Hoon Park[1], Silki Arora[1], Alesia Antoine[1], and Debopam Chakrabarti[2] — [1]Physics Department and College of Optics and Photonics, University of Central Florida, Orlando, FL 32816-2385, USA — [2]Burnett School of Biomedical Sciences, University of Central Florida, Orlando, USA

High pressure can change the cell morphology and membrane fluidity. We combine microscopy and spectroscopic probes to study pressure effects at the single cell level. In individual red blood cells large, reversible volume changes are observed over the pressure range from 0.1 to 200 MPa. In erythrocytes infected with the malaria parasite Plasmodium falciparum we observe clear differences in the deformability and between the compression and decompression curves. A possible mechanism for the reversible volume change may involve transport of water through the phospholipid membrane.

BP 7.45 Mon 17:30 P3

**Mechanical properties of human neutrophils in sepsis** — •Maik Herbig[1], Andrew Ekpenyong[1], Leon Menschner[2], Nicole Töpfner[2], Li Wenlong[1], Reinhard Berner[2], and Jochen Guck[1,3] — [1]Biotechnology Center, Technische Universität Dresden, 01307 Dresden, Germany — [2]University Hospital Carl Gustav Carus, 01304 Dresden, Germany — [3]Cavendish Laboratory, Dept. of Physics, Univ. of Cambridge, CB3 0HE, UK

Recent studies have suggested the use of cell mechanical properties as a diagnostic marker for cancer. Similar use in infectious diseases has received considerably less attention. Using an optical stretcher we have measured the mechanical properties of neutrophils during infection by various sepsis-inducing bacteria. Tractable alterations in cell mechanics due to pathogens could engender its use as a diagnostic marker for sepsis. Furthermore, our work may offer new insights into the complex interactions between immune cells and pathogens.

BP 7.46 Mon 17:30 P3

**Shape fluctuations and osmotic pressure in rounded fibroblasts** — •Samaneh Rezvani and Christoph Schmidt — Drittes Physikalisches Institut - Biophysik, Georg-August-Universität Göttingen, Germany

The structure of the cytoskeleton is complex and controls a broad variety of dynamical behaviors.Oscillatory dynamics observed in certain cell types, most prominently in muscle cells such as, insect flight muscle cells which have evolved to generate rhythmic and rapid contractile forces.

Fibroblasts are the most common cells of connective tissue in animals and play an important role, for example, in wound healing. Shape studies of non-adhering rounded fibroblast cells showed a slow oscillatory behavior that can last many hours at a constant frequency.

Here, we further investigate periodic oscillations of 3T3 fibroblast cells in order to establish the driving forces. Using confocal microscopy, we follow the oscillation frequencies under controlled osmotic conditions in 3D.

BP 7.47 Mon 17:30 P3

**Non-Equilibrium Cell Mechanics Probed with a Feedback-Controlled Dual Optical Trap** — •Florian Schlosser, Florian Rehfeldt, and Christoph F. Schmidt — Drittes Physikalisches Institut - Biophysik, Georg-August Universität Göttingen, Göttingen

Cellular processes not only respond to biochemical, but also to mechanical stimuli. Cells sense the mechanical properties of their surroundings and can adapt to the mechanical properties of their micro-environment. Acto-myosin structures are key players in the generation of contractile forces that cells use to probe the outside world.

We study the contributions of acto-myosin fibers to the force produced by a cell. We attach fibronectin-coated beads to opposite sides of suspended 3T3 fibroblast cells and analyze the correlated motions of the two beads. Using a combination of active and passive microrheology, we could identify the non-equilibrium fluctuations and simultaneously probe the viscoelastic properties of the cell. With a feedback-controlled force clamp we were able to measure the cellular response to a constant external force.

Here, we present data on contractile forces and elastic properties of the cell. Biochemical perturbation experiments demonstrate the key role of myosin motors for contractile force generation. Using the optical trap in force-feedback mode (e.g. force clamp) allowed us to analyze the cellular fluctuations at different levels of pre-stress. Combination with confocal scanning microscopy allows us to directly image the fluorescently tagged actin distribution during the trapping experiments and correlate structure and function.

BP 7.48 Mon 17:30 P3

**Force-induced nuclear shape changes in suspended cells** — •Chii Jou Chan[1,2] and Jochen Guck[1,2] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, UK — [2]Biotechnology Center, TU Dresden, Dresden, Germany

While studies in the past on nuclear mechanotransduction have focused mostly on adherent cells attached to rigid substrates, we study how physical stress propagates and regulates nuclear shape changes for cells in suspended state using an optical stretcher. Intriguingly, we observed distinctly different nuclear response for both naturally suspended and adherent cells, when the cells were subjected to external mechanical stress. Specifically, the cell nucleus of a naturally suspended cell undergoes compression in response to membrane stretch while the cell nucleus for a naturally adherent cell experiences positive deformation, which correlates well with membrane stretch. Our studies suggest that while the vimentin intermediate filaments may play a dominant role in transmitting intracellular forces to cell nuclei of naturally suspended cells, the LINC complex found in many of the naturally adherent cells appear to regulate nuclear shape changes in response to whole cell deformation. Our findings shed new light on the different mechanical pathways from the force-responsive cytoskeleton to the nucleus which may lead to downstream cellular signaling events as the cells adapt to changes in the physical environment.

# BP 8: Posters: Active cell and tissue mechanics

Time: Monday 17:30–19:30 Location: P3

BP 8.1 Mon 17:30 P3

**The 3D Vertex Model for Epithelial Mechanics** — •Silvanus Alt, Frank Jülicher, and Guillaume Salbreux — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Deutschland

Understanding how mechanical forces drive epithelia deformations is crucial to shed light on processes involved in morphogenesis. Here we introduce a 3D vertex model, which represents cells in epithelia in three dimensions by a network of vertices joined by triangulated surfaces. Surface and line tensions, arising from forces generated in the actomyosin cytoskeleton, and the cells* intracellular elasticity act on the vertices to generate cellular deformations. Using this framework, we are interested in understanding the 3D cell shape in epithelia as well as the 3D deformations of epithelia, such as folding, formation of furrows, and invagination of structures.

In my talk, I focus on the physical mechanism for the formation of cysts, out-of-plane bulges which form in the Drosophila wing discs as a result of ectopic expression of a wide range of transcription factors. The 3D vertex model quantitatively captures the observed tissue deformations by considering an increase in line tension at the boundary of the cyst. The increase in tension at the boundary results in a planar pressure driving out of plane deformations. We propose that this constitutes a general mechanism for both invagination and evagination of epithelia.

BP 8.2 Mon 17:30 P3

**Mechanical cues during early embryogenesis of *C. elegans*** — •Philipp Struntz, Rolf Fickentscher, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

The impact of biochemical signaling on developmental processes has been studied intensively during the last decades. However, the role of mechanical cues during embryogenesis has received much less attention. To elucidate the latter in the developmental model organism *C. elegans*, we have used a custom-made selective plane illumination microscope (SPIM) [1]. SPIM allowed us to quantitatively follow cell divisions and subsequent cell migration in three dimensions with a high spatiotemporal resolution. Comparison of different individuals showed only small deviations of cell trajectories, hence indicating a robust cellular arrangement process. A simple mechanical model revealed that cell organisation until gastrulation is determined by the cells' quest for a position with least repulsive interactions imposed by surrounding cells and the engulfing eggshell of the embryo. The model also predicts key features of the developing tissue that are in favorable agreement with experimental observations.

[1] Rolf Fickentscher, Philipp Struntz & Matthias Weiss: *Mechanical cues in the early embryogenesis of Caenorhabditis elegans*. Biophys. J, 105:1805 – 1811 (2013)

BP 8.3 Mon 17:30 P3

**Broken detailed balance: A tool for identifying non-equilibrium dynamics** — •Christopher Battle[1,4], Nikta Fakhri[1,4], Chase Broedersz[2,4], Fred C. MacKintosh[3], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Lewis-Sigler Institute for Integrative Genomics and Department of Physics, Princeton University, Princeton, NJ, USA — [3]Dept. of Physics & Astronomy, Vrije Universiteit, Amsterdam, Netherlands — [4]These authors contributed equally to this work

Living systems exist far from thermal equilibrium, with active processes undergirding many of their functions. While some cellular processes show unmistakable non-equilibrium characteristics, e.g. persistent directed motion, others are more subtle, exhibiting non-thermal, random motion which is similar in appearance to Brownian motion, e.g. cortical stress fluctuations or active cellular mixing. Some techniques such as combined active and passive microrheology can quantify the non-equilibrium component of such processes, but they require comparisons between different measurement modalities. We here present an alternative and very general technique to identify non-equilibrium processes, searching for violations of detailed balance in an appropriately chosen phase space of the system. Our approach has the advantage of not requiring comparisons between different measurement techniques, and also allows us to determine a lower limit on the work dissipated by an active system.

BP 8.4 Mon 17:30 P3

**Morphological analysis of epithelial tissues** — •Sara Kaliman[1], Damir Vurnek[1], Florian Rehfeldt[2], and Ana-Sunčana Smith[1] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg — [2]3rd Institute of Physics-Biophysics, University of Göttingen

Tissue growth is an inherently complex process, the details of which need to be understood not only from a biological standpoint but also in terms of the purely physical and geometrical aspects. In the most common scenario, epithelial tissue exhibits an increase in cell density during the growth of a colony until such time as a steady state is reached. Using the growth of MDCK II epithelial tissue as an example, we show that several millimeter-sized compartments organize radially, within the typically circular colony, over several days. To characterize these compartments, we study the intensity of the cell-cell and cell-substrate adhesion, as well as the structure of the cellular actin cortexes within each compartment. These data are correlated with information about the local cell density and division rate. Furthermore, we show that the cells within the colony divide the space according to a Voronoi tessellation, based on the shape of the cell nuclei. We use this realization to study the development of the morphological measures (the cell area, orientation, elongation and volume) in the process of densification. We find that as the cell density increases, the tissue structure approaches, but never reaches, a Centroidal Voronoi tessellation. This reorganization is achieved by positioning the nuclei closer to the centers of mass of the cell bodies and by decreasing the area associated with the intercellular contacts.

BP 8.5 Mon 17:30 P3

**Cellular chirality derives from active torques generated in the actomyosin cytoskeleton** — •Sundar Naganathan[1], Sebastian Fürthauer[2], Frank Jülicher[3], and Stephan Grill[1,3,4] — [1]MPI-CBG, Pfotenhauerstr. 108, 01307, Dresden — [2]Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, N.Y. 10012 — [3]MPI-PKS, Nöthnitzerstr. 38, 01187, Dresden — [4]Biotechnology Center, TU Dresden, Tatzberg 47/49, 01307, Dresden

Many developmental processes break left/right (L/R) symmetry with a consistent handedness, which require cells to be chirally asymmetric. The mechanisms by which cell chirality is established remain unclear, but the actomyosin cytoskeleton appears to be involved. To address this problem, we investigated flows in the actomyosin cortex of the one-cell stage C. elegans embryo. In addition to anterior-directed cortical flow, we observe the cortex to break chiral symmetry by counter-rotating flow with a consistent handedness in the anterior and posterior halves. Using active chiral fluid theory, we demonstrate that this motion derives from an active torque-generation process of defined chirality in the actomyosin cortex. This torque generation depends on myosin activity and can be independently regulated from tension generation though mild changes in Rho pathway activity, which we show by weak perturbation RNAi experiments. Our experiments suggest that chirality and torque generation is an emergent network property of the cortex. Interestingly, genes that affect the establishment of the C. elegans L/R body axis also regulate active torques, setting the stage for a mechanistic understanding of chiral morphogenesis in development.

BP 8.6 Mon 17:30 P3

**Uncovering the slow mode dynamics of migrating tumor cells** — •Christoph Mark, Claus Metzner, Julian Steinwachs, and Ben Fabry — Biophysics Group, University of Erlangen

Cell migration is usually analyzed by statistical methods that assume temporal homogeneity of the random process. Using long-time migration data from MDA-MB-231 tumor cells on 2D surfaces and in 3D collagen matrices, we show that this random walk process is highly inhomogeneous in time and accross the ensemble. Analysing the cell trajectories with a Hidden Markov Model reveals distinct migration modes with small mode switching rates. We thus describe the measured velocity time series $\vec{v}_t$ as a first-order autoregressive process $\vec{v}_{t+1} = q_t\vec{v}_t + \sigma_t\vec{g}_t$, in which the correlation factor $q_t$ and the noise amplitude $\sigma_t$ are treated as slowly varying superstatistical parameters. We show that the joint distribution $p(q, \sigma)$ and the temporal correlations of these super-parameters provide a characteristic fingerprint of the cell's migration mechanisms in different environments, whereas

traditional time-averaging measures, such as the mean squared displacement, mask such differences almost entirely. An inhomogeneous model, based on the extracted superstatistics can reproduce a large set of characteristic data features quantitively.

BP 8.7 Mon 17:30 P3

**Mobility of semi-flexible chains coupled with hydrodynamics** — •Won Kyu Kim and Roland Netz — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We study the hydrodynamic coupling and the effect of fluctuations on semi-flexible chains propulsion dynamics, where the chains are externally driven by an oscillating force or torque. By use of the linear response theory and Brownian dynamics simulations, we find optimal conditions for the chain propulsive force which can be maximized by proper driving frequencies and chain flexibilities. And we discuss how can the chain dynamics attain the effective propulsion in a collective manner.

BP 8.8 Mon 17:30 P3

**AFM-based indentation measurements of adult zebrafish spinal cord tissue** — •Stephanie Möllmert[1], Veronika Kuscha[1,2], Anna V. Taubenberger[1], Michael Brand[1,2], and Jochen Guck[1,3] — [1]BIOTEC, TU Dresden, Germany — [2]CRTD, TU Dresden, Germany — [3]Cavendish Laboratory, Department of Physics, University of Cambridge, UK

Severe injury to the mammalian spinal cord triggers a complex cascade of biochemical signals that eventually lead to the formation of a glial scar. In addition to inhibiting neuronal regrowth and causing loss of motor function, the glial scar has been proposed to act as a mechanical barrier preventing successful axon regeneration. Studies on spinal cord regeneration in adult zebrafish have revealed that zebrafish - in contrast to mammals - are able to successfully regain motor function after complete spinal cord transection. Therefore, the mechanical description of live spinal cord tissue poses an intriguing addition to biochemical analysis and might shed light on previously unknown mechanisms involved in successful spinal cord regeneration or the failure thereof. To efficiently investigate inherent mechanical properties of live spinal cord tissue from adult zebrafish, we have established a reliable protocol to prepare viable transverse acute spinal cord sections. Indentation type atomic force microscopy (AFM) was then employed to determine apparent elastic moduli (Young's moduli) of these sections under near physiological conditions. The presented work serves as a basis to investigate mechanical properties of neuronal tissue in vivo and test their importance in addition to biochemical and genetic factors.

BP 8.9 Mon 17:30 P3

**Coordinated actomyosin kinetics in generating pulsatory dynamics** — •Masatoshi Nishikawa[1,2,3], Sundar Naganathan[1,2,3], Guillaume Salbreux[1], and Stephan Grill[1,2,3] — [1]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]BIOTEC, Dresden, Germany

The cell cortex, which consists of cross-linked actin filaments and non-muscle myosin and is located beneath the cell membrane, is responsible for driving cell mechanical events. The cortex has been shown to be inherently unstable, displaying pulsatory dynamics characterized by transient accumulations of myosin at $\mu m$ length scales. We sought to identify the regulatory mechanism of coordinated actomyosin kinetics to generate pulsatory dynamics, and that ensures the robust cellular processes. To this end we develop a new method to characterize, in the comoving frame of reference, turnover timescales of cortical components as a function of the concentration of actin and myosin, which we term Comoving Mass Balance Imaging (CoMBI). We applied this method to the cortical flow in the one-cell stage *C. elegance* embryo, and succeeded to extract the actomyosin kinetics in spatially and temporally resolved manner. This method provides us with a detailed description of actomyosin mechanochemical dynamics, relevant for the cellular scale.

BP 8.10 Mon 17:30 P3

**Simulation of force transmission in random fiber networks** — •Arne Monsees, Julian Steinwachs, Claus Metzner, and Ben Fabry — Biophysics Group, University of Erlangen

Self-organizing random networks of biopolymers, such as collagen gels, are routinely used as three-dimensional matrices for cell migration experiments. Methods for reconstructing the cell's traction forces from displacement fields take into account nonlinear mechanical properties of the networks, but usually approximate it as a continuum material. In the close vicinity of the cell, this approximation fails, since there the transmission of a point force is not spherically symmetric but focused into a small set of individual fibers. We present first simulation results for networks of realistic fibers with built-in curvature and cross-links. The fibers are represented as chains of straight segments, and the discrete chain units have a stiffness with respect to streching, bending and torsional deformations. The response to a static perturbation is found by minimizing the potential energy of the system. By comparing the results to a mean field theory, we map out the limits of applicability of both approaches and explore the combined effects of nonlinearity and inhomogeneity.

## BP 9: Posters: Biotechnology and bioengineering

Time: Monday 17:30–19:30 Location: P3

BP 9.1 Mon 17:30 P3

**Quantum-mechanical study of crystalline and amorphous calcite** — Gernot Pfanner[1], •Martin Friák[1,2], Li-Fang Zhu[1], Svetoslav Nikolov[3], Anna Maria Janus[1], Helge Otto Fabritius[1], Pavlína Hemzalová[1], Duancheng Ma[1], Dierk Raabe[1], Julia Huber[4], Andreas Ziegler[4], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Institute of Physics of Materials AS CR, v.v.i. Brno, Czech Republic — [3]Institute of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria — [4]Central Facility for Electron Microscopy, University of Ulm, Ulm, Germany

Arthropoda, that represent nearly 80 % of all known animal species, are protected by an exoskeleton formed by their cuticle. The cuticle represents a hierarchically structured multifunctional bio-composite based on chitin and proteins. Some groups like Crustacea reinforce the load-bearing parts of their cuticle with calcite. We present a theoretical parameter-free quantum-mechanical study of the phase stability and structural and elastic properties of both crystalline and amorphous (ACC) calcite employing a supercell approach. Computational supercells employed as structural models for crystalline and amorphous calcite contain six and twenty $CaCO_3$ formula units, respectively. Our comparative study shows that the density of amorphous calcite is lower than that of its crystalline form and that also the studied single-crystalline elastic constants are lower in case of ACC. Both findings are in qualitative agreement with available experimental data.

BP 9.2 Mon 17:30 P3

**Hardware implementation of artificial memristors for neural networks** — •Bernhard Kaltschmidt, Marius Schirmer, Savio Fabretti, and Andy Thomas — Bielefeld University, Bielefeld, Germany

Recently, we developed a circuit board, which is able to simulate a memristor like behavior. This circuit board was combined with *Lego Mindstorms NXT*. With this strategy, it was possible to emulate associative memory in an autonomous robot. Currently, we are working on our next step. Here, we want to replace the *Lego Mindstorms NXT* with a combination of a *Raspberry Pi* mini computer and a circuit board (*Brick Pi*), which offers the ports to connect original *Lego*-elements. The intention of this project is to upgrade the weak processing unit of the *Lego Mindstorms NXT* with a device, which has all the abilities of a complete computer system. This is supported by the simulation of the Pavlov model network in *Brian*.

BP 9.3 Mon 17:30 P3

**Bioactive Surfaces by Polymer Pen Lithography** — •Ravi Kapoor[1], Falko Brinkmann[1,2], Sylwia Sekula-Neuner[1], Michael Hirtz[1], and Harald Fuchs[1,2] — [1]Institut für Nanotechnologie (INT) & Karlsruhe Nano Micro Facility (KNMF), Karlsruher Institut für Technologie (KIT), 76021 Karlsruhe, Germany — [2]Physikalisches In-

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Polymer pen lithography (PPL) is a promising soft lithography technique which has the capability of patterning large areas with precision without denaturing or damaging delicate organic and biologically active compounds. PPL is actually combination of microcontact printing and dip-pen nanolithography, and it takes the advantage of microcontact printing for patterning large areas and dip-pen nanolithography for precisely delivering the ink molecules on the surface. The ink transfer mode is alike microcontact printing or pen spotting approaches, depending on the ink / substrate combination. Multiplexing, i.e. patterning more than one ink compound in close proximity onto the surface is highly demanded in biological applications and can be provided by PPL. Here we present the application of PPL for patterning with different bio-active ink / substrate combinations, e.g. a DNP azide ink on an alkyne-terminated surface with copper catalyzed azide-alkyne cycloaddition (CuAAC). The retained functionality of the DNP allergen head group is confirmed by detection of allergen specific Immunoglobin E (IgE) antibodies. This will offer important improvements for substrates used in the study of mast cell activation in the future.

BP 9.4 Mon 17:30 P3

**Single molecule detection of insulin autoantibodies in type 1 diabetes** — •Juliane Beyer[1], Ralf Paul[2], Ezio Bonifacio[2], and Stefan Diez[1,3] — [1]B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden, Germany — [2]CRTD - Center for Regenerative Therapies Dresden, Germany — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Type 1 diabetes (T1D) is characterized as a chronic autoimmune disease caused by a selective inflammatory destruction of the insulin producing beta cells in the pancreatic islets of Langerhans. Closely associated to T1D are insulin autoantibodies (IAAs), representing early markers of the disease. Therefore the reliable detection is needed to i) predict the onset of T1D, ii) implement successful regenerative therapies and iii) to prevent loss of the beta cell mass.

For this purpose, we developed a novel optical assay for the detection of insulin autoantibodies using single molecule detection. This quantitative approach specifically detects IAAs in the low pM range using quantum dots and total internal reflection microscopy (TIRF).

So far, for clinically diagnostics, IAAs are detected using an antigen radiolabelling approach which is time consuming, hazardous and expensive. With our novel assay we are able to specifically detect high affinity antibodies without using radiolabelled antigens.

In the future our assay could be used as a point of care measurement for T1D, readily usable in the health care sector combining the prognostic and diagnostic measurements of autoantibodies in T1 D.

BP 9.5 Mon 17:30 P3

**Programmable patterning of protein bioactivity on surfaces using visible light** — •Cordula Reuther[1,2], Robert Tucker[2,4], Leonid Ionov[2,3], and Stefan Diez[1,2] — [1]B CUBE, TU Dresden, Dresden, Germany — [2]Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Leibnitz Institute for Polymer Research, Dresden, Germany — [4]Hansen Medical, Mountain View, California, USA

Patterning functional proteins on engineered surfaces is of interest for the development of nanotechnology, tissue engineering, biosensors and cell biology. Here, we report on the programmable patterning of proteins as well as the local activation of enzymes using patterned widefield illumination by visible light. Specifically, the light locally heats the carbon-coated surface and switches the conformation of a thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) polymer layer in aqueous solution between the swollen state at $T < 30°C$ (protein-repelling conformation) to the collapsed state at $T > 33°C$ (protein-binding conformation). Thereby, functional protein patterns with different geometries and sizes could be successfully generated in situ. Moreover, we demonstrated the specific patterning of multiple kinds of proteins side-by-side by sequential processing without the need for specific linker molecules or elaborate surface preparation. Additionally, while performing microtubule-based gliding motility assays, the accessibility of kinesin-1 motor proteins could be switched reversibly in a localized manner.

BP 9.6 Mon 17:30 P3

**DNA origami nanopores for controlling DNA translocation** — Silvia Hernandez Ainsa, Nicholas Bell, Vivek Thacker, Kerstin Göpfrich, Karolis Misiunas, and •Ulrich F Keyser — Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, CB3 0HE, Cambridge, UK

DNA origami nanopores are emerging as sensors for biological molecules [1]. Here, we combine DNA origami structures with glass nanocapillaries to reversibly form hybrid DNA origami nanopores. Trapping of the DNA origami onto the nanocapillary is proven by imaging fluorescently labeled DNA origami structures and simultaneous ionic current measurements of the trapping events [2]. We show three applications highlighting the versatility of these DNA origami nanopores. First, by tuning the pore size we can control the folding of dsDNA molecules. Second, we show that the specific introduction of binding sites in the DNA origami nanopore allows selective detection of ssDNA as a function of the DNA sequence [2]. Third, we are able to use voltage to change the state of our DNA origami nanopores to lower the frequency of DNA translocation and explain this with a mechanical model [3].

[1] N. A. W. Bell et al. DNA origami nanopores. Nano Letters 12(1):512-517, 2012.

[2] S. Hernandez Ainsa et al.DNA origami nanopores for controlling DNA translocation. ACS nano, 7(7):6024-6030 2013.

[3] S. Hernandez Ainsa, et al. Voltage responsive DNA origami nanopores. submitted. 2013.

## BP 10: Posters: Molecular Motors

Time: Tuesday 9:30–12:30 Location: P1

BP 10.1 Tue 9:30 P1

**The role of kinesin-8 in chromosome movements on the mitotic spindle** — •Anna H. Klemm[1], Nenad Pavin[2], and Iva M. Tolic-Norrelykke[1] — [1]Max Planck Institute CBG, Germany — [2]Department of Physics, University of Zagreb, Croatia

During cell division, replicated chromosomes move back and forth around the spindle midzone before they are segregated evenly on the two daughter cells. In a screen in the fission yeast Schizosaccharomyces pombe we studied the role of all known fission yeast kinesin-motors, dynein heavy chain and the microtubule (MT) crosslinking protein ase1 on these movements. We found that the movement was only changed by deletion of the kinesin-8 motor klp5/6, but not by deletion of the other motors. It is known that the motor protein kinesin-8 influences chromosome movements by regulating MT catastrophe. However, the mechanics of how the cell coordinates the movement is unknown. Here we saw that in cells lacking klp5/6 replicated centromeres move over the entire spindle length and switch less often the direction of motion, whereas in wild-type cells, the replicated centromere covers only the central third of the spindle. The centromeres spend a significantly longer time in proximity of the spindle pole body in klp5/6-deleted cells in comparison with wild-type cells. Also, comparable to interphase MT and in vitro studies, klp5-GFP accumulates at the plus-end of polar spindle MTs as they grow and then disappears when the polar spindle MT undergoes catastrophe. We conclude that klp5/6 causes centromere movements away from the spindle pole bodies, most likely by increasing microtubule catastrophe in a length-dependent manner.

BP 10.2 Tue 9:30 P1

**Synchronization of elastically coupled processive molecular motors and regulation of cargo transport** — •Felix Kohler and Alexander Rohrbach — Universität Freiburg, Germany

In biological systems, many energetic processes are quantized by the hydrolysis of ATP-molecules enabling elementary reactions and conformation changes of proteins. In this way, molecular motors step discontinuously along cytoskeletal filaments to transport cargos such as vesicles or to translate filaments for cytoskeletal reorganization [1]. Most motors operate in groups and thereby enable a more efficient cargo transport [2]. A few studies have shown indications for a coordi-

nation between the motors and thus a coherent stepping of motors in vitro [3] and in vivo [4]. In order to analyze collective work of motor proteins by a theoretical approach, we introduce the synchronization q as a new observable for elastic coupling, which is identified with the probability to find a stochastic system in its ground state. The synchronization q can be read out from the ratio of the mean times of motor resting and stepping. For the motor proteins myosin V and kinesin I we show that the transport velocity and power can increase significantly for certain motor synchronizations or couplings.

[1] J. Howard, Mechanics of Motor Proteins and the Cytoskeleton
[2] F. Jülicher and J. Prost, prl 75 (1995)
[3] C. Leduc, F. Ruhnow, J. Howard, and S. Diez, pnas 104, (2007)
[4] X. Nan, P. A. Sims, P. Chen, and X. S. Xie, jpc B 109, (2005)

BP 10.3 Tue 9:30 P1

**Single and multi motor measurements of the kinesin-like protein KIF20A** — •Alice Wiesbaum[1], Nikta Fakhri[1], I-Mei Yu[2], Anne Houdusse-Juille[2], and Christoph F. Schmidt[1] — [1]Georg-August Universität Göttingen, De — [2]Institut Curie, Paris, Fr

The Kinesin-like protein KIF20A is necessary for different processes in human cells. It was found to have an essential role during cell division. There KIF20A is required for chromosome passenger complex mediated cytokinesis. Following phosphorylation by PLK1, KIF20A creates a docking site for PLK1 and recruits it at the central spindle. Knocking out KIF20A leads to defects in the cleavage furrow formation. A down-regulation of KIF20A showed an attenuate growth of pancreatic cancer cells. All this makes KIF20A an interesting object to study.

To understand the genetic structure and the function of single parts of KIF20A, we did in vitro experiments with different KIF20A mutants. KIF20A shows a flexible extension at the N-terminal, of which we partly removed different amounts of amino acids. We investigated KIF20A and the obtained constructs in surface gliding assays, as well as in single molecule tracking, using fluorescent nanotubes bound to the motor protein. In addition we had a look at the shape of KIF20A using small angle x-ray scattering (SAXS).

BP 10.4 Tue 9:30 P1

**Bimodal transport in a system of active and inactive kinesin-1 motors** — •Lara Scharrel[1,2], Rui Ma[3], Frank Jülicher[3], and Stefan Diez[1,2] — [1]B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden, Germany — [2]Max Planck Institute of Cell Biology and Genetics, Dresden, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Long-range directional transport in cells is facilitated by microtubule-based motor proteins. One example is transport in a neuron where groups of motor proteins, such as kinesin-1 and cytoplasmic dynein, ensure the supply and clearance of cellular material along the axon. Defects in axonal transport have been linked to Alzheimer and other neurodegenerative diseases. However, it is not known how in detail multi-motor transport is impaired if a fraction of motors is defective. To mimic impaired multi-motor transport in vitro, we performed gliding motility assays with varying fractions of active kinesin-1 and inactive kinesin-1 mutants. We found that impaired transport manifests in multiple motility modes: (i) a fast mode with gliding at single-molecule velocity, (ii) a slow mode with gliding at close-to zero velocity or stopping, and (iii) a mode with switches between fast and slow mode. Notably, the transition from fast to slow mode occurred at a threshold fraction of active motors. Furthermore, we developed a theoretical description which explains the bimodal motility as well as the sharp transitions between fast and slow motility. Our results demonstrate that, depending on the fraction of active motors, impaired multi-motor transport is either performed close to full speed or is out of action.

BP 10.5 Tue 9:30 P1

**Synthetic molecular motors: a model study** — •Amartya Sarkar and Alexander S. Mikhailov — Fritz Haber Institute, Faradayweg 4-6, Berlin 14195

A model of a synthetic molecular machine, whose operation closely resembles that of real molecular motors, is constructed and numerically investigated. The machine, described in terms of an elastic network, is able to perform cyclic conformational motions. These mechanochemical motions result from repetitive and sequential events - binding of a ligand, its conversion to a product, and the product release. The machine has two domains (arms) connected by a flexible hinge; while one of the arms is pinned, the other is able to perform cyclic swinging motions. Due to ratchet interactions between the swinging arm and a stiff filament, internal cyclic motions in the machine become converted into directed translational motion of the filament. Stochastic simulations of this model motor system under the conditions of both weak and strong coupling are performed. Further simulations with a stall force applied to the rigid filament have also been performed. Various statistical and mechanical properties of this model have been studied in detail.

BP 10.6 Tue 9:30 P1

**Measurements of single fluorescent motor proteins: The Right Way** — •Felix Ruhnow, Linda Kloss, and Stefan Diez — B CUBE, Technische Universität Dresden

Cytoskeletal motor proteins are required in many cellular processes, such as intracellular transport and mitosis. Therefore, the biophysical characterization of motor protein movement along their filamentous tracks is essential. Commonly, stepping motility assays are used to determine the stepping and detachment rates of various molecular motor proteins by measuring their speed, run length and interaction time. However, comparison of these results proved to be difficult because the experimental setup (e.g. bead assay vs. single-molecule fluorescence assay), the experimental conditions (e.g. temperature, buffer or filament preparation) and data analysis (e.g. normal vs. exponential distribution) can influence the results. Here, we describe a method to evaluate traces of fluorescent motor proteins and propose an algorithm to correct the measurements for photobleaching and the limited length of the filaments. Additionally, bootstrapping is used to estimate statistical errors of the evaluation method. The method was tested with numerical simulations as well as with experimental data from kinesin-1 stepping experiments to show that the run length of kinesin-1 is independent of the microtubule length distribution. Our work will not only improve the evaluation of experimental data, but will also allow for better statistical comparison of two or more populations of motor proteins (e.g. motors with distinct mutations or motors linked to different cargos).

BP 10.7 Tue 9:30 P1

**Microtubule Guiding on Nano-Patterns of Molecular Motors Generated by Laser-Ablation** — •Matthäus Mittasch[1,2], Cordula Reuther[1,2], Stephan Grill[1,3], and Stefan Diez[1,2] — [1]Max Planck Institute of Molecular Biology and Genetics, 01307 Dresden, Germany — [2]B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden, 01307 Dresden, Germany — [3]Biotechnology Center, Technische Universität Dresden, 01307 Dresden, Germany

Molecular motors such as kinesin-1 are highly optimized biological nano-machines that can be immobilized within engineered environments for the transport of cytoskeletal filaments such as microtubules in order to miniaturize and revolutionize hybrid nano-devices. However, for many applications it is of great importance to control the direction of the filament motion on planar surfaces to fulfill unique tasks such as the specific sorting of molecular entities. Here, we demonstrate the generation of highly-localized binding sites for kinesin-1 on poly(L-lysine)-g-poly(ethylene glycol)-coated surfaces using laser-ablation. Thereby, specific patterns of molecular motors with freely programmable shapes and feature-sizes down to a few hundred nanometers were generated. Straight lines, having a width of about 500 nanometers were shown to guide microtubules reliably. Moreover, we tested the guiding behavior on curved lines to investigate experimentally, if complex patterns can be used to sort microtubules, as was recently predicted theoretically (Rupp and Nédélec, Lab Chip (12), 2012).

BP 10.8 Tue 9:30 P1

**Dynamics of diffusing particles interacting with directionally moving particles on a polar filament** — •Denis Johann, Debajit Goswami, and Karsten Kruse — Saarland University, Saarbrücken, Germany

During cell division, pairing of sister chromosomes and their segregation is driven by the mitotic spindle, which is a stable bipolar structure consisting of overlapping microtubules, motor and other associated proteins. However, how the interplay between these proteins and microtubules render stability to the spindle structure is still unknown. Passive mobile cross-linkers called Ase1 have been found to dynamically adapt the dynamics of microtubule sliding induced by molecular motors to the length of the microtubules' overlap region [1].

Here, we study the effect of Ase1 on molecular motors in presence of steric interactions in terms of a stochastic lattice model. We find that

the Ase1 accumulate towards the end of the lattice in the direction of motor hopping and characterise their distribution through a mean-field theory.

[1] Braun et al., Nature Cell Biology 13, 1259-1264 (2011)

BP 10.9 Tue 9:30 P1

**Directionality of Single Kinesin-5 Cin8 Molecules is Mediated by the Tail Domains** — •André Düselder[1], Christina Thiede[1], Alice Wiesbaum[1], Vladimir Fridman[2], Dieter Klopfenstein[1], Larisa Gheber[2], and Christoph F. Schmidt[1] — [1]Georg-August-Universität, Göttingen, Deutschland — [2]Ben-Gurion University of the Negev, Beer-Sheva, Israel

Cin8, the tetrameric Kinesin-5 from budding yeast, shows the striking ability to move toward both the plus as well as the minus end of a microtubule. The molecular mechanism for this switch of directionality remains unknown. We have investigated this mechanism by examining the role of the C-terminal tail domains of Cin8 in the regulation of its directionality and motor function. To remove only the head-tail-interactions in the otherwise native tetramer, we built a Cin8 variant lacking the tail domains. In contrast to the wild type motor, this construct moves with a low velocity toward a randomly-chosen, but persistent direction. To look solely at the motility-generating subunits of Cin8, we fused the head domains and neck linker of Cin8 to the stalk of Kinesin-1 to construct a dimeric chimera. As a single molecule, this chimera is bidirectional with frequent changes in direction, indicating that the Cin8 head domains are inherently bidirectional. In optical trapping experiments, the probability of a switch of directionality increases with an increase of the force acting on the motor. We performed extensive power spectral analysis of the motor under various loads and different nucleotide conditions. Our findings suggest a force sensitive mechanism for a switch of directionality in Cin8.

BP 10.10 Tue 9:30 P1

**Rotation eines Proteinkomplexes in einer Lipidmembran: Molekulardynamik-Simulationen** — •Michael Becker — Universität Duisburg-Essen 47057 Duisburg

Wir befassen uns mit der Simulation des $F_{0c}$-Unterkomplexes der ATP Synthase und dessen Interaktion mit den Membranlipiden bei der Rotation. Zu diesem Zweck wird eine MD Simulation, bestehend aus einer Membran und des in ihr eingebetteten c-Ringes durchgeführt. Die Rotation des c-Ringes wird mittels einer gesteuerten Molecular Dynamik Simulation realisiert, wobei die Geschwindigkeit und somit der Impuls der Atome des c-Ringes alle 0.1 $[ps]$ angepasst wird. Das hieraus resultierende Drehmoment ist durch $\vec{M} = \vec{r} \times \frac{\partial \vec{P}}{\partial t}$ gegeben. Unsere Idee ist es also, dem c-Ring alle 0.1 $[ps]$ einen festen Drehimpuls $\vec{L}$ zu geben und anhand der Änderung dieses Drehimpulses, in der Zeit von eben diesen 0.1 $[ps]$, dass durch die Reibung wirkende Drehmoment mittels $\vec{M} = \frac{\vec{L}(t) - \vec{L}(t0)}{\Delta t}$ zu bestimmen, da im Gleichgewicht dieses Drehmoment dem angelegten entspricht.

## BP 11: Posters: Cytoskeleton

Time: Tuesday 9:30–12:30 Location: P1

BP 11.1 Tue 9:30 P1

**Time-resolved study of vimentin aggregation mediated by multivalent cations** — •Christian Dammann and Sarah Köster — Institute for X-Ray Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Besides actin filaments and microtubules, intermediate filaments (IFs) are a major component of the cytoskeleton, forming networks and bundles in the cell. Attractive interactions between purified negatively charged IFs can be mediated by small cations and the understanding of these interactions increases the knowledge of the cytoskeleton on a fundamental level. Here, we directly image the attractive interaction of vimentin IFs in the presence of multivalent cations using time-lapse fluorescence imaging. The dynamics of this process are followed in a drop-based microfluidic device that allows for rapid imaging shortly after the first protein-cation contact. Given a necessary threshold cation concentration, we find that the aggregation process takes place on the order of a few minutes. During this process the initially freely fluctuating filaments form highly compacted networks. We interpret our findings with regard to competitive binding of mono- and multivalent cations onto the filaments and find an explanation for the observed attraction mechanism. Our result emphasizes the important role of electrostatics for cytoskeletal proteins. The findings are likely to be representative for the class of vimentin-like IFs.

BP 11.2 Tue 9:30 P1

**Entropic contraction of actin networks** — •Carsten Schuldt, Tom Golde, Jörg Schnauss, Martin Glaser, and Josef A. Käs — Universität Leipzig , Institut für Experimentelle Physik I, Physik der weichen Materie, Linnéstr. 5, 04103 Leipzig, Germany

Retraction at the rear of a cell is a fundamental part of its migration process. This contraction can be accomplished by actin-myosin interaction. However, myosin knock-out cells have been shown to be still capable of migration. Alternatively, the depolymerization of the cytoskeleton was proposed to cause contractile forces only by a gain in entropy in the absence of molecular motors. This concept has been demonstrated on polymer mesh-works of nematode's major sperm protein.

We study the depolymerization of actin networks. In particular, the mesoscopic details and the forces associated with this process are of interest. We employ a micro-rheology approach in conjunction with light induced softening of actin networks [1] to measure both softening and contraction of the depolymerizing mesh-work.

[1] Golde *et al.* 2013. PRE 88:044601

BP 11.3 Tue 9:30 P1

**Dynamics of active actin network contraction** — •Dominic Jourdain[1], Anne Bernheim[2], and Karsten Kruse[1] — [1]Universität des Saarlandes, Germany — [2]Ben Gurion University, Israel

Recent in vitro experiments on actin filaments together with myosin motors reveal characteristic contraction patterns. The contraction speed increases linearly at first, before it decays exponentially. For asymmetric initial x-y-aspect-ratios, the contraction seems to follow this asymmetry. Using a continuous nonlinear Neo-Hookian elastic model for the filaments with a density dependent extra term to take the motor activity into account, we are able to qualitatively reproduce the asymmetric contraction and the contraction speed curves. To this end, a triangular finite element simulation is used.

BP 11.4 Tue 9:30 P1

**Visco-elastic properties of artificial biopolymer networks** — •Matthias Koch, Dominic Ruh, and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Microtubules (MT) are biopolymers which self-organize over a large spatial and temporal scale in living cells as a response to a variety of external stimuli. Most of the highly complex intracellular processes like cell-division or mechanotransduction are based on MT networks. The mechanical properties of single biopolymers like actin filaments or microtubules have already been studied in a wide context. However, the role of the meshwork geometry on the transport of mechanical momentum in a two dimensional MT network has not been studied so far.

Optical tweezers allow generating an array of anchor points for artificial polymer networks consisting of fluorescently labelled MT filaments attached to optically trapped 1$\mu$m spheres. We use multiple time-multiplexed optical traps which are displaced at rates up to 50kHz for both 3D force generation and measurements. The positions of the trapped particles can be evaluated using back focal plane interferometry, allowing resolving momentum propagation through the network. This configuration allows probing the visco-elastic properties of biopolymers in synthesized networks in a bottom-up approach and might reveal deeper insights in their complex interaction as part of the cytoskeleton. Results from first experiments with fluorescently labelled MT filaments attached to optically trapped 1$\mu$m spheres are presented.

BP 11.5 Tue 9:30 P1

**On the homogeneity of in vitro assembled keratin 8/18 networks** — •Tobias Neckernuss[1], Katinka Mertens[1], Ines Martin[1], Tobias Paust[1], Michael Beil[2], Raphael Blumenfeld[3], and Oth-

MAR MARTI[1] — [1]Department of Experimental Physics, Ulm University, D-89069 Ulm — [2]Clinic of Internal Medicine I, Ulm University, D-89069 — [3]Department of Earth Science & Engineering, Imperial College London, GB-London SW7 2BP

The cytoskeleton of epithelial cells consists of three types of filament systems: microtubules, intermediate filaments IFs and actin filaments. In our work, we have a closer look on in vitro assembled intermediate filaments consisting of keratin 8/18 and $MgCl_2$, serving as a crosslinker. With an optical trap we are able to determine mechanical properties of the network by trapping and exciting an embedded polystyrene bead which motion is transferred via the network to response beads in the surrounding. Correlating the motion of the excited beads with the ones of the response beads allows us to determine the homogeneity of the network. The setup for such a multibead microrheology measurement is presented as well as the evaluation methods. Furthermore the linearity of the networks response is tested with single bead measurements.

BP 11.6 Tue 9:30 P1

**thermal fluctuation of branched biopolymers and resulting entropic force** — •MOHAMMADHOSEIN RAZBIN[1,2], PANAYOTIS BENETATOS[3], MARTIN FALCKE[4], and ANNETTE ZIPPELIUS[1,2] — [1]Institute for Theoretical Physics, Georg-August University , Friedrich-Hund-Platz 1, 37077 Goettingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077, Goettingen, Germany — [3]Department of Physics, Kyungpook National University, South Korea — [4]Mathematical Cell Physiology, Max-Delbrück-Center for Molecular Medicine, Robert-Rössle-Straße 10, D-13092 Berlin, Germany

We consider branched structures of biopolymers, such as actin polymerized by Arp2/3. The polymers are modeled as weakly bending chains, which are grafted at one end and form branches at a given angle. we compute the thermal fluctuation of the endpoints and the resulting entropic forces on a flat membrane, restricting the fluctuations of the endpoints. The entropic forces are shown to depend sensitively not only on the persistence length but also on the geometry of the structure.

BP 11.7 Tue 9:30 P1

**Impact of cell-sized confinement on the dynamics of actin polymerization** — •ZOE SWANK, SIDDHARTH DESHPANDE, and THOMAS PFOHL — University of Basel, Basel, Switzerland

Components of the cytoskeleton are generally geometrically confined in cells, thus the range of physical dynamics exhibited by polymers in response to external confinement is connected to our understanding of biological systems. Using a microfluidic platform, we have studied the effects of varying geometrical confinements on the semi-flexible biopolymer actin. We have designed microfluidic devices, containing separate micro-confinements of differing geometries, which may exchange macromolecules and ions with a connected inlet channel via diffusion. Hence, we are able to observe the polymerization of actin filaments in vitro within diffusion-controlled micro-confinements, subject to various geometrical parameters. Furthermore, it is possible to create a macromolecular concentration gradient across the micro-confinements, enabling the control of actin filament polarity during polymerization. Observations of single-filament and multiple-filament fluctuations are correlated, and the distribution of single filaments and filament networks are analyzed. Imposing a progressively narrower confinement has been shown to dampen polymer fluctuations and alter their distribution, while constraining filaments to increasing angles of external curvature is found to primarily affect the distribution of polymers within the confinement.

BP 11.8 Tue 9:30 P1

**Active Microrheology: Mechanical Properties of In Vitro Assembled Keratin Networks** — TOBIAS PAUST[1], KATINKA MERTENS[1], INES MARTIN[1], TOBIAS NECKERNUSS[1], MICHAEL BEIL[2], and •OTHMAR MARTI[1] — [1]Institute of Experimental Physics — [2]Department of Internal Medicine I

Macro- and microrheology is extensively used to characterize complex networks of biopolymers. From this data one infers mechanical properties affecting migration or the response to external stresses. So far macro- and microrheology give similar but not identical responses.

The aim in these studies is to gather information about the dynamic mechanical properties of in vitro assembled keratin 8/18 networks realized by an optical tweezers setup.

In this work we explore the possibility of multi-point microrheology to determine locally the complex tensorial elastic response of heterogeneous networks. We use the measurements to find possible differences between macro- and microrheology. A careful analysis of the data provides additionally the frequency response of the complex elastic tensor. Furthermore, it is possible to determine phase dependencies between excitation and response. We show the data of measurements of in vitro assembled keratin 8/18 networks with varying Mg2+ concentrations.

BP 11.9 Tue 9:30 P1

**Nonlinear elasticity of cross-linked networks** — •KARIN JOHN[1], DENIS CAILLERIE[2], PHILIPPE PEYLA[1], ANNIE RAOULT[3], and CHAOUQI MISBAH[1] — [1]Université Grenoble 1/CNRS, LIPhy UMR 5588, F-38041 Grenoble, France — [2]L3S-R, B.P. 53, F-38041 Grenoble Cedex 9, France — [3]Laboratoire MAP5 UMR 8145, Université Paris Descartes/CNRS, F-75270 Paris Cedex 06, France

Cross-linked semiflexible polymer networks are omnipresent in living cells. Typical examples are actin networks in the cytoplasm of eukaryotic cells, which play an essential role in cell motility, and the spectrin network, a key element in maintaining the integrity of erythrocytes in the blood circulatory system. We introduce a simple mechanical network model at the length scale of the typical mesh size and derive a continuous constitutive law relating the stress to deformation. The continuous constitutive law is found to be generically nonlinear even if the microscopic law at the scale of the mesh size is linear. The nonlinear bulk mechanical properties are in good agreement with the experimental data for semiflexible polymer networks, i.e., the network stiffens and exhibits a negative normal stress in response to a volume-conserving shear deformation, whereby the normal stress is of the same order as the shear stress. Furthermore, it shows a strain localization behavior in response to an uniaxial compression.

The presented theory provides a basis for the continuum description of polymer networks such as actin or spectrin in complex geometries and it can be easily coupled to growth problems, as they occur, for example, in modeling actin-driven motility.

BP 11.10 Tue 9:30 P1

**Equilibrium Dynamics of Helical Polymers** — •LORENZ HUBER, PHILIPP LANG, and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Germany

Biopolymers like DNA, cytoskeletal filaments or artificially designed DNA-origami fibres are elastic nanoparticles that form helical configurations in their ground state. The handedness, radius and pitch of these helices are determined by their curvature $\kappa$ and torsion $\tau$. Their statistical mechanics is described by the helical wormlike chain model, where $\kappa, \tau$ are identified as the filaments' intrinsic bending and twisting rates, respectively.

Here we employ Brownian dynamics simulations to investigate the thermal end-to-end distance fluctuations. We find that $\langle \delta R^2(t) \rangle$ exhibits a rich scaling behavior with varying $\kappa$ and $\tau$. For $\kappa = 0$ the initial relaxation resembles the $t^{3/4}$-scaling law as predicted by semiflexible polymer theory. In contrast, helices with a low ascending pitch angle, i. e. $\kappa > \tau$, show power law exponents exceeding 3/4 due to the additional elastic modes of the spring-like polymer conformation. The crossover region with $\kappa < \tau$ reveals a sudden intermediate relaxation regime with a scaling exponent well below 3/4. With rising $\tau$ this domain only slowly converges towards the semiflexible limiting case.

Our findings demonstrate the intriguing influence of helical parameters on the dynamics of single polymer systems and can in principle help to determine structural details beyond the resolution of (static) experimental techniques.

BP 11.11 Tue 9:30 P1

**Mechanical Properties of Keratin Bundles in Living Cells** — •JENS-FRIEDRICH NOLTING and SARAH KÖSTER — Institute for X-Ray Physics, University of Göttingen, Germany

Intermediate filaments are a major component of the eukaryotic cytoskeleton along with microtubules and microfilaments and play a key role in cell mechanics. Here, we present a study of keratin intermediate filament bundles in living cells. Intracellular forces in combination with cytoskeletal cross-talk lead to buckling of the keratin bundles. By investigating these buckling events *in situ* we conclude upon the mechanical properties of the keratin bundles and their environment. In brief, we measure the buckling wavelength and the bundle diameter of the events using live cell confocal microscopy. From these data we then deduce the elastic modulus of the surrounding matrix and the persis-

tence length of the bundle. Furthermore, we evaluate the strength of the coupling between the individual filaments inside a keratin bundle by fitting a coupling factor to our data. Our findings suggest that the coupling between the filaments within a bundle is predominantly strong but it allows for some movement of filaments with respect to each other.

BP 11.12 Tue 9:30 P1

**Subunit exchange in vimentin intermediate filaments** — •Bernd Nöding and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

Intermediate filaments, together with actin filaments and microtubuli and in combination with motorproteins and binding proteins make up the cytoskeleton of eukaryotic cells. While assembly mechanisms for different intermediate filaments have been modeled in the past, insights into the dynamic changes in the filament cross-section are still largely missing. Thus, we perform measurements of the exchange of fluorescently labeled subunits on fully assembled vimentin intermediate filaments. We find that an exchange of subunits occurs at a temperature dependent rate. Likely, polymorphism of the filament cross-section is an important factor in this process. With these findings, we aim to contribute to a more comprehensive description of the assembly and subunit exchange mechanism.

BP 11.13 Tue 9:30 P1

**Studying the assembly of intermediate filaments in microfluidic channels using fluorescence cross correlation spectroscopy (FCCS)** — •Viktor Schroeder[1], Bernd Nöding[1], Anja Niedermayr[2], Harald Herrmann[3] und Sarah Köster[1] — [1]Institute for X-Ray Physics, Georg-August-University Göttingen, Göttingen, Germany — [2]Department of Neurophysiology and Cellular Biophysics, Georg-August-University Göttingen, Göttingen, Germany — [3]Division of Molecular Genetics, German Cancer Research Center (DKFZ), Heidelberg, Germany

The cytoskeleton of eukaryotes consists of three different filamentous systems: microtubules, actin filaments and intermediate filaments (IFs). While both tubulin and actin are highly conserved, IF proteins occur in many different variations, depending on cell type and organism. All cytoskeletal filaments consist of distinct subunits and assemble in a characteristic way. For vimentin IFs, which are found in cells of mysenchymal origin, a principal assembly model exists. However, measurements of the assembly process with high time resolution, which would yield insight especially into the early assembly steps, are still largely missing. To approach this problem, we use fluorescence cross correlation spectroscopy (FCCS) in combination with microfluidic continuous flow mixers to access time scales in the millisecond range and directly follow binding events.

BP 11.14 Tue 9:30 P1

**Magnetic interactions in the magnetosome chain of magnetotactic bacteria** — •Bahareh Kiani and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Magnetotactic bacteria are aquatic microorganisms that swim and orient in the direction of magnetic field due to the presence of the magnetosome chain, a chain of vesicle-enclosed magnetic nanoparticles that are aligned on a cytoskeletal filament [1]. Here we investigate magnetic interactions between the nanoparticles to study the contribution of magnetism to the persistence length of the chain. The calculation of the energy of a curved magnetosome chain shows that magnetic interactions contribute only little to the stiffness of the chain, which should be mostly attributed to the filament. Furthermore, magnetic interactions favor closed-ring chains, and attachment to the filament can stabilize the chain against ring closure.

[1] Dirk Schüler, *Magnetoreception and Magnetosomes in Bacteria* (Springer, 2006).

BP 11.15 Tue 9:30 P1

**Elastic response of pre-stressed 3D filamentous networks with compliant crosslinks** — •Knut Heidemann[1], Meenakshi Prabhune[2], Florian Rehfeldt[2], Christoph Schmidt[2], and Max Wardetzky[1] — [1]Institut für Numerische und Angewandte Mathematik, Georg-August-Universität Göttingen — [2]Drittes Physikalisches Institut - Biophysik, Georg-August-Universität Göttingen

The cytoskeleton of cells is a composite network of filaments ranging from stiff rod-like microtubules to semiflexible actin filaments that together play a crucial role for cell structure and mechanics. The collective dynamics of these cytoskeletal filaments with widely different mechanical properties yet remain to be understood completely.

To model a strongly heterogeneous composite, we set up 3D simulations of filamentous networks with compliant crosslinks, and extract elastic moduli via quasistatic deformations.

Furthermore, We introduce an affine theory that captures the simulation results correctly. In particular, we derive asymptotic exponents for the scaling of the differential modulus with stress in the limit of infinite crosslink densities. Numerical results for finite numbers of crosslinks are presented as well.

In addition, we analyze the effects of pre-stress, which is easily tunable in our simulations. It turns out that the initial normal stress can be related to the linear shear elastic modulus, and might therefore be of importance for experimental studies as well.

## BP 12: Posters: Imaging

Time: Tuesday 9:30–12:30 Location: P1

BP 12.1 Tue 9:30 P1

**Homo-Fret to Investigate the Oligomeric State of Proteins** — •Franz-Josef Schmitt, Matthias Broser, Cornelia Junghans, and Thomas Friedrich — Institute of Chemistry, Biophysical Chemistry, TU Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany

The combination of various microscopic techniques allows to address complex problems in biophysics. We present a multi-parameter setup based on to a Nikon TI Eclipse microscope that combines time resolved fluorescence microscopy and simultaneous anisotropy microscopy by splitting the detector optically into two independent areas. All microscopic techniques (confocal, wide field, total internal reflection) can be done with a high photon throughput up to 2 Mio. photons/sec. with spectral and polarization resolution. Förster Resonance Energy Transfer (FRET) between identical fluorophores without the discrimination between donor and acceptor (Homo-FRET) allows the determination of the aggregation state of identical chromophors. Microscopic measurements of time resolved Homo-FRET were used to determine the aggregation state of a model system of fluorescence proteins (FKBP-GFP constructs) that can dimerize or form larger aggregates (up to pentamers) by adding a specific membrane-permeable agent. The technique has great application potential for the observation of the repair cycle of the D1 protein in the photosystem II.

BP 12.2 Tue 9:30 P1

**Diffusion in Living Cells Determined by Multiparameter Imaging** — •Franz-Josef Schmitt, Cornelia Junghans, Matthias Sturm, Marvin Schlischka, and Thomas Friedrich — Institute of Chemistry, Biophysical Chemistry, TU Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany

Multiparameter microscopy is close to becoming a standard technique in live cell imaging. The synergistic interplay between highly resolved fluorescence microscopy and photoswitchable fluorescence proteins lead to a brilliant new methodology that broke the diffraction barrier of optical microscopy. We show how the photoswitchable genetically expressed Dreiklang Protein is used to determine the local diffusion coefficients in the cell cytoplasm and the cell nucleus as well as the kinetics of the Dreiklang protein diffusion across membranes. The technique shows preferred pathways of proteins across the cell nucleus which are not visible by constantly fluorescing labels due to the strong overlap of the emission of single molecules that lead to homogeneous fluorescence patterns. The dynamics of selectively marked mitochondria is tracked and the mean square displacement is calculated showing regimes of hampered diffusion, free diffusion and active transport.

BP 12.3 Tue 9:30 P1

**An insight into structural changes induced to cells by chemical fixatives using X-ray nano-diffraction** — •Clémenet Hémonnot, Britta Weinhausen, Rita Graceffa, Robin Wilke, and Sarah Köster — Institute for X-Ray Physics, University of

Göttingen, Germany

Various research methods have been developed to study the structure and composition of biological cells, the most prominent ones being fluorescence and electron microscopy. However, for most of these methods, sample preparation such as chemical or cryogenic fixation, staining or labeling, or tissue sectioning is prone to introduce artifacts. Thus, our aim was to use a label-free technique that probes cells in their native, aqueous environment at high resolution. We have applied X-ray nano-diffraction to image cells in microfluidic devices. High spatial resolution due to small wavelengths is combined with high penetration depth, enabling us to study entire cells. The microfluidic devices allow us to keep the cells alive as well as reducing the radiation damage by cooling the sample and by decreasing the concentration of free radicals through constant buffer or media flow. We have performed X-ray nano-diffraction experiments on fixed-hydrated and living eukaryotic cells. In particular, we have compared three widely employed chemical fixatives and analyzed the overall structure of the nucleus and cytoplasm. The different fixatives indeed introduce a different degree of structural changes on length scales on the order of 35 to 45 nm.

BP 12.4 Tue 9:30 P1

**Assessing reptation motion with the WormTracker** — Matthias Weiss and •Carsten Schade — Experimental physics 1, University of Bayreuth

The locomotion pattern of C. elegans (a small transparent roundworm) is complex and depends on the properties of the environment. To gain a better understanding of the locomotion mechanism of C. elegans, it is mandatory to take a closer look on the motion of individual worms. To get the exact movement pattern of C. elegans in different environments, we have constructed a worm imaging platform. This platform monitors in a time-resolved fashion the accurate shape and center of mass of worms during their movement.The tracking station allows single- and multi worm tracking. In the single tracking mode it is possible to track a single worm for any period of time. Therefore it is possible to track the complete lifetime of a single worm. In the multi tracking mode, it is feasible to track all worms on the plate and therefore to get comparative data from the movements of a worm ensemble in the same environment. The tracking software and the hardware are programmed with Matlab and LabView, i.e. it is easy to develop additional software packages for customized measurements.

BP 12.5 Tue 9:30 P1

**Sub-diffraction imaging of cellular organelles** — •Andreas Veres and Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Eukaryotic cells are highly compartmentalized. One of the most prominent organelles is the endoplasmic reticulum (ER) which assumes the morphology of a sponge-like web that spans throughout the cell. The full structure of the ER, however cannot be resolved by conventional light microscopy approaches as the typical mesh size is below the diffraction limit. To overcome this limitation, we have used SOFI (Superresolution optical fluctuation imaging) which provides a means to overcome the diffraction limit by exploiting fluorescence fluctuations of quantum dots. Based on our SOFI images we have determined the fractal dimensions of the ER and its porosity in cells at different stages.

BP 12.6 Tue 9:30 P1

**Preparation of colloidal CdSe quantum dots for medical fluorescence labelling** — •Svenja Herbertz[1], Lothar Houben[2], Kathrin Scheckenbach[3], and Thomas Heinzel[1] — [1]Solid State Physics Laboratory, Buildg. 25.23., Heinrich-Heine University Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf — [2]PGI-5, FZ Jülich, Wilhelm-Johnen-Str. , D-52425 Jülich — [3]HNO-Klinik, Buildg. 13.76, Heinrich-Heine University Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf

The size dependence of their energy bandgap allows producing quantum dots of various fluorescence wavelengths in one production process. We fabricated colloidal CdSe QDs with tunable emission via kinetic growth with TOP as stabilizer [1] and investigated the influence of various growth parameters on the fluorescence behavior. The produced QDs have a size-dependent fluorescence line with typical FWHM of about 40 nm. Via X-ray diffraction and HR-TEM nanocrystal diameters of about 2 to 6 nm were measured and a hexagonal wurtzite crystal structure was identified. The surface of the QDs as-fabricated was chemically modified to establish solubility in aqueous media. In the context of detecting drugs in cell cultures by fluorescence labelling with QDs, an agent of particular interest is the chemotherapeutic cisplatin. The interaction of cisplatin with QDs, for a start without a direct connection of the molecules, was investigated. It was found that the presence of cisplatin quenches the fluorescence intensity of QDs in water.

[1] E. M. Boatman et al., J. Chem. Educ. 82, 1697(2005).

BP 12.7 Tue 9:30 P1

**Age related changes in human RPE cells, imaged by multicolor SIM microscopy.** — •Florian Schock[1,2], Gerrit Best[1,2], Nil Celik[2], Alina Bakulina[6], Martin Hagmann[1,2], Rainer Heintzmann[4,5], Jürgen Hesser[6], Stefan Dithmar[2], and Christoph Cremer[1,3] — [1]Kirchhoff Institute for Physics, University of Heidelberg — [2]Department of Ophthalmology, University of Heidelberg — [3]Institute of Molecular Biology, Mainz — [4]Institute for Physical Chemistry, University of Jena — [5]Institute of Photonic Technology, Jena — [6]Institute for Medical Technology, Mannheim

In our society old-age diseases are becoming more frequent. One reason for these are non-degradable deposits of degradation products. These are generated in normal cell-processes, but their accumulation during the human lifespan leads to dysfunction of cell-activity. This is believed to be the case in age related macula-degeneration, where the deposits form granules of the size of about 0.5$\mu$m to 3$\mu$m. Structured Illumination Microscopy is used to study auto-fluorescent proteins in this deposits, allowing us to separate and image them. In contrast to electron-microscopy, fluorescence microscopy has less stringent constraints to sample preparation and is generally less invasive. Additionally, it offers the possibility to separate different kinds of deposits by using multicolor excitation. This allows us to search for differences in the composition of the deposits. We analysed several histological samples by donors of different age. We present quantitative data to the relation between donor age and granula quantity. All work on human tissue was done according to the Declaration of Helsinki.

BP 12.8 Tue 9:30 P1

**Apertureless Scanning Near-Field Optical Microscopy of Tobacco Mosaic Viruses and Intermediate Filament Desmin** — •Niklas Biere[1], Alexander Harder[1], Mareike Dieding[1], Volker Walhorn[1], Sven Degenhard[2], Andreas Brodehl[3], Christina Wege[2], Hendrik Milting[3], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanoscience, Bielefeld University — [2]Dpt. of Molecular Biology and Plant Virology, Institute of Biology, University of Stuttgart — [3]Heart and Diabetes Center NRW, Bad Oeynhausen

Aperture-less scanning near-field optical microscopy (aSNOM) makes use of both, high resolution topographic and fluorescence imaging. Atomic force microscopy (AFM) allows for a topographic resolution down to the atomic scale. Furthermore it can be operated in ambient conditions, liquids or in vacuum which makes it ideal for a large variety of different samples. The evanescent illumination of the AFM cantilever tip induces enhanced electromagnetic fields that are strongly confined to the tip apex. These can serve to excite and image single dye molecules. Here we report on our custom built aSNOM setup using commercially available monolithic silicon cantilevers. We investigated sparsely labelled tobacco mosaic viruses and the intermediate filament protein desmin. Both of which are complex structures composed of mixed building blocks. The simultaneous recording of topography and fluorescence data and their inherent alignment allows for the exact localization of distinct fluorescently labelled building blocks within the superordinate macromolecular structures.

BP 12.9 Tue 9:30 P1

**Space- and time-resolved information of refraction index in a microresonator** — •Tobias Menold[1,2], Michael Metzger[1], Alexander Konrad[1], Andreas Horrer[2], Sabrina Rau[1], Günther Gauglitz[1], Dai Zhang[1], Alfred J. Meixner[1], Dieter Kern[2], Marc Brecht[1,3], and Monika Fleischer[2] — [1]IPTC, University of Tübingen — [2]Institute for Applied Physics, University of Tübingen — [3]Zürcher Hochschule für Angewandte Wissenschaften, Institute of Applied Mathematics and Physics

The aim of our research is to determine the change of the refractive index within a Fabry Perot microresonator, consisting of a flat and a curved mirror in close distance ($\lambda$/2-region), in space and time using a standard colour CCD camera. Using white light illumination yields a position dependent transmission. If a flat and a convex mirror are used the transmission shows a spectrally well-defined Newton ring pattern. The possibility to sense small changes of the refractive index within the

cavity depends on the resonator properties and the wavelength resolution of the CCD camera. The main issue is to extract the wavelength with high resolution out of the RGB values determined by the CCD camera. For this purpose we calibrated the CCD-chip using the transmission pattern of monochromatic light with a spectral range between 380 nm and 650 nm. Based on these images we were able to calculate the hue-value of HSV colour space. With that calibration it is possible to translate information from the CCD-camera into refraction index information. The calibration enables us to determine the refraction index within a microresonator with spatial and temporal resolution.

BP 12.10 Tue 9:30 P1

**Probing quantum coherence in light-harvesting (LH1) complexes using FRET from a single nitrogen vacancy center** — •Priyadharshini Balasubramanian[1], Anna Ermakova[1], Chris Schroeder[2], Liam McGuinness[1], Felipe Caycedo-Soler[2], Caroline Autenrieth[3], Susana Huelga[2], Martin Plenio[2], Robin Ghosh[3], and Fedor Jelezko[1] — [1]Institute for Quantum Optics, University of Ulm — [2]Institute for Theoretical Physics, University of Ulm — [3]Institute of Biology, University of Stuttgart

The formidable quantum efficiency of light harvesting complexes in photosynthetic organisms have been attributed to the long-lived quantum coherence effects. Experiments with ensemble of LH1 complex, have reported the observation of quantum coherence in the time scale of picoseconds range, but the results suffer from ensemble averaging over inhomogeneous distribution of site energy. Here we propose single molecule - Fluorescence Resonance Energy Transfer(FRET) experiment between a single NV center in diamond and the LH1 complexes, to probe the inter-ring coherence dynamics. The path of excitonic energy transfer(EET) between the rings will be measured by injecting excitation locally to a chromophore via a single NV center attached to an AFM tip, and the fluorescent emission is detected from a single red-shifted LH1 in the membrane. The distance traversed by the excitation energy in the membrane gives insight on the contribution of quantum coherence to the inter-ring energy transfer dynamics. Unraveling the role of coherent dynamics in the process of light-harvesting could provide inspiration for artificial photosynthesis.

BP 12.11 Tue 9:30 P1

**Refractive index studies of biological cells and nuclei using digital holographic microscopy** — •Mirjam Schürmann[1], Jana Scholze[1], Chii J. Chan[2], Paul Müller[1], Andrew E. Ekpenyong[1], Kevin J. Chalut[2], and Jochen Guck[1,2] — [1]Biotechnology Center, TU Dresden, Tatzberg 47/49, 03107 Dresden, Germany — [2]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK

In recent years, digital holographic microscopy (DHM) has increasingly been used in biophysical and cell biological studies for the determination of the refractive index of cells. This quantitative phase microscopy technique is non-invasive, in comparison to other traditional imaging techniques, which often require external labelling of biological samples. Previous work in our group on cell differentiation revealed a lineage-specific modulation in the cells' refractive index, suggesting the use of DHM as a useful tool for marker-free studies of cell differentiation. Recently we have also used DHM to study the optical properties of the cell nucleus, which may reflect its epigenetic nature. In contrast to other studies suggesting a high refractive index of cell nuclei compared to the cytoplasm, the present study reveals that the refractive index of isolated cell nuclei of a variety of cell types can be lower than the refractive index of the cell. In addition, nuclear refractive index was found to be highly sensitive to external salt concentrations. This characterisation of the optical properties of nuclei is important for the proper interpretation of laser trapping experiments of cells or the use of light scattering techniques in tissues, such as optical coherence tomography, for diagnostic purposes.

BP 12.12 Tue 9:30 P1

**Towards a zone plate based ultra compact HHG driven XUV/soft X-ray scanning transmission microscope** — •Christian Späth, Jürgen Schmidt, Huaihai Pan, Alexander Guggenmos, and Ulf Kleineberg — Ludwig-Maximilians-Universität München, Lehrstuhl für Experimentalphysik - Laserphysik, 85748 Garching, Germany

X-ray microscopy is an invaluable imaging method in many research areas with applications in physical, medical and biological problems as well as material science. Especially XUV/soft X-ray microscopy offers the great potential for investigating sensitive biological samples in their natural environment with low dose to reduce radiation damage and high spatial and energy resolution to address questions concerning sub cellular features or elemental composition. Here we report on our concept of an ultra compact microscope utilizing laser driven high harmonic radiation with ˜ 73 eV energy as a light source and a zone plate operated in transmission as the main focussing element combined with different detectors which enables us to run this system in scanning mode as a STXM but also in a modified version as a high resolution instrument in diffraction mode employing the CDI (coherent diffractive imaging) technique. Furthermore due to our pulsed light source the possibility of time-resolved microscopic analysis is given with a possible few-femtosecond temporal resolution.

BP 12.13 Tue 9:30 P1

**Following the topography during abscission using SICM** — •Ulrich Fromme[1], Natalie Elia[2], and Christph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Fakultät für Physik, Georg-August-Universität, Göttingen — [2]Department of Life Sciences and the National Institute for Biotechnology in the Negev, Ben-Gurion University, Beer-Sheva, Israel

The last step in the division cycle of animal cells is abscission. It is defined as the cutting of the small intracellular bridge which remains as a connection between the two daughter cells after the cytoplasm has been divided. This bridge, the so-called midbody, is of an interesting structure, as it contains dense tubulin structures which originate from the cell division- and DNA-separation process. Due to the compactness of this structure, a complex system of membrane constriction and tubulin disassembly molecules are recruited for abscission. In this study we used Scanning-Ion-Conductance-Microscopy (SICM) to create topological movies of these structures in living MDCK cells. SICM can produce images with a resolution that is superior to standard optical methods without damaging or deforming the structures. This makes it possible to acquire high-resolution images and to observe the morphological changes of the intracellular bridge during the abscission process.

# BP 13: Posters: DNA/RNA and related enzymes

Time: Tuesday 9:30–12:30 Location: P1

BP 13.1 Tue 9:30 P1

**Local melting of ds-DNA within ultrathin amphiphilic films** — •Caroline Falk, Hua Liang, Nikolai Severin, and Jürgen P. Rabe — Department of Physics Humboldt-Universität zu Berlin

DNA-replication is an important process in the human body. Replication of double-stranded (ds)-DNA requires its local unwinding, i.e. melting into two single strands (1). DNA, when stretched in solution, overwinds and melts (2). This was argued to give insight onto the replication mechanism. It is difficult, however, to access the direct conformational changes during stretching in solution. Preliminary work has demonstrated that this transition can be investigated on a graphite surface, pre-coated with an amphiphilic layer imaged with scanning force microscopy (3). ds-DNA can be stretched by an amphiphilic layer. This leads to a local splitting of the ds-DNA into two single strands and overwinding of the rest of the vector ds-DNA. This effect can be analyzed as a function of plasmid length and base sequences. We demonstrate here our efforts to identify the location of the local melting within the ds-DNA by marking specific locations within the DNA.

(1) D.Coman, I.M.Russu, Journal of Biological Chemistry 280, 20216 (2005).

(2) J.Adamcik, S.Tobenas, G.Di Santo, D.Klinov, G.Dietler, Langmuir, 25, 3159 (2009).

(3) H.Liang, W.Zhuang, N.Severin, J.P.Rabe Control of Single DNA Conformation on a Nanostructured Template (to be published).

BP 13.2 Tue 9:30 P1

**Quantitative DNA Overstretching Using Optical Tweezers** — Roland Hillmann, André Spiering, Andy Sischka, and •Dario Anselmetti — Experimental Biophysics, Bielefeld University, 33615 Bielefeld, Germany

We investigated the binding of histonecomplexes to DNA by monitoring the dynamic structure of individual nucleosomes by optical tweezers with single molecule force spectroscopy. 16.4um long biotinylated dsDNA is attached to two streptavidin coated microspheres, one held by a micropipette, as well as the other by the optical trap, respectively. The histones in our experiment contain all of the natural proteins (H2a, H2b, H3, H4) including the linker histone-like protein (H1) to form higher order structures. We observed distinct sawtooth patterns, that can be interpreted as the release of individual nucleosome complexes and will discuss the observed phenomena in the framework of histone complex formation.

BP 13.3 Tue 9:30 P1

**Nucleosome Breathing Facilitates Rapid DNA Packaging Into Chromatin** — •Brendan Osberg, Johannes Nuebler, and Ulrich Gerland — Arnold-Sommerfeld Center for Theoretical Physics and Center for NanoScience, Theresienstraße 37, 80333 München

In eukaryotic cells DNA is packaged into chromatin: Nucleosomes, each consisting of 147 base pairs of DNA wrapped around a histone protein octamer, cover approximately 90% of the DNA. However, the mechanisms whereby cells achieve such a high coverage within a short time, e.g. after DNA replication, remain poorly understood.

It is well known that random sequential absorption processes of hard particles on a line lead to extremely slow filling kinetics beyond about 75% coverage, due to a "jamming" behavior. Of course, ATP consuming "remodeler" enzymes can speed up the filling of the DNA with nucleosomes.

However, we show that the breathing property of nucleosomes, where DNA transiently partially unwraps from the histones due to thermal fluctuations, can already eliminate the jamming behavior and alleviate the kinetic problem. We also consider effects whereby the steady progression of the replication fork could enable fast filling in its wake.

BP 13.4 Tue 9:30 P1

**Measuring DNA translocation through nanopores in graphene and carbon nanomenbranes with Optical Tweezers** — •Sebastian Knust, Andre Spiering, Andy Sischka, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

The forces acting on DNA during translocation through a nanopore were measured with Optical Tweezers. We developed a video-based force detection and analysis system allowing for virtually interference-free axial force measurements with sub-piconewton precision [1].

We previously measured the translocation of dsDNA through 20 nm thick Si2N3 membranes (0.1 pN/mV for pores $\geq$ 30 nm) [2, 3]. Carbon nanomembranes and graphene with a thickness of 3 nm and 0.3 nm respectively allow for even more sensitive measurements.

We show the controlled translocation of a single dsDNA strand attached to a microbead with an overall force resolution of $\pm$0.5 pN at a sample rate of 123 Hz.

[1] S. Knust et. al., Rev. Sci. Instrum. **83**, 103704 (2012)

[2] A. Spiering et. al., Nano Lett. **11**, 2978 (2011)

[3] A. Sischka et. al., in preparation

BP 13.5 Tue 9:30 P1

**Single Molecule Localization Microscopy of Chromatin Structures** — •Udo Birk[1,2], Kirti Prakash[1], Aleksander Szczurek[1], Hyun-Keun Lee[1], and Christoph Cremer[1,2] — [1]Institute of Molecular Biology (IMB), Ackermannweg 4, 55118 Mainz, Germany — [2]Kirchhoff Institute for Physics, Heidelberg University, 69120 Heidelberg, Germany

Understanding the structural and organizational aspects of chromatin at different stages of cell differentiation as well as at various phases of the cell cycle is one of the many promising applications of super-resolution microscopy. It is challenging to study e.g. the organization of the different proteins which form the basis of chromosomal superstructures, due to limitations of conventional Light Microscopy (LM) and of Electron Microscopy (EM). To this end, structured illumination microscopy (with an optical resolution of about 100 nm in the object plane) could provide an improved resolution of intact cell nuclei and of the chromatin therein.

We report results on visible light based single molecule localization microscopy (SMLM) of chromatin structures in intact cell nuclei, and studied these structures at different stages of the cell cycle using the SMLM method of Spectral Position Determination Microscopy (SPDM). We analyzed the distribution of DNA and of associated proteins. The images obtained show a dramatic increase in light optical resolution of chromatin structures. Novel labeling techniques are required to make full use of SMLM visualization of DNA also directly labeled, i.e. without fluorescence in-situ hybridization.

BP 13.6 Tue 9:30 P1

**Effects of molecular crowding on promoter finding** — •David Gomez and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

All biological functions of DNA depend on the recognition of specific sequences by site-specific DNA-binding proteins. Binding of these proteins to their binding sites is believed to occur through a facilitated diffusion process that combines one-dimensional diffusion along the DNA with three-dimensional diffusion in the bulk solution.

This model has been assumed to be general for all DNA-binding proteins even though the conditions, such as protein concentrations, are different for different DNA-binding proteins. The objective of this work is to model the dynamics of the RNAP-promoter binding under different concentrations of RNAPs and other proteins that act as 'obstacles.' To do that, we place a linear DNA template with its promoter, RNAPs and obstacles on a 3D lattice, and determine the RNAP-promoter binding rates at different conditions. Our results suggest that an acceleration in the binding process occurs only at some obstacle concentrations and non-specific binding times of the RNAP on the DNA.

BP 13.7 Tue 9:30 P1

**Dielectric spectroscopy of DNA up to 110 GHz** — Elena Ermilova, Frank Bier, and •Ralph Hölzel — Fraunhofer Institute for Biomedical Engineering Am Mühlenberg 13, 14476 Potsdam-Golm, Germany

Dielectric studies of DNA aqueous solutions still contribute to a better understanding of the interaction mechanisms between biological molecules, solvent, their ionic environment and electromagnetic fields at upper GHz and lower THz frequencies. Reflection measurements using a vector network analyzer allow a fast and uncomplicated determination of permittivity spectra from the measured complex reflection

coefficient. In the present study we report the experimental results on dielectric relaxation of Na-DNA at various concentrations. Permittivity measurements were performed in the broad frequency range between 25 MHz and 110 GHz in a single sweep by means of a vector network analyzer. The permittivity spectra of DNA solutions exhibit a complex behaviour with several dispersion regions attributed to different relaxation mechanisms. Resulting from fitting to the double Cole-Cole model we resolved two dispersion regions: around 100 MHz and 20 GHz, respectively, and analysed their relaxation strengths and relaxation times.The wide frequency range provides possibilities for better analysis of the relaxation process attributed to the water dipoles in the presence of DNA macromolecules. The small dimension of the coaxial sensor allows to reduce the sample volume, which opens new possibilities for dielectric spectroscopy of well defined highly concentrated DNA solutions, as well as biological and synthetic polymer solutions.

BP 13.8 Tue 9:30 P1

**Experiments of DNA-Ligand-Complexes with Optical and Magnetic Tweezers** — •Ying Wang[1], Susan Haji Samo[1], Andy Sischka[1], Helene Schellenberg[1], Katja Tönsing[1], Thomas Jany[2], Thorsten Glaser[2], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanoscience, Bielefeld University, 33615 Bielefeld, Germany — [2]Lehrstuhl für Anorganische Chemie I, Bielefeld University, 33615 Bielefeld, Germany

We investigated the specific binding of Co-, Cu- and Ni-dinuclear metal complexes (DNMCs) to dsDNA with optical (OT) and magnetic tweezers (MT). DNMCs bind to the DNA backbone, hydrolyse phosphate esters (cutting functionality) and thus prevent the particular DNA segment from being replicated or transcribed. In the OT stretching experiments, we have observed force peaks, suggesting knot or coil formation of DNA entanglements, since the aromatic groups of neighbouring DNMCs can interact with each other via $\pi$-stacking. Detecting these complexations have proved the binding of DNMCs to DNA. In twisting experiments with MT, we have evidenced that 200$\mu$M Cu-DNMC shows cutting functionality. Because of the created nicks, the DNA molecule can no further be twisted. Combining with molecular recognition techniques DNMCs could be utilized on medical applications as a possible drug dealing with cancers in the future.

## BP 14: Posters: Protein Structure and dynamics

Time: Tuesday 9:30–12:30 Location: P1

BP 14.1 Tue 9:30 P1

**Langevin simulations of conformational changes in proteins under temperature gradients** — •Anne Dorothee Müller and Martin E. Garcia — Theoretische Physik, Universität Kassel, Fachbereich 10, Kassel, Germany

We developed a program to simulate conformational changes in small, globular proteins under temperature gradients by integrating the Langevin equations of motion. This program uses a potential based on the coarse-grained model developed by Nan-Yow Chen et al. [PhysRevLett.96.078103(2006)]. Chen's force field does not need any a priori information about the native state of the protein and is known to be able to describe the folding of proteins to both alpha-helices and beta-sheets. Hence we investigated the protein 3ZNF which has part alpha-helix part beta-sheet as its native structures.

BP 14.2 Tue 9:30 P1

**A multiscale model for fibrinogen** — •Stephan Köhler[1,2], Martin McCullagh[3], Friederike Schmid[1], and Giovanni Settanni[1,4] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Graduate School Materials Science in Mainz — [3]Department of Chemistry and Institute for Biophysical Dynamics, University of Chicago, Chicago, Illinois, United States — [4]Max Planck Graduate Center mit der Johannes Gutenberg-Universität Mainz

The blood protein fibrinogen (fg) plays an important role in the coagulation cascade and the immune response to injury. However, these functions may also be initiated by fg aggregation on extraneous bodies such as, e.g. medical implants. In our previous work, atomistic molecular dynamics simulations have been used to characterize fg flexibility in solution [1]. Due to the size of the protein complex, however, atomistic simulation of fg aggregates at surfaces are not possible with current computers. Lower resolution models are required to address these systems. Here we present a new coarse grained (CG) model for fg that systematically incorporates data from all atom molecular dynamics simulations. This model reduces the resolution from nearly 31000 interacting particles in an all atom model to 45 CG beads.A heterogeneous elastic network connecting the beads is able to capture the dynamics on large and intermediate scales while the charges assigned to the coarse grained beads elucidate the charge structure of fibrinogen.

[1] Fibrinogen flexibilty and adsorption properties investigated using atomistic molecular dynamics simulations - S. Köhler, F. Schmid and G. Settanni, DPG meeting '14 abstract BP205

BP 14.3 Tue 9:30 P1

**Photoswitchable Dynamics of the Orange Carotenoid Protein (OCP) in Living Cells of Synechocystis sp. PCC6803** — •Franz-Josef Schmitt[1], Evgeny Maksimov[2], Vladimir Z. Paschenko[2] und Thomas Friedrich[1] — [1]Institute of Chemistry, Biophysical Chemistry, TU Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany — [2]Department of Biophysics, Biology Faculty, Lomonosov Moscow State University, 119991 Moscow, Russia

The cyanobacterium Synechocystis sp. PCC6803 contains a photoswitchable protein, the orange carotenoid protein (OCP) which undergoes conformational changes under illumination in the blue spectral regime. After activation by light the OCP binds to the membrane extrinsic phycobilisome (PBS) complexes and leads to non-photochemical quenching (NPQ) of the PBS fluorescence reducing the flow of energy into the photosystems (PS) under high light conditions as protection mechanism. We investigated the energy migration in the PS II by time- and wavelength-resolved fluorescence spectroscopy in a wide temperature range between 4 K and 300 K. The decay associated spectra calculated from the time resolved spectra were simulated by rate equation systems to analyse the pathway of energy migration in the PBS of Synechosystis sp. WT and two mutants that exhibit PBS of reduced complexity. The simulations show that NPQ of PBS by OCP occurs in the PBS core with an apparent time constant of about 100 ps. At kryostatic temperatures the efficient NPQ by OCP is hampered showing that the protein flexibility and/or mobility is essential for NPQ.

BP 14.4 Tue 9:30 P1

**Glass-like transition in a dry protein: evidence from neutron scattering study** — •A.V. Frontzek[1], S.V. Strokov[1], J.P. Embs[2], and S.G. Lushnikov[1] — [1]Ioffe Physical Technical Institute, St.Petersburg, Russia — [2]Paul Scherrer Institut, Switzerland

The interest in proteins dynamics is stimulated by its close relation to the biological activity and mechanisms of functioning. Generally, biopolymers demonstrate the dynamical features typical for disordered systems. Such phenomena as the dynamical transition and a glass transition in hydrated proteins have been revealed and intensively investigated in past decades. However, it still remained an open question if a glass transition occurs in dry biopolymers. Our purpose was to study the vibrational and relaxational dynamics of two dry model proteins, bovine serum albumin and alpha-lactalbumin form bovine milk, at temperatures at which a glass or dynamical transition can occur (200-340K). The lyophilized powders of both proteins have been used for neutron scattering experiments at a neutron time-of-flight spectrometer FOCUS (SINQ). As a result, the inelastic incoherent dynamic structure factors and the density of states have been obtained and analyzed in broad temperature range. Anomalous temperature behaviour has been revealed for relaxational and low-frequency vibrational dynamics of investigated proteins in the vicinity of 250 K. The mean square atomic displacement has been demonstrated to exhibit a change in the slope of temperature dependence near the same temperature. The presented results point out that the glass-like transition occurs also in dry protein.

BP 14.5 Tue 9:30 P1

**Computational clarification of structural detail in polyglutamine aggregation** — •Markus Miettinen — FU Berlin, Berlin, Germany

In many neurodegenerative diseases, such as Altzheimer's, Parkinson's and Huntington's, cell death is associated with protein misfolding and aggregation. We studied the events leading to aggregation of polyglutamine, the aggregation-prone part of the disease-associated protein in Huntington's and eight other diseases. It is believed that some structures in the initial stages of aggregation are highly toxic, but due to their fleeting nature it has been difficult to obtain direct experimental data on them. Combining a criterion based on available experimental data with extensive molecular simulations, we demonstrated the infeasibility of several structures, and could single out one motif as crucial for the initiation of aggregation. We suggest a pathway that could provide new insight into developing strategies to alleviate toxicity.

BP 14.6 Tue 9:30 P1

**Local averaging of single particle cryo-electrom microscopy data** — •Amudha Kumari Duraisamy[1] and Gunnar F. Schroeder[1,2] — [1]Institute of Complex Systems, Forschungszentrum Juelich, 52425 Juelich, Germany — [2]Physics Department, Henrich-Heine-Universitaet, Duesseldorf, Germany

Single particle cryo-EM is a powerful technique to study the structure of biomolecular assemblies that are often large, flexible and conformational heterogeneous. Most of the density maps obtained from cryo-EM experiments are limited in resolution by this conformational heterogeneity. Improving the resolution of the density maps, thus, requires to account for the structural heterogeneity. In principle, the resolution can be reached to the atomic level, if the images of the structures are aligned accurately [1]. In the biological macromolecules, the conformational motions leads to global structural changes, however there are often rather rigid domains. Those rigid domains could be used to align and average the density to reach higher resolution. This is analogous to NCS averaging used to improve the phase information in the field of X-Ray crystallography [2]. An algorithm is presented to average rigid domains and to improve the resolution of cryo-EM density maps.

References: [1] Henderson. R, Q. Rev. Biophys. 28 171-193 (1995). [2] Kleywegt. G and Read. R, Structure 5 1557-1569 (1997).

BP 14.7 Tue 9:30 P1

**Ultrafast Side Chain Dynamics of Peptides at the Air-Water Interface** — •Michael Donovan, Mischa Bonn, and Tobias Weidner — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Proteins possess fluctuating structural forms, and very little is known about their dynamics at the interface between two bulk phases. Few tools are available to study dynamics at interfaces. For this reason we chose to use a time resolved variant of the intrinsically surface specific vibrational spectroscopy Infrared-Visible Sum Frequency Generation. The rotational dynamics of side chains are followed by orthogonal infrared pump pulses and SFG probe pulses. The IR pulse bleaches specific side chain orientations. The recovery of the steady state signal, related to side chain rotational motion, is monitored in real time. Specifically, model amphiphilic LK peptides which consist of alternating leucines and lysines have been probed at the air water interface. Further experiments which utilize isotopically labeled side chains along the peptide backbone will allow us to resolve the rotational dynamics in further detail.

BP 14.8 Tue 9:30 P1

**Thermodynamic characterization of protein folding using Monte Carlo methods** — •Nana Heilmann, Moritz Wolf, Julia Setzler, and Wolfgang Wenzel — INT, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

The study of protein folding has been a difficult challenge in molecular biology and simulation science. Up-to-date research showed reproducible folding of small protein using molecular dynamics simulations. These results can be only achieved by using time-consuming, specialized supercomputers [1]. In contrast to molecular dynamics simulations, Monte Carlo based simulations are not constrained solving Newton's equation of motion and therefore protein folding simulations can be compute on conventional computer architectures. In this study, we show reproducible all-atom folding transition of the villin headpiece 1VII, which was simulated by using SIMONA[2], a Monte Carlo based simulation package for nanoscale simulations including a variant of the Amber99SB*-ILDN[3]. The results of these simulations demonstrate that Monte Carlo simulation techniques are generally applicable to the investigation of large-scale conformational changes of protein on conventional computer architectures. The thermodynamic characterization of simulated proteins can be compared with the experimental results while the computing time for observing folding/refolding events can be significantly reduced in comparison with molecular dynamics simulations. [1] Shaw et al. Science 330 (2010). [2] Wolf et al. J Comput Chem (2012). [3] Lindorff-Larsen et al. Science 334 (2011).

BP 14.9 Tue 9:30 P1

**Dynamics of the family of protein disulfide isomerases.** — •Jack Heal[1], Stephen Well[2], Emilio Jimenez-Roldan[1], Rudolf Römer[1], and Robert Freedman[1] — [1]University of Warwick, Coventry, England, CV4 7AL — [2]University of Bath, Bath, England, BA2 7AY

Protein disulfide isomerase (PDI) is a multifunctional enzyme that facilitates protein folding by disulfide bond formation and isomerisation. PDI consists of four thioredoxin-fold domains; the other members of the PDI family are formed of a small number of homologous domains. The function of some of the members is not well understood or characterised. Recently, the structure of human PDI has been determined for the first time through X-ray crystallography. These data add to a small number of previous X-ray crystal structures of the PDI family members that are available in the protein data bank. With these structures as input, we use rapid computational methods to simulate their overall flexibility and dynamics. We study quantitatively the relative domain orientations as well as the distance between functional sites, extending our recent study on yeast PDI. From this information, we construct a map of these motions and discuss the protein dynamics of the PDI family in the context of structure, sequence and function. We aim to use these techniques along with the experimental data available to fully characterise the whole family and use structure-derived information to inform discussion of protein function in general.

BP 14.10 Tue 9:30 P1

**Influence of surface and subsurface properties on the structure and activity of adsorbed bactericidal proteins** — •Christian Spengler[1], Christian Kreis[1], Stéphane Mesnage[2], Hendrik Hähl[1], and Simon Foster[2] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken — [2]University of Sheffield, Krebs Institute, Department of Molecular Biology and Biotechnology, Sheffield S10 2TN, United Kingdom

Protein adsorption is the first step in biofilm formation: Protein films serve as a conditioning layer that enables and affects the attachment of bacteria and other organisms. Hence, the understanding and control of protein layers is an important task that is relevant to life sciences and engineering. Previous studies revealed that the structure and density of adsorbed proteins and the adhesion force of bacteria depend on both the surface properties and the subsurface composition of the adsorbent material [1,2]. These findings raise the question whether or not the activity of adsorbed proteins is also influenced by the properties of the underlying material. In this study, we investigate how the activity – the bactericidal effect – of adsorbed lysozyme and lysostaphin is affected by surface properties. The activity is thereby characterized by measuring the turbidity of a very sensitive protein assay containing purified peptidoglycan.

[1] Hähl et al., Langmuir **28** (2012) 7747-7756
[2] Loskill et al., Langmuir **28** (2012) 7242-7248

BP 14.11 Tue 9:30 P1

**Resolving conformational switching of AAA+ protease FtsH in real time using single-molecule FRET** — •Martine Ruer, Philip Gröger, Nadine Bölke, and Michael Schlierf — B CUBE - Center for Molecular Bioengineering, TU Dresden, 01307 Dresden

FtsH is a highly conserved, homo-hexameric AAA+ protease embedded in the bacterial membrane, where it recognizes, unfolds, translocates and degrades protein substrates to be degraded. Previous crystal structure data of Thermotoga maritima FtsH in an ADP and an ATP-bound state show an ATPase and a protease domain linked by a flexible hinge, facilitating a large conformational change event upon ADP/ATP binding. Based on these structural data, a model was presented where the unfolding and proteolytic mechanism are tightly coupled. However, in protease assays FtsH shows an ATP independent mechanism. How is the chemical energy converted into mechanical work for protein unfolding and translocation? We are using single-molecule Förster Resonance Energy Transfer (smFRET) experiments to resolve the conformational changes of FtsH upon ATPase and protease activities. Therefore, we have developed an in vitro assay with vesicle encapsulated, self-assembled FtsH hexamers in absence or presence of degradation substrates. In absence of a degradation substrate, the labeled FtsH protease shows 2 or 3 conformational states and the

conformational switching is strongly dependent on the ATP concentration. In further experiments, we study the ATP dependent kinetics of the different conformational states in dependence of various protein substrates.

BP 14.12 Tue 9:30 P1

**Friction between hydrogen bonding peptides** — •Julian Kappler and Roland Netz — Institut für Theoretische Physik, Freie Universität Berlin, 14195 Berlin, Germany

Understanding how friction arises from microscopic interactions is not only important for improving the efficiency of machines, but also for a detailed understanding of biologically relevant systems. We use all-atom MD simulations to study the friction between pairs of various kinds of stretched homo-polypeptide strands in water: While fixing one peptide strand, we pull the second one with constant velocity along its axis, thereby simulating a non-equilibrium steady state. In our analysis we particularly focus on the roles of i) the hydrogen bonds (and cooperative effects thereof) between the pairs and ii) the interaction of the pulled peptide with the surrounding water.

BP 14.13 Tue 9:30 P1

**Fluorescence Lifetime Spectroscopy of Free and Enzyme-bound NADH** — •André Weber[1,2], Werner Zuschratter[2], and Marcus Hauser[1] — [1]Abteilung Biophysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Leibniz-Institut für Neurobiologie, Speziallabor Elektronen- und Laserscanmikroskopie, Brenneckestr. 6, 39118 Magdeburg, Germany

NADH plays a keyrole in energy metabolism of cells and its autofluorescence acts as an indicator for metabolic states of a cell. Certain enzymes, so called dehydrogenases, build up products from substrates by a transport of hydrogen to $NAD^+$.

The fluorescence lifetimes of NADH allow for differentiation between free diffusing and protein-bound NADH and are sensitive to pH, temperature and ionic strength.

We investigate the concentration dependent reaction dynamics of dehydrogenases while binding to NADH and substrates in solution with various pH values via fluorescence lifetime spectroscopy of NADH fluorescence. Through time and space correlated single photon counting we analyse the wavelength dependence of the fluorescence decays.

BP 14.14 Tue 9:30 P1

**Adsorption kinetics and structure of hydrophobins at interfaces** — •Jonas Raphael Heppe[1], Hendrik Hähl[1], Philipp Hudalla[2], Ludger Santen[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken — [2]Saarland University, Theoretical Physics, D-66041 Saarbrücken

Protein adsorption to interfaces is a common, but complex process with many applications. Besides the attachment to the solid/liquid interface, the adsorption to the interface between water and other liquids or air is of major technological interest. Amphiphilic proteins stabilize this interface and hence serve as emulsifying or foaming agent. To control the processes, a deeper understanding of the competitive processes and interactions leading to the final adsorbate is necessary.

Hydrophobins (HFB) are a class of proteins that may serve as ideal model candidates. Produced by filamentous fungi, they are conformationally stable, highly surface active, and form ordered monolayers at the water surface [1]. We studied the adsorption of HFB wild types and specifically designed mutants featuring different geometry or charge.

To access the adsorption kinetics, we used ellipsometry to record *in situ* the adsorbed amount at the air/water interface and on solid substrates varying the conditions of surface and solution. Moreover, we analyzed the resulting structure of the adsorbates by applying XRR.

Our results reveal differences in the adsorption kinetics depending on the electrical and steric properties of the proteins as well as the ambient parameters. The experiments are accompanied by theoretical modeling. [1] S. Varjonen et al., Soft Matter 7 (2011) 2402

BP 14.15 Tue 9:30 P1

**Sorting cryo-EM images into classes of similar molecular conformations** — •Michaela Spiegel[1] and Gunnar Schröder[1,2] — [1]ICS-6 Computational Structural Biology, Forschungszentrum Jülich, Germany — [2]Physics Department, Heinrich-Heine-Universität Düsseldorf, Germany

The resolutions of density maps which are reconstructed from single-particle cryoelectron microscopy (cryo-EM) images are often limited by the conformational heterogeneity of the biological macromolecules. To increase the resolution, the images have to be sorted into groups of similar conformations. The common approaches of sorting images typically compare densities (either in 2D or 3D). However, a large difference in conformation does not necessarily lead to a large difference in density. We are developing a new sorting method that is based on comparing conformations. For this we are using a bootstrapping approach and refine pseudo-atomic models against an ensemble of bootstrapped density maps. These models capture the conformational variance and can be used for sorting the images. This procedure also reveals the conformational heterogeneity and is able to determine global conformational motions of large macromolecular structures and assemblies.

BP 14.16 Tue 9:30 P1

**Optical activity of chiral molecules and its analog on a macroscopic scale** — •Carina Häusler, Hendrik Bettermann, and Mathias Getzlaff — Institute of Applied Physics, University of Duesseldorf

Optical activity of chiral molecules like proteins in nm-range is barely understood due to its complex behavior but it may provide a new non-invasive blood sugar measurement for diabetes patients. It is the goal to develop an experimental setup for students which demonstrates the analogy between nm-sized molecules and cm-sized helices. The latter creates a simple approach for this optical phenomenon without the use of chemical processes. The measurement setup consists of a source for linearly polarized light and an analyzer to determine the degree of rotation of the electric field vector after transmission. Biologically relevant substances like glucose, fructose, and camphor are studied by visible light whereas chiral copper helices with dimensions in the cm-regime are studied by radiation in the GHz range. The specific amount of rotation is identified in both scales in the same way which is not known for molecules in cm-range yet. The data also shows a direct comparison of enantiomeric excess in both scales. Furthermore, the experiment demonstrates the mutarotation of glucose and a wavelength depending amount of rotation in the nm-range.

BP 14.17 Tue 9:30 P1

**Competing paradigms of protein dimerization tested by solution SAXS** — •Stefano Da Vela[1], Fajun Zhang[1], Vasyl Haramus[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik - Universität Tübingen, Tübingen, Germany — [2]Helmholtz-Zentrum Geesthacht: Zentrum für Material- und Küstenforschung GmbH, Geesthacht, Germany

Small Angle X-Ray Scattering (SAXS) is a versatile and popular tool for the characterization of proteins in solution. In this contribution we use the capabilities of SAXS, Size Exclusion Chromatography and complementary Dynamic and Static Light Scattering techniques to investigate the association and interactions of Ovalbumin, Bovine Serum Albumin and Immunoglobulin G. These proteins are chosen as different paradigms for protein dimerization. We explore the architecture, the effective dimensions and hydration state of monomers and dimers in relation to the solution parameters. Furthermore, we assess the influence of the dimerization on the quality of the information which can be obtained from SAXS data and the effect of the resulting shape polidispersity on the overall protein-protein interaction parameters. A deeper insight into the dimerization process can serve as basis for further studies on its influence on protein phase behaviour and on protein dynamics in concentrated solutions.

BP 14.18 Tue 9:30 P1

**Diffusion of peripheral membrane proteins on intracellular membranes** — •Julia Hoffmann and Matthias Weiss — University of Bayreuth, Bayreuth, Germany

Biological processes, such as secretion and signaling in living cells, depend crucially on the diffusive properties of the involved proteins. The mobility of proteins is determined by their environment as well as by their size and thus by their ability to form oligomers. Fluorescence correlation spectroscopy (FCS) is a common and sensitive technique to characterize the diffusive processes of proteins *in vivo*. We used this technique to investigate different peripheral membrane protein types, including membrane anchored Ras proteins and proteins involved in the cell's secretion machinery. FCS measurements of membrane anchored N-Ras mutants for example, show predominantly anomalous diffusion on intracellular membranes. In contrast, FCS experiments on Sec16, a regulating protein of the COPII machinery in the early secretory pathway, show slowed diffusion on membranes of endoplasmic reticulum due to oligomerization. These insights into the diffusion and

oligomerization of peripheral membrane proteins yield valuable information about physico-chemical mechanisms that support, for example, secretion events.

BP 14.19 Tue 9:30 P1

**Using Molecular Dynamics Simulation to Obtain Protein Pigment Interaction in Photosynthetic Pigment Protein Complex** — •Xiaoqing Wang, Sebastian Wuester, and Alexander Eisfeld — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany

Protein pigment interaction is very important on the electronic excitation energy transfer and spectral properties in photosynthetic pigment-protein complex. However, investigating the interaction from full quantum mechanics is out of reach because of the large number of protein atoms and the complicated arrangement of pigment molecules. In our work classical molecular dynamics simulation is used to simulate the dynamics of pigment-protein complex on the ground state. The local excitation energies and transition dipole-dipole couplings which used to build the Hamiltonian of the complex are extracted from the structure information of the molecular dynamics trajectories. In order to investigate the protein pigment coupling interaction the spectral density is calculated. Since the excitation energy is calculated by electrostatic energy shift caused by the atomic charge of protein environment we can investigate the influence of various parts of the protein. The method also might help to understand the effects on the molecular dynamics parameters.

## BP 15: Posters: Systems biology and neurosciences

Time: Tuesday 9:30–12:30 Location: P1

BP 15.1 Tue 9:30 P1

**Optimization of collective enzyme activity via spatial localization** — •Filipe Tostevin, Alexander Buchner, Florian Hinzpeter, and Ulrich Gerland — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität, Munich, Germany

The spatial organization of enzymes often plays a crucial role in the functionality and efficiency of enzymatic pathways. To understand the design and operation of enzymatic pathways, it is therefore important to analyze how the relative arrangement of enzymes affects pathway function. Here we investigate the effect of enzyme arrangements on the flux of a minimal two-enzyme pathway within a reaction-diffusion model. We consider different reaction kinetics, spatial dimensions, and loss mechanisms for intermediate substrate molecules. Our systematic analysis of the different regimes of this model reveals both universal features and distinct characteristics in the phenomenology of these different systems. In particular, the distribution of the second pathway enzyme that maximizes the reaction flux undergoes a generic transition from co-localization with the first enzyme when the catalytic efficiency of the second enzyme is low, to an extended profile when the catalytic efficiency is high. However, the critical transition point and the shape of the extended optimal profile is significantly affected by specific features of the model. We explain the behavior of these different systems in terms of the underlying stochastic reaction and diffusion processes of single substrate molecules.

BP 15.2 Tue 9:30 P1

**Reaction kinetics modeling of RNAi: gene silencing dependence of target mRNA concentration** — •Simon Dornseifer[1], Georg Szakiel[1], Tobias Restle[1], and Jens Christian Claussen[2] — [1]IMM, Universität zu Lübeck, Germany — [2]Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

The discovery of post-transcriptional gene silencing via RNA interference (RNAi) gave rise to the development of new nucleic acid-based tools. Mechanistic key details of RNAi in human need to be deciphered yet. Here we propose and investigate a computational model of siRNA-mediated RNAi in human cells in order to link precise quantitative kinetic data and new molecular findings with a quantitative and time-resolved understanding of RNAi in the human system. Cell culture experiments suggest that the RNAi machinery adopts to large variations in target mRNA level, independent of siRNA or Ago2 concentrations. These experimental findings are not explained by the common literature view of RNAi, here termed dissociative mechanism, where the departing ligand (here, cleaved RNA fragments) leaves the complex in a slow step. Here, we investigate an alternatice, associative mechanism of target strand recognition by Argonaute 2 (Ago2). The associative model is compatible with the high multiple turnover rates of RNAi-based gene silencing in living cells and accounts for target mRNA concentration-dependent acceleration of the RNAi machinery. The associative model proposed here suggests that the efficacy of an siRNA or miRNA depends on the expression level of its target RNA such that high target levels allow better regulation via RNAi.

BP 15.3 Tue 9:30 P1

**Biophysics of mechanosensation in the fruit fly Drosophila** — •Achintya Prahlad[1], Christoph F. Schmidt[1], and Martin Göpfert[2] — [1]Third Institute of Physics - Biophysics, Georg-August University, Göttingen — [2]Schwann-Schleiden Research Centre, Faculty of Biology, Georg-August University, Göttingen

The fruit fly Drosophila uses mechanosensation for several purposes. Much of the literature is on a class of organs called chordotonal organs, such as the auditory organ attached to the antennae, and the larval pentamere organ (or lch5). The sensory neurons at the core of these organs have one dendrite, which terminates in a cilium. The cilia are said to be the main transducers. The lch5 organ aids in locomotion by giving feedback to the central nervous system.

Molecular and anatomical aspects of these organs have been studied. Also, there have recently been some exciting discoveries about the mechanics of the external sound receiver. However, an understanding of the internal transduction mechanics and the manner in which membrane channels are activated upon deflection of the cilium is still elusive. Since the inner parts of the antenna organ of an adult fly are difficult to access in a functional state and since flies don't survive under water, we are using a preparation of larvae under buffer solution that allows us to directly access the sensory neurons of the lch5. Our approach is to then use optically-trapped beads to give stimuli to the cilia, and couple that with calcium imaging in the cells.

# BP 16: Poster - Glasses / Stat. Phys. Bio. / Networks (joint DY/BP/CPP/SOE)

In this poster session there are contribution from
- Focus Session: Slow Dynamics in Glasses and Granular Matter
- Focus Session: Feedback Control - Soft and Hard Matter
- Glasses
- Statistical Physics in Biological Systems
- Networks - Statistics and Dynamics

Time: Tuesday 9:30–12:30 Location: P1

BP 16.1 Tue 9:30 P1

**Investigation of the behavior of binary mixtures upon variation of the dynamic asymmetry** — •Marie-Luise Braatz[1], Sebastian Schramm[1], Thomas Blochowicz[1], Bernd Stühn[1], and Bernhard Frick[2] — [1]Experimental Condensed Matter Physics, TU Darmstadt, Germany — [2]Institut Laue Langevin, Grenoble, France

We study dynamically asymmetric binary mixtures comprised of polystyrene and the small molecule methyl tetrahydrofuran (MTHF). The blends are fully miscible on supercooling but still exhibit two glass transition temperatures. Between these two temperatures MTHF relaxes in a matrix of polystyrene, showing the signature of geometrical confinement on the nanoscale in its dynamic properties. Among the interesting characteristics observed, is a transition from fragile to strong behavior of the time constants and in some cases features of a type-A glass transition are found.

We study the behavior of these characteristics upon varying the molecular weight and thereby the dynamic asymmetry of the mixture as well as the concentration of the small molecules. Dielectric spectroscopy, depolarized dynamic light scattering and quasielastic neutron scattering are combined to cover a dynamic range of 1ps to 1000s.

Our results are compared to theoretical predictions that expect fragile-strong transitions and type-A glass transitions to be most pronounced at low concentrations of the small molecules and large dynamic asymmetries.

BP 16.2 Tue 9:30 P1

**Mesoscale modeling of aeolian sand transport** — •Anne Meiwald, Marc Lämmel, and Klaus Kroy — Institut für Theoretische Physik, Leipzig, Germany

Aeolian transport of sand is one of the most important geological processes on Earth and other rocky planets, creating a wide range of self-organised dynamic structures, like ripples or sand dunes. To make the complex grain physics more amenable to analytical studies, it was proposed to coarse-grain the ensemble of grain trajectories by two types representing low-energetic reptating grains and high-energetic saltating grains [1]. We recently showed that our analytically tractable and numerically efficient continuum model reliably reproduces sand flux measurements obtained in various wind tunnel experiments [2].

Here, we scrutiny the potential of our approach to predict important grain-scale properties and find remarkable agreement with various experimental data. We also speculate about the reason for the success of the coarse-grained description, even in comparison to more detailed numerical models, despite its allegedly unfaithful representation of some of the grain-scale details [3]. Finally we conclude that the two-species continuum approach provides an appropriate starting point for analytical and efficient numerical modelling of seemingly complex aeolian saltation process and the structures it creates.

[1] Bagnold, *The physics of blown sand and desert dunes.* Dover Publ. (2005).
[2] Lämmel, Rings, and Kroy, New J. Phys. 14, 093037 (2012).
[3] Kok, and Renno, J. Geophys. Res. 114, D17204 (2009).

BP 16.3 Tue 9:30 P1

**Railway buckling safety: From Theory to application** — •János Török[1], László Halma[2], and István Fejér[2] — [1]Department of Theoretical Physics,Budapest University of Technology and Economics, H-1111 Budapest, Hungary — [2]Vasútépítök Kft, H-9023 Györ, Csaba utca 9

Using numerical simulation and mesoscopic theory we show that in granular materials the effective friction coefficient at walls depends heavily on the wall roughness. We show that it can be used in real application. In continuous welded rails the standard railbed in small radius curves are not able to resist the radial load arising from temperature and train movement. Today many different and expensive methods are used to tackle this problem. We show that by making the bottom of the sleepers rough we can increase the buckling safety of the track.

BP 16.4 Tue 9:30 P1

**Continuum Mechanics Simulations of Nonlinear Deformation of Viscoplastic Solids** — •Heliana Cardenas[1] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — [2]Zukunftskolleg und Fachbereich Physik, Universität Konstanz, Konstanz, Germany

When amorphous solids are formed by solidification of dense liquids slow intrinsic relaxation plays a determining role on describing their behavior. Systems like this can be perturbed by external mechanical fields driving it to a non-equilibrium regime following then non-linear deformation laws. The mode-coupling theory of the glass transition (MCT) has been extended to describe the interplay between strong external forces and slow relaxation.

A non-linear extension of the Maxwell model of viscoelastic fluids is proposed. This model takes into account the relaxation time dependence on the shear rate and thereby mimics microscopic processes identified by MCT. Combining this constitutive equation with the Navier-Stokes equations we can describe the evolution of macroscopic flows. Attention will be focused on shear-thinning fluids where the fluid's viscosity decreases with an increasing rate of shear stress.

To solve non-linear integro-differential equations finite element modeling (FEM) is used through a computational fluid dynamics tool. The effect of different relaxation times for a pressure driven flow is studied by analyzing velocity profiles, among other measurable quantities.

BP 16.5 Tue 9:30 P1

**Mechanical Properties of Sheared Wet Granular Piles** — •Somnath Karmakar[1], Marc Schaber[1], Anna-Lena Hippler[1], Martin Brinkmann[2], Mario Scheel[3], Marco Di Michiel[3], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]MPI for Dynamics and Self-Organization, Göttingen, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France

Adding small amount of wetting fluid to dry granulates typically leads to the granular stiffness which arises due the formation of minute liquid contacts between individual granules by the virtue of capillary forces. We experimentally study the mechanical properties of wet granulates, composed of monodisperse spherical glass or basalt beads. The glass microspheres are almost perfectly wetted by water whereas the basalt microspheres have a rather large contact angles with water. The different wettability causes a difference in the shape and volume distribution of the appeared liquid morphologies. We have investigated the shear strength, measured under cyclic shear deformation for various system parameters like liquid content, shear rate and absolute pressure. At large absolute pressures, the associated energy dissipation of a sheared wet granulate is considerably smaller than that of a completely dry bead assembly; where the wetting fluid might act as a 'liquid lubricant' by lowering the wet bead pile's shear stiffness. With time resolved X-ray microtomography, we could shed some light on the underlying microscopic mechanisms of the sheared wet granulates.

BP 16.6 Tue 9:30 P1

**Stability of Barchan Dune Fields** — •Sven Auschra, Marc Lämmel, and Klaus Kroy — Institut für theoretische Physik, Leipzig, Germany

Crescent-shaped barchan dunes are among the most impressive structures observed in arid regions on Earth and Mars. Although they are isolated from nearby dunes by bedrock, models suggests that truly isolated barchans would be unstable with respect to their mass balance

[1]. This suggests that some sort of interactions between the dunes in a dune field give rise to some size stabilization resulting in the empirically observed uniform size distribution along the dune field [2, 3].

To uncover the underlying mechanism, we perform a mass stability analysis for a pair of consecutive dunes in a barchan field. Sand supplied from the horn of the windward dune to its downwind neighbor initiates a complex response of its shape and mass. Based on a dimensionally reduced description justified by a closeby shape attractor, a one-dimensional fixed-point equation for the mass balance of the downwind dune is derived and analyzed for stable solutions.

[1] Fischer, Cates and Kroy, Phys. Rev. E 77, 031302, 2008.
[2] Hersen, Andersen, Elbelrhiti, Andreotti, Claudin and Douady, Phys. Rev. E 69, 011304, 2004.
[3] Duran, Schwämmle, Lind and Herrmann, Nonlin. Processes Geophys. 69, 455-467, 2001.

BP 16.7 Tue 9:30 P1

**Ab-inito MD parameter estimation for Na diffusion in glasses** — •Lars Winterfeld and Erich Runge — Institut für Physik, TU Ilmenau, 98693 Ilmenau

Molecular dynamics (MD) simulation provide a scalable method for the investigation of disordered systems like glasses. However, there is no generally accepted method for the determination of the MD model parameters. We present a new first-principle approach that allow us to self-consistently obtain such parameters by sampling an ensemble of representative configurations. We use MD to create these configurations and run ab-initio DFT calculations as basis for the subsequent fitting procedure. Results of this approach are compared for $(Na_2O)_x - SiO_2$ glass systems with those from the literature.

BP 16.8 Tue 9:30 P1

**Non-universal dielectric properties of glasses at very low temperatures** — •Annina Luck, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, INF227, D-69120 Heidelberg

The universal behaviour of amorphous solids at low temperatures, governed by two level tunneling systems, has long been a generally accepted fact. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling sytems can cause specific material-dependent effects in magnetic fields.

To study the possible influence of nuclear electric quadrupoles connected with atomic tunneling systems on the low frequency dielectric properties of glasses down to a temperature of 10 mK, we measured the multicomponent glass N-KZFS11, which contains 25 mass percent of tantalum oxide and a glass containing a similar amount of holmium oxide. As $^{181}$Ta and $^{165}$Ho carry very large nuclear electric quadrupole moments,these glasses seem to be ideal candidates to determine the influence of nuclear electric quadrupole moments on the physical properties of glasses at low temperatures.

Our measurements not only show a non-universal dieletric behaviour in the two glasses, but also differ significantly from various predictions of the standard tunneling model. We discuss these new findings in the framework of the tunneling model.

BP 16.9 Tue 9:30 P1

**Understanding the properties of two dimensional silica systems** — •ProjeshKumar Roy[1] and Andreas Heuer[2] — [1]Graduate school of chemistry, University of Muenster — [2]Institute of physical chemistry, University of Muenster

Recently, STEM and SPM studies were performed by Lichtenstein et al, [1] in a virtually two dimensional silica bilayer; which was grown by depositing vaporised Si atoms on a [Ru(0001)] metal surface in an oxygen atmosphere. Silica bilayers were generated, which could be either amorphous or crystalline, depending on the preparation conditions. Under specific conditions even both states could be generated in the same layer, including a short-range transition between them. Remarkably, even in the amorphous case both layers were virtually identical. Due to the atomic resolution the ring statistics in the amorphous structure could be characterized in detail.

We report about computer simulations which have the aim to reproduce the properties of two-dimensional silica layers and, consequently, obtain an improved microscopic understanding of this system. In particular we want to learn, under which conditions crystalline and amorphous structures can be generated, respectively. For this purpose, an appropriate silica potential has to be developed which can be used in the two-dimensional case and is able to generate the observed structural features.

[1] Lichtenstein L; Heyde M; Freund H.J.; J. Phys. Chem. C 2012, 116, 20426.

BP 16.10 Tue 9:30 P1

**Understanding the energy landscape of a simple water model** — •Katharina Ferling and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster

Liquid water plays an important role not only in our everyday life but also in simulations and experiments where it serves as a solute with many applications. The understanding of the water behaviour, including its anomalies, can play an important role in improving the description of water. Here the emphasis lies on the property of building H-bonds which is believed to be one major factor for many anomalies such as the density change or the liquid-liquid phase transition at low temperatures. For the present investigation a simple model has been chosen which focuses on the distinction between a close-packed and an open structure. The one dimensional model - which was first introduced by Ben-Naim [1,2] - has now been extended with additional long range interactions in the underlying potential to get rid of the mean-field character of that model. First, simulations are performed in the NPT-ensemble with the aim to show water-like behaviour such as a high-density liquid and low-density liquid (HDL-LDL) transition. Second, from simulations in the NVT-ensemble for different volumes (lengths, resp.) a closer understanding of the possible anomalies can be reached, related to properties of the underlying potential energy landscape.

[1] Arieh Ben-Naim, J. Chem. Phys. 128, 024505 (2008)
[2] Lotta Heckmann and Barbara Drossel, J. Chem. Phys. 137, 064503 (2012)

BP 16.11 Tue 9:30 P1

**Compressed exponential decays in correlation experiments: The influence of temperature gradients and convection** — •Jan Gabriel, Thomas Blochowicz, and Bernd Stühn — Institut für Festkörperphysik, Darmstadt

In a wide range of correlation experiments using laser light or partially coherent X-rays so called compressed exponential correlation functions were reported [1] i.e. decays $c(\tau) \propto \exp(-(t/\tau)^\beta)$ with $\beta > 1$. The source of this phenomenon is still a point of discussion. For example for colloidal particles in supercooled liquid [2] it is claimed that near $T_g$ hyperdiffusive behavior appears, which leads to compressed correlation functions.
We performed multispeckle-dynamic light scattering experiments in a temperature range from 230 K to 300 K with a sCMOS camera in a system of Polystyrene spheres in supercooled propanediol. At low temperatures compressed exponential decays are observed. At the same time, however, the speckle pattern shows indication for convection in the sample due to a slight temperature gradient, across the sample cuvette mounted on a cold finger cryostat. These effects increase with decreasing temperature and after a temperature jump and can be corrected for by assuming convective flow at constant velocity. Such corrections reduce or remove compressed exponential behavior.

[1] A Madsen, R. L. Leheny, H. Guo, M Sprun and Orsolyal, New J. Phys., **12**, 055001 (2010)
[2] C. Caronna, Y. Chushkin, A. Madasen and A. Cupane, Phys. Rev. Lett., **100**, 055702 (2008)

BP 16.12 Tue 9:30 P1

**Temperature and pressure dependence of the supramolecular structure of 2-ehyl-1-hexanol and 4-methyl-3-heptanol** — •Thomas Büning[1], Christian Sternemann[1], Catalin Gainaru[2], Michael Paulus[1], Kolja Mende[1], Florian Wirkert[1], Irena Kiesel[1], Johannes Möller[1], Julia Nase[1], Stefan Bauer[2], Roland Böhmer[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund — [2]Fakultät Physik/E3, Technische Universität Dortmund, D-44221 Dortmund

Hydrogen bonds are essential for structure and dynamics of e.g. alcohols, aqueous solutions and water. Due to their low tendency to crystallization and large variability in molecular configuration, monohydroxy alcohols are a typical system that is studied to learn about the impact of hydrogen-bonding on molecular liquids. Because of the hydrogen bonds alcohols form supramolecular structures in the liquid phase. Here, the molecular arrangements of monohydroxy alcohols such as 2-ethyl-1-hexanol (2E1H) and 4-methyl-3-heptanol (4M3H) strongly depend on the position of the OH group within the molecule.

Based on dielectric spectroscopy molecular arrangements in chain-like (2E1H) and, ring-like (4M3H) structures have been proposed. We present an x-ray diffraction study of 2E1H and 4M3H, providing new information regarding the supramolecular structure in pressure up to 4 kbar and temperature down to -110 °C.

BP 16.13 Tue 9:30 P1

**Molecular Order and Dynamics of Nanometric Thin Layers of Poly(styrene-b-1,4-isoprene) Diblock Copolymers** — •Wycliffe K. Kipnusu[1], Mahdy M. Elmahdy[1], Martin Tress[1], Emmanuel U. Mapesa[1], Detlef-M. Smilgies[2], Jianqi Zhang[3], Christine M. Papadakis[3], and Friedrich Kremer[1] — [1]Institute of Experimental physics I, Linnstr.5, 04103, Leipzig — [2]CHESS, Wilson Laboratory, Cornell University, Ithaca, NY 14853, USA — [3]Technische Universität München, Physik-Department, James-Franck-Straße 1, 85748 Garching, Germany

Order and dynamics of poly(styrene-block-1,4-isoprene), P(S-b-I) diblock copolymers in nanometer thin layers with different isoprene volume fraction (fPI) and identical molecular weight of the styrene blocks are studied by a combination of Grazing-Incidence Small-Angle X-ray Scattering (GISAXS), Atomic Force Microscopy (AFM) and Broadband Dielectric Spectroscopy (BDS). GISAXS and AFM reveal randomly oriented lamellar structures in the films and a parallel orientation at the top surface, respectively. Using BDS, three well separated relaxation processes are detected, (i) and (ii) the dynamic glass transitions (segmental mode) in the styrene and isoprene blocks respectively and (iii) the normal mode relaxation representing fluctuations of the isoprene chain as a whole or parts of it. While the two former do not show any thickness dependence in their spectral positions, the latter becomes faster with decreasing sample thickness. This reflects the difference in the length-scale on which the molecular fluctuations take place.

BP 16.14 Tue 9:30 P1

**Intra- and inter-molecular dynamics in the course of vitrification in organic glasses** — Ludwig Popp, Benjamin Suttner, •Wilhelm Kossak, and Friedrich Kremer — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik I, Linnestr. 5, 04103 Leipzig

FTIR and BDS are utilized to study the vitrification of various well known glass formers in a wide temperature range around the calorimetric glass transition temperature, Tg. Measurements on Propylene glycol, Glycerol, Salol, Benzophenone, Sorbitol, Xylitol, etc. are compared and the sub-molecluar specificity of the different moieties in their contribution to thermally activated processes including the dynamic glass transition are discussed. By that the necessity of atomistic models of the glass transition beyond coarse grained models is revealed.

BP 16.15 Tue 9:30 P1

**The potential energy landscape of sheared glass-forming systems** — •Markus Blank-Burian and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster, Deutschland

We performed molecular dynamics simulations of small supercooled binary Lennard-Jones mixtures ($65 <= N <= 1040$) under a constant shear rate. The shearing is achieved by applying Lees-Edwards periodic boundary conditions to the system. The potential energy landscape (PEL) is most informative for small systems. However, we also study the influence of finite size effects on our results.

In previous work, it was shown, that the finite size effects in unsheared systems is quite small for thermodynamic observables and for the diffusivity. The dynamics of these systems can be described by a continous time random walk (CTRW) between minima in the potential energy landscape. Our focus now lies on comparing these results with the constantly sheared system.

In the sheared system, we test for finite size effects in general properties like the velocity profile or the shear viscosity. Since the potential energy landscape is now time-dependent, we use affine transformations to understand the temporal evolution of its minima. With this insight, we can use the same continuous time random walk analysis as with the unsheared system.

BP 16.16 Tue 9:30 P1

**Self-stabilizing Learning Rules in Neural Models driven by Objective Functions** — •Rodrigo Echeveste and Claudius Gros — Institut für Theoretische Physik, Johann Wolfgang Goethe Universität, Max-von-Laue-Str. 1, Frankfurt am Main, Germany

In the present work, learning rules for a neuronal model are derived from two objective functions. On the one hand, the neuron's firing bias is adjusted by minimizing the Kullback-Leibler divergence with respect to an exponential output distribution. On the other hand, learning rules for the synaptic weights are obtained by minimizing a Fisher information that measures the sensitivity of the input distribution with respect to the growth of the synaptic weights. In this way, we obtain rules that both account for Hebbian/anti-Hebbian learning and stabilize the system to avoid unbounded weight growth. As a by-product of the derivation, a sliding threshold, similar to the one found in BCM models, is obtained for the learning rules.

As a first application of these rules, the single neuron case is studied in the context of principal component analysis and linear discrimination. We observe that the weight vector aligns to the principal component when the input distribution has a single direction of maximal variance but, when presented with two directions of equal variance, the neuron tends to pick the one with larger negative Kurtosis. In particular, this fact allows the neuron to linearly separate bimodal inputs. Robustness to large input sizes ( 1000 inputs) is also studied, observing that the neuron is still able to find the principal component in a distribution under these conditions.

BP 16.17 Tue 9:30 P1

**Fluctuations of Probe Particles Coupled to Molecular Motors** — •Patrick Pietzonka, Eva Zimmermann, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

In recent years, many experiments have been carried out in which the motion of molecular motors is probed by the observation of attached colloidal particles. For the experimental determination of the torque exerted by the rotational motor $F_1$-ATPase onto such a particle, the application of a fluctuation theorem (FT) for the motion of the colloid has been proposed [1].

However, we show that this approach is generally valid only in the limit of fluctuations on short timescales. The statistics of fluctuations during larger time-intervals depends significantly on the intrinsic behavior of the motor and the linker, which is not observable in experiments. In particular, we investigate a simple model characterized by discrete motor jumps and harmonic coupling between the motor and the colloid [2]. Using the framework of the theory of large deviations, we calculate the distribution of fluctuations of the colloid in the long-time limit. This result implies a refined formulation of the FT-like relation observed in experiments. Moreover, we gain general insight into the properties of stochastic processes with hidden degrees of freedom.

[1] K. Hayashi *et al.*, Phys. Rev. Lett. **104**, 218103 (2010)
[2] E. Zimmermann and U. Seifert, New J. Phys. **14**, 103023 (2012)

BP 16.18 Tue 9:30 P1

**Detention time of a model microswimmer at a plane surface: importance of hydrodynamic interactions** — •Konstantin Schaar, Andreas Zöttl, and Holger Stark — TU Berlin, Institut für Theoretische Physik

We discuss the detention time of a microswimmer at a plane no-slip surface taking into account hydrodynamic interactions of the swimmer with the surface and rotational diffusion. To evaluate the detention time, we use the formalism of the mean first-passage time (MFPT) based on an appropriate Smoluchowski equation. The microswimmer operates in 'squirmer' mode and can easily be tuned between a 'pusher' and a 'puller'. The hydrodynamic interactions with the surface are described by lubrication theory.

We examine the MFPT and also the distribution of first passage times at the surface and achieve good agreement of our results with direct simulations of the squirmer motion close to the no-slip surface using the method of multi-particle collision dynamics. The detention time of the squirmer is clearly determined by hydrodynamic interactions with the surface. They rotate the squirmer away from the surface and therefore reduce the detention time considerably compared to pure rotational diffusion. We find that pushers have a larger detention time than pullers.

BP 16.19 Tue 9:30 P1

**Thermodynamically consistent coarse graining of molecular motor models** — •Eva Zimmermann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

In many single molecule experiments probe particles that are attached to molecular motors are used to infer properties of the motor protein from the analysis of the particle's trajectory and to manipulate the

system by exerting external forces on the motor protein via the probe particle. Theoretical modelling used to describe such assays should comprise at least two coupled degrees of freedom. However, many simple theoretical models applied to molecular motor experiments contain only one degree of freedom representing the motor.

We use a simple illustrative model consisting of two coupled degrees of freedom for the molecular motor and the probe particle to introduce a coarse graining method that allows to eliminate the explicit dynamics of the probe particle in a dynamically and thermodynamically consistent way. We discuss under which conditions the coarse grained model reduces to the widely-used one-particle models.

BP 16.20 Tue 9:30 P1

**Active Turing Systems** — •Silke Bergeler, Florian Thüroff, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Active Turing systems combine the ideas of active matter and reaction diffusion systems showing Turing patterns. We investigate such systems analytically and numerically starting within the framework of Boltzmann-like equations. Adapting previous analytical approaches for active systems we derive a set of hydrodynamic equations and perform a linear stability analysis of the isotropic uniform steady state. We find that the stability against homogeneous perturbations switches from unstable to stable by crossing a threshold noise from below. From direct simulations of the Boltzmann equation we observe that activity changes the form of the Turing patterns and broadens the parameter range for which patterns emerge. Analytical investigations on the stability of the isotropic homogeneous steady state are confirmed by numerical analysis.

BP 16.21 Tue 9:30 P1

**Application of a random fitness landscape model to a long term evolution experiment** — •Mares Barekzai[1], Su-Chan Park[2], and Joachim Krug[3] — [1]Department of Physics, University of Cologne,Germany — [2]Department of Physics, Catholic University of Korea, Bucheon, South Korea — [3]Department of Physics, University of Cologne,Germany

Since 1988, a long term microbial evolution experiment has attracted attention in the scientific community. In the experiment 12 populations of Escherichia coli are propagated in a daily refreshed minimal medium for more than 50000 generations. One of many results are the fitness trajectories of these asexually evolving populations, where fitness is measured as relative growth rate compared to the founding population. Is there a simple model to interpret the observed microbial evolution? We approached this question using the House of Cards Model introduced in 1978 by Kingman, which models the evolution of an asexual population on an uncorrelated random fitness landscape in the limit of infinite genome size. This limit implies that all mutations generate new fitness values drawn from a fixed probability distribution. The model produces fitness trajectories that are in qualitative agreement with the experimental data. Based on an analytical solution for the long term behavior of the model, we estimate the model parameters from the experimental data and provide a biological interpretation of our results.

BP 16.22 Tue 9:30 P1

**Event chain simulations of polymer bundles** — •Tobias Alexander Kampmann and Jan Kierfeld — TU Dortmund, Germany, NRW

We study simulation methods for large polymer systems forming locally dense structures such as polymer or filament bundles. In order to simulate such systems effectively using Monte-Carlo methods, we propose a novel event chain algorithm adapted from hard sphere systems [E. P. Bernard, W. Krauth, Phys. Rev. E, 80: 056704 (2009)]. The algorithm works rejection-free and reduces autocorrelation and equilibration times significantly.

We demonstrate the advantages of the algorithm by investigating the diffusive behaviour of bundle structures. Using the event chain algorithm a polymer bundle exhibits the correct scaling of diffusion constants with bundle size, which is not obtained using simple local displacement moves. We apply the algorithm to bundle networks formed by semiflexible filaments with short-range attractive interactions.

BP 16.23 Tue 9:30 P1

**Estimation of sleep stages and sleep depth dynamics by neural clustering** — •Stephan Volkland[1] and Jens Christian Claussen[2,1] — [1]INB, Universität zu Lübeck, Germany — [2]Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

The quantitative analysis of sleep from polysomnographic date (i.e., simulataneous recording of EEG, EMG and EOG) is practically limited by the final step of sleep scoring, i.e. extensive manual inspection of data according to the Rechtschaffen and Kales rules or the recent AASM counterpart, leading to a manually classified time series of sleep stages on a discrete scale of six values (wake, REM, S1, S2, S3, S4). Starting from the observation that the stages S2, S3, and S4 are merely defined by spectral properties, namely by activity in the delta and sigma band, here we present a neural clustering approach to assess sleep stages automatically by unsupervised neural clustering and a posteriori assignment of sleep stages. One particular goal is to provide a finer resolution in time as well as a finer interpolation in sleep depth than obtainable from manual scoring. We find that EOG and EMG data are still needed to improve classification of wake and REM states, and still an interpolation of states at the borders of wake, REM and S1 is difficult. In the range between the NonREM stages S1–S4 an interpolation with higher resolution is feasible, as expected.

BP 16.24 Tue 9:30 P1

**Extended diffusion model of sleep depth dynamics** — •Anna Barkentien[1] and Jens Christian Claussen[2,1] — [1]INB, Universität zu Lübeck, Germany — [2]Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

The duration of wake bouts during sleep has puzzled complex systems scientists since a decade since [1], as these distributions eventually resemble a power-law. The theoretical understanding is incomplete, biologically plausible models still are not available. A pure Markov analysis [2] assuming random switching however ignores any deterministic components in the dynamics which are manifest in time correlations. The phenomenological model proposed in [1] describes sleep depth by a one-dimensional diffusion process with a reflecting border for sleep and a restoring force for wake. We extend this model in [3] to account for the REM state and modify the restoring force law to account for deviations to the power law that are observed in data from some (but not all) labs and obtain a better fit to data [3]. We conclude that a refined model as [3] is necessary to account for the different experimental results, but significantly larger cohorts of sleep studies would be needed to distinguish between the two-regime and the one-regime distributions. This concerns only the wake $\rightarrow$ sleep transition, the sleep $\rightarrow$ wake transition remains consistant with a random process homogeneous in time.

[1] C.C. Lo et al, EPL 57, 631, 2002. [2] J.W. Kim et al, PRL 102, 2009. [3] A. Barkentien and J.C. Claussen (in preparation).

BP 16.25 Tue 9:30 P1

**Multidimensional epistasis and the transitory advantage of sex** — •Johannes Neidhart, Stefan Nowak, Ivan G. Szendro, and Joachim Krug — THP, Universität zu Köln, Deutschland

The benefit of sex and recombination is a long standing problem. We numerically study evolutionary dynamics on high dimensional epistatic fitness landscapes, with focus on the temporal development of the evolutionary advantage of recombination. We show that the adaptive advantage of recombination on static landscapes is strictly transitory. These findings are explained by means of well established results for a setup with two loci. It is further shown that the transitory advantage can be prolonged indefinitely in fluctuating environments.

BP 16.26 Tue 9:30 P1

**Adaptive walks in Kauffman's NK-Landscape** — •Stefan Nowak and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Deutschland

We study evolutionary dynamics in a high-dimensional genotype space in the limit of rare mutations and strong selection. In this regime the population performs an uphill walk which terminates at local fitness optima. We analyze the length and attained fitness of such walks with our focus on the influence of different genetic interaction patterns.

BP 16.27 Tue 9:30 P1

**Coexisting autocatalysts generate increasing complexity** — •Emanuel Gregor Worst[1], Philipp Zimmer[2], Eva Wollrab[1], Karsten Kruse[2], and Albrecht Ott[1] — [1]Biologische Experimentalphysik, Universität des Saarlandes, Deutschland — [2]Theoretische Biologische Physik, Universität des Saarlandes, Deutschland

The evolution towards more complex structures from the earliest building blocks of life remains poorly understood. Here we present an experimental realization that exhibits evolutionary properties in one dimension and generates multiple coexisting species. Molecular chains of a certain length (identified as a species) are autocatalytically reproducing, and new species form randomly by spontaneous concatenation. We use DNA strands and DNA ligase, covalently linking single-stranded DNA, as an experimental model system. Reproduction occurs by template-directed ligation. Spontaneous and random generation of new species is a consequence of thermal fluctuations. We show that the system evolves towards more complex structures in a non-trivial way if the ratio between autocatalytic reproduction and spontaneous generation of new species exceeds a critical value. An outstanding characteristic of this system is the iterated production of more complex species while coexistence is maintained.

BP 16.28 Tue 9:30 P1

**Identifying molecular expression dynamics in practice - how to distinguish between noise regulation and direct deterministic control using experimental data** — •Martin Hoffmann[1] and Jörg Galle[2] — [1]Fraunhofer ITEM, Project Group Personalized Tumor Therapy, Biopark I, Josef-Engert-Strasse 9, 93053 Regensburg, Germany — [2]Interdisciplinary Centre for Bioinformatics, University of Leipzig, Haertelstr. 16-18, 04107 Leipzig, Germany

Biological noise plays an important role in generating phenotypic diversity and contributes to unspecific environmental adaptation. However, the classical pathway view of cell biology focusing on deterministic stimulus-response relationships may well accommodate the majority of biological phenomena. It is thus necessary to develop combined theoretical and experimental approaches that can dissect the relative contribution of noise regulation and direct deterministic control. Accordingly, we define molecular level conditions for noise-driven and deterministic dynamics and compare corresponding modeling results to published experimental data. We show that both models can fit the FACS data for the toggle switch system equally well while simulated dynamic mRNA labeling results in distinct observations for both models. Using synthetic time course data we demonstrate that complete system identification can be achieved based on single cell tracking. As demonstrated, noise regulation can be an effective second layer of cell regulation that may be associated with active short term search processes.

BP 16.29 Tue 9:30 P1

**Propagation and propagation failure of waves on excitable tree networks** — Nikos Kouvaris[1], •Thomas Isele[2], Alexander Mikhailov[3], and Eckehard Schöll[2] — [1]Department of Physics, University of Barcelona, Marti i Franques 1, 08028, Barcelona, Spain — [2]Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [3]Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

We study the properties of pulse solutions on excitable tree networks by means of numerical (simulation and continuation) as well as analytical methods. We focus on the dependence of the propagation velocity and the change of stability properties with respect to the branching ratio (i.e. degree) of the nodes. But we also consider different coupling strengths and the continuous (thermodynamic) limit of our model.

BP 16.30 Tue 9:30 P1

**Dynamics of neural networks with transient synaptic plasticity rules** — •Bulcsú Sándor and Claudius Gros — Institut für Theoretische Physik, Goethe Universität, Frankfurt am Main, Deutschland

Working memory makes it possible to hold information temporarily for processing purposes; as such it has an important role in the execution of cognitive tasks. Its operation may possibly be mediated via short-term or transient synaptic plasticity effects. Thus the standard Tsodyks-Markram model for transient synaptic dynamics, built upon short-term synaptic plasticity effects, is a promising candidate to investigate the underlying dynamical behavior of these systems.

In our work we propose a simplified continuous time model for presynaptic plasticity rules, called full depletion model, which may allow a stricter control of the dynamics. The model is implemented for clique encoding recurrent networks with a Mexican-hat connection profile of synaptic weights. These systems show a wide variety of dynamical states as a function of the control parameters. We study the different types of behaviour emerging from transient synaptic plasticity rules from a dynamical system's point of view.

BP 16.31 Tue 9:30 P1

**Optimization of complex network for minimizing traffic congestion: case study for a popular internet based service in Serbia** — •Igor Stanković[1], Vladica Tinotor[2], and Jovan Radunović[3] — [1]Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [2]Republic Agency for Electronic Communications, Višnjićeva 8, 11000 Belgrade, Serbia — [3]School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia

We present a case study of network parameter optimization for a popular internet based service in Serbia. The physical layer of the network consists of two existing nation-wide optical networks, i.e., a commercial telecommunication network and a network of public power grid operator. The second network is build for synchronization and control of the power grid and is not currently used commercially. Information traffic is directed by standard Open Shortest Path First routing protocol and in our case initial link weights are assigned according to the link costs [1]. We apply optimization algorithm aimed at avoiding, if possible, link overload by a judicious link weight tuning. The output characteristics which enter into quality of service function are link utilization and total cost of the service. The input parameters of the optimization algorithm are network topology, relevant protocol, link costs and capacities.

[1] J. Smiljanic, I. Stankovic, "Efficient Routing on Small Complex Networks Without Buffers", Physica A **392**, (2013) 2294.

BP 16.32 Tue 9:30 P1

**Motifs in Triadic Random Graphs Based on Steiner Triple Systems** — •Marco Winkler and Jörg Reichardt — Institute for Theoretical Physics, University of Würzburg, Germany

Conventionally, pairwise relationships between nodes are considered to be the fundamental building blocks of complex networks. However, over the last decade so-called motifs have attracted much attention. It has been hypothesized that these motifs, rather than links, serve as the building blocks of network structures. Although the relation between a network's topology and its function, its robustness against perturbations, or its efficiency in spreading information, is the central theme of network science, there is still a lack of sound generative models needed for testing the functional role of subgraph motifs. Our work aims to overcome this limitation. We employ the framework of exponential random graph models (ERGMs) to define models based on triadic substructures. The fact that only a small portion of triads can actually be set independently poses a challenge for the formulation of such models. To overcome this obstacle, we use Steiner triple systems (STSs). These are partitions of sets of nodes into pair-disjoint triads, which thus can be specified independently. Combining the concepts of ERGMs and STSs, we suggest generative models capable of generating ensembles of networks with nontrivial triadic Z-score profiles. Further, we discover inevitable correlations between the abundance of triad patterns, which occur solely for statistical reasons and need to be taken into account when discussing the functional implications of motif statistics.

BP 16.33 Tue 9:30 P1

**Architecture of biologically inspired adaptive transport networks** — •Johannes Gräwer[1], Carl Modes[2], Marcelo O. Magnasco[2], and Eleni Katifori[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Laboratory of Mathematical Physics, The Rockefeller University, New York, NY, USA

We study self-organized adaptation mechanisms of biologically inspired transport networks (e.g. plasmodial veins of slime moulds). Therefore, evolving network architectures are simulated using a generic dynamical system and weighted graphs. The graphs' edges represent tubes with Hagen-Poiseuille flow, connected through junctions, represented by their nodes. A local update rule, that changes the conductivity of the tubes (edge weights) according to the flow through them, is used as a self-organizing adaptation principle. We model these interrelated transportation and adaptation processes on paradigmatic complex network topologies (e.g. Watts-Strogatz, Barabási-Albert, Erdös-Rényi) with random initial edge weights. We examine the adaptation dynamics and find, that it exhibits discrete, cascade reorganization events until the network reaches a hierarchically organized state.

BP 16.34 Tue 9:30 P1

**Quantum walks on 1D and 2D quasi-crystals** — •Chi-Hung Weng and Oliver Mülken — Institute of Physics, University of Freiburg, Germany

We study the dynamics of quantum walks on a quasi-crystals modelled by the tight-binding Aubry-André-Harper (AAH) equation. We numerically solved both the diagonal/off -diagonal AAH in both 1D and 2D cases. It is known that the 2D diagonal AAH can also be regarded as a model for the Integer Quantum Hall Effect (IQHE), a phenomena when a 2D electron gas is subjected to strong magnetic fields at a low temperature. As a consequence we also observe the edge states which are responsible for carrying the current. Those states can be changed from localized to de-localized, as a topological phase within the aperiodic modulated on-site potential varies. In order to identify how localized the states are, as well as how fast the transport is, the Inverse Participation Ratio (IPR) and Mean Squared Displacement (MSD) are calculated, respectively. Moreover, we also study the impact of disorder and non-Hermitian settings ( i.e. system with absorbers or Parity-Time (PT) symmetric modulated aperiodicity) on the dynamics.

BP 16.35 Tue 9:30 P1

**Transport efficiency in complex networks** — •Marco Tabarelli and Oliver Mülken — Albert-Ludwigs-Universität, Freiburg, Germany

We examine complex networks of two-level quantum systems regarding their efficiency to transport exitons through the network. Our model uses the so-called Quantum Stochastic Walk (QSW), a version of a quantum master equation in Lindblad form (LME) which allows to parametrize the classical-quantummechanical crossover. To describe a circular probability current an external node is coupled to two "ends" of the network acting as a source to an entrance node and a trap to an exit node. These links are directed and their effect is realized with additional Lindblad operators in the dissipative term of the LME. Comparing stationary solutions of node populations sheds light on the probability current through the network. In addition to the geometry of the network, parameters varied include the internal coupling constant, source- and trap strength and the ratio of coherent and decoherent transitions. Networks studied include modified linear chains and networks with self-similarity properties.

BP 16.36 Tue 9:30 P1

**Feedback control of vorticity in a Newtonian fluid** — •Maria Zeitz and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Our goal is to explore feedback control strategies to stabilize novel dynamic flow patterns in microfluidic model systems. As an example, we investigate a Couette flow geometry without the inner cylinder filled with a Newtonian fluid. Its vorticity satisfies a diffusion equation. To stabilize a mean vortex strength in the flow field, we use feedback control with hysteresis. We either set the angular velocity of the outer cylinder or apply a torque at the boundary and switch velocity or torque value in a hysteretic fashion depending on the actual mean vortex strength. Since the boundary condition changes with time, the system does not reach a stationary state. In this setup, we explore the possibility of time-periodic solutions and spatial flow patters. In a second step, we will also implement time-delayed feedback in our system.

BP 16.37 Tue 9:30 P1

**Fractal distributions in a cyclic information-engine with optimal feedback** — •Michael Bauer, Andre C. Barato, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

It is known that information obtained by measurements can be converted into work, the paradigmatic example being Szilard's engine. For a two level system coupled to a heat bath and a work reservoir we obtain the optimal protocol corresponding to the maximal work extraction. Moreover, we consider a controller performing cyclic measurements and changing the protocol accordingly. Analyzing this optimal cyclic machine we find a recursion relation for the initial occupation probability of the level with higher energy, which depends on the measurement error. Through the numerical analysis of this relation we obtain a fractal histogram, which is a strange attractor (common in chaos theory). This fractal structure can be explained with a simplified model leading to the Cantor set.

BP 16.38 Tue 9:30 P1

**Feedback control of non-equilibrium dynamics of a multilayer system of confined colloidal particles in planar shear flow** — •Sascha Gerloff, Tarlan A. Vezirov, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We perform computer simulations of charged colloidal particles in planar shear flow combined with feedback control. The particles interact via a combined Yukawa- and softsphere-potential. The system is known to form shear-induced multi-layer configurations in confinement and to show different intra-layer structures which depend on the applied shear rate [1]. The parameters are set to suit experimental data for ludox silica particles, which where previously studied [2, 3].
We employ overdamped Brownian dynamics simulations to investigate the structure and the rheological behavior of the considered system. We then supplement our equations of motion by an additional dynamical equation, which corresponds to a feedback control mechanism for the shear rate via the shear stress. This enables the system to select between steady states dependent on the control parameters. Furthermore we present an approximation which estimates the transtion between steady states in the control parameter space analytically.
[1] T. A. Vezirov and S. H. L. Klapp, Phys. Rev. **E 88**, 5 (2013).
[2] S. Grandner and S. H. L. Klapp, J. Chem. Phys. **129**, 244703 (2008).
[3] S. H. L. Klapp, Y. Zeng, D. Qu and R. v. Klitzing, Phys. Rev. Lett. **100**, 118303 (2008).

## BP 17: Microswimmers (joint DY/BP)

Time: Tuesday 9:30–12:30 Location: ZEU 146

BP 17.1 Tue 9:30 ZEU 146

**Aftrican trypanosomes swim faster in small capillaries and heterogeneous environment** — •Davod Alizadehrad and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Germany

Human African trypanosome (HAT), the causative agent of the deadly sleeping sickness in sub-Saharan Africa, is a protozoan or single- celled microorganism that propels itself with the help of a beating flagellum. Despite good recent progress [1], refined models and further numerical simulations are necessary to uncover the heavily debated propulsion mechanism of the trypanosome, in particular, how the flagellum is attached to the cell body.

In this study, to simulate the swimming trypanosome, we construct a refined elastic network model of trypanosome based on experimental data and combine it with the mesoscale simulation technique called multi-particle collision dynamics (MPCD) to model the fluid environment. We reproduce several key features of trypanosome motility. First, we simulate the swimming and rotation speed of the trypanosome and find excellent agreement with experiments [2]. Second, we show that confinement has profound effects on trypanosome locomotion. In narrow circular channels the swimming speed increases up to 6 times its bulk value. Finally, we demonstrate that randomly distributed obstacles in a fluid help the trypanosome to swim more efficient.

[1] S.B. Babu and H. Stark, New J. Phys. 14, 085012 (2012).
[2] N. Heddergott, et al., PLoS Pathog, 8, e1003023 (2012).

BP 17.2 Tue 9:45 ZEU 146

**Energetic efficiency of ciliary propulsion** — •Andrej Vilfan and Natan Osterman — J. Stefan Institute, Ljubljana, Slovenia

Energetic efficiency of swimming has long been considered a non-issue in microorganisms, but newer studies show that ciliates can use more than half of their energy for propulsion. To estimate how close the ciliates are to the theoretically optimal way of swimming we address the following problems: i) we determine the optimal stroke of a cilium, ii) we determine the optimal beating pattern of a ciliated surface and

iii) we calculate the optimal shape of a ciliated swimmer.

For a single cilium we define the efficiency in a scale-invariant way and show that the optimal stroke consists of a working stroke with a stretched cilium and a recovery stroke where the cilium bends and moves closer to the surface. When optimizing an array of cilia we additionally show that metachronal waves improve the efficiency and that the optimal efficiency is achieved for antiplectic waves. The resulting beating patterns, as well as the optimal ciliary density, show remarkable similarity with those observed in ciliated microorganisms. In order to optimize the shape of the whole swimmer we use a simplified description where we replace the ciliated layer with a surface slip velocity. The optimal shapes again resemble those of different ciliates. If we combine the results of our optimization with experimental efficiency estimates we can show that Paramecium has a propulsion efficiency that is within a factor of 2 of the theoretical optimum.

[1] N. Osterman and A. Vilfan, PNAS 108, 15727 (2011) [2] A. Vilfan, Phys. Rev. Lett. 109, 128105 (2012)

BP 17.3 Tue 10:00 ZEU 146

**Hydrodynamics of spherical microswimmers in a quasi-2D geometry** — •Andreas Zöttl and Holger Stark — TU Berlin

Microorganisms like bacteria, sperm cells or algae live in aqueous environments and their motion is therefore governed by low-Reynolds-number hydrodynamics, but also influenced by thermal and biological noise. Experiments with artificial microswimmers, which are used to study collective motion of self-driven particles out of equilibrium, are often performed in a quasi-2D geometry or in thin films, where dynamic clustering and motility-induced phase separation is observed.

Motivated by recent experiments of active colloids and emulsion droplets in confinement, we also study the collective motion of spherical squirmers moving in a quasi-2D geometry by means of multi-particle collision dynamics. Hydrodynamic near-field interactions between swimmers lead to hydrodynamic rotational diffusion, while hydrodynamic interactions between the channel walls and swimmers strongly influence the preferred swimmer orientations and therefore the formation of hexagonal clusters. Neutral squirmers in particular separate into a gas-like and a crystalline phase which we characterize by a structural order parameter. Varying the density of the swimmers from low to high area fraction results in a steep increase of the order parameter at the critical density, accompanied by strong fluctuations indicating a non-equilibrium phase transition which is absent for strong pullers and pushers.

BP 17.4 Tue 10:15 ZEU 146

**Optimization of bead-spring micro-swimmers and study of dense swimmer solutions** — •Jayant Pande[1,2] and Ana-Sunčana Smith[1,2] — [1]Institute for Theoretical Physics, Friedrich-Alexander University, Erlangen, Germany — [2]EAM: Cluster of Excellence, Friedrich-Alexander University, Erlangen, Germany

With the increasing need to understand and predict the locomotion of natural organisms and machines at the micro-scale, the theoretical modelling of micro-swimmers has become an important field of study. Contributing to its development, we present analytical results on the geometric and kinematic optimization of three-ellipsoid microswimmers, based on the three-sphere model of Najafi and Golestanian. Assuming a sinusoidal driving protocol, we identify different drag-related regimes and determine the exact shapes which maximise the swimming velocity and efficiency in each regime. Conditions on the optimal forcing parameters as well as the push/pull nature of the swimmer are elucidated. The analytical work is supported by simulations using an in-house framework based on the lattice-Boltzmann method. Its versatility and massively-parallel capabilities allow us to explore near-field effects as well as those arising from asymmetry in the swimmer design. We show that these effects, while inaccessible to an exact theoretical treatment, are nevertheless amenable to an approximate description. In the last part of our contribution, we employ our simulation system to study large populations of passive and active particles in fluids. For different concentrations, we observe previously-known effects as well as departures from theory.

BP 17.5 Tue 10:30 ZEU 146

**Statistical properties of tracer positions, sedimenting in an active fluid** — •Thomas John, Matthias Mussler, and Christian Wagner — Experimentalphysik, Universität des Saarlandes

Fluid dynamics on $\mu$m scale at velocities in $\mu$m/s is characterized by very low Reynolds numbers. Therefore no turbulent behavior and characteristics is expected. Nevertheless, a spatial-temporal random flow field can be present in a media if the fluid contains a lot of active, irregular moving micro-swimmers. We consider trajectories of passive sedimenting beads in such fluids. This trajectories are strongly influenced from the random flow field if the passive particle (tracer) diameter comparable or less then the diameter of the micro-swimmers. We measured such trajectories in suspensions of the green alga chlamydomonas reinhardtii. The alga has two flagella, a diameter of 10 $\mu$m and swims as a puller with 50 $\mu$m/s. We extract statistical properties of the passive bead positions, e.g. the mean square displacement or the probability density function. Our results are compared with the Brownian motion characteristics of sedimenting particles in very dilute systems and the known non-Brownian characteristics in passive sedimenting particles at higher volume concentrations where the hydrodynamic interactions becomes important.

BP 17.6 Tue 10:45 ZEU 146

**Propulsion of droplets by rigidly tethered traction forces** — •P. Sekhar Burada, Reiner Kree, and Annette Zippelius — Institute for Theoretical Physics, University of Göttingen, Germany

We study the dynamics of an active droplet, with both translational- and rotational degrees of freedom. A field of interfacial traction forces, which is time independent in a body-fixed reference frame drives the system. Using the general solution of the Stokes equation, with the appropriate boundary conditions, we are able to calculate the hydrodynamic flow pattern both inside and outside of the droplet. Also, using force- and torque balance conditions the translational- and rotational velocities of the droplet are calculated. We derive the conditions, in terms of mode amplitudes of the traction force, which need to be satisfied in order to preserve the shape of the droplet.

**15 min break**

BP 17.7 Tue 11:15 ZEU 146

**Transport powered by bacterial turbulence** — •Andreas Kaiser[1], Anton Peshkov[2], Andrey Sokolov[3], Borge ten Hagen[1], Hartmut Löwen[1], and Igor S. Aranson[3] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf — [2]Service de Physique de l'Etat Condensé, Gif-sur-Yvette — [3]Materials Science Division, Argonne National Laboratory

We show that turbulence in a bacterial bath can be exploited to power and steer directed transport of mesoscopic carriers through the suspension. In our experiments and simulations, a microwedge-like "bulldozer" is exposed to a bacterial bath of varied concentration and obtains a maximal transport speed in the turbulent state of the bacterial suspension.

BP 17.8 Tue 11:30 ZEU 146

**Cell body rocking is dominant mechanism for flagellar synchronization in a swimming alga** — Veikko Geyer[1], Frank Julicher[2], Jonathon Howard[1], and •Benjamin Friedrich[2] — [1]Max Planck Institute for Cell Biology and Genetics — [2]Max Planck Institute for the Physics of Complex Systems

The eukaryotic flagellum is a best-seller of nature: These slender cell appendages propel sperm and many other microswimmers, including disease-causing protists. In mammalian airways and the oviduct, collections of flagella beat in synchrony to pump fluids efficiently. Here, we report on theory and experiment that elucidate a mechanism of flagellar synchronization in the model organism *Chlamydomonas*, a green algal cell that swims with two flagella like a breaststroke swimmer. Our analysis shows how synchronization arises by a coupling of swimming and flagellar beating and characterizes an exemplary force-velocity relationship of the flagellar beat. Any perturbation from the synchronized state causes the cell body to rock, which changes the hydrodynamic friction forces acting on the flagella and thus their speed, which restores their synchronization.

Geyer *et al.*: Proc. Natl. Acad. Sci. U.S.A. **110**, 2013.

BP 17.9 Tue 11:45 ZEU 146

**Direct Measurements of Active Flagellar Fluctuations** — •Benjamin Friedrich[1], Rui Ma[2], Gary Klindt[1], Frank Julicher[1], and Ingmar Riedel[3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Institute for Advanced Study, Tsinghua University, Beijing, China — [3]Department of Bioengineering, Stanford University, Stanford, CA, USA

The eukaryotic flagellum beats regularly, driven by the oscillatory dynamics of molecular motors, to propel cells and pump fluids. Small, but

perceivable fluctuations in the beat of individual flagella have physiological implications for synchronization in collections of flagella as well as for hydrodynamic interactions between flagellated swimmers. Here, we characterize phase diffusion and amplitude fluctuations of sperm flagellar beat patterns. We employ shape mode analysis and limit cycle reconstruction for a low-dimensional representation of flagellar bending waves. We find that flagellar fluctuations are dominantly of active origin. Using a minimal model of collective motor oscillations, we demonstrate how active fluctuations can naturally arise from the stochastic dynamics of individual motors.

BP 17.10 Tue 12:00 ZEU 146

**Synchronization of rigid microrotors by time-dependent hydrodynamic interactions** — •Mario Theers and Roland Winkler — Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Juelich, D-52425 Juelich, Germany

The synchronized beating of flagella is fundamental for the coordinated motion of microswimmers such as spermatozoa, bacteria, protozoa, or algae. It is a longstanding conjecture that this microscopic synchronization could be induced by hydrodynamic interactions. However, synchronization is not easily achieved for low Reynolds-number fluids, which are described by Stokes equations. The presence of kinematic reversibility combined with swimmer symmetries may prevent synchronization.

We provide an extension of previous low-Reynolds number studies by analyzing the linearized, time-dependent Navier-Stokes equations instead of the usually adopted Stokes equations. As a model system, we investigate the emergent dynamical behavior of hydrodynamically coupled microrotors and demonstrate that time-dependent hydrodynamic interactions inevitably lead to synchronization of their rotational motion, which is not achieved on the basis of Stokes equations. We show that the system can be described by coupled nonlinear integro-differential equations and derive analytical results for the the phase difference. Additionally, results are compared to mesoscale hydrodynamic simulations. Our studies provide a deeper insight into the nature of hydrodynamic interactions between microswimmers.

BP 17.11 Tue 12:15 ZEU 146

**A close look at the tumbling of bacteria** — •Tapan Chandra Adhyapak and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin

Peritrichous bacteria such as Escherichia coli propel themselves by using multiple flagella, each rotated at the base by a rotary motor. Hydrodynamic interactions together with an intricate balance of elasticity of the flagella cause them to synchronize and form a single bundle leading to propulsion in a straight line. Such straight runs of a bacterium frequently terminate at relatively short lived tumbling events during which one or more of the flagella leave the bundle disrupting uniform motion and causing the bacterium to change its course. In addition to hydrodynamic interactions and elasticity, rotation-induced polymorphic transitions between different flagellar states [1] is observed to play an important role in re-orientating the bacterium. The detailed process however is complex and very little understood. We investigate the tumbling strategy of an E. Coli modelling its propulsion using an extended continuum theory of elasticity in presence of hydrodynamic interactions. We examine, in particular, the effect of rotation-induced polymorphic transitions of flagella during such processes.

[1] R. Vogel and H. Stark, Phys. Rev. Lett. **110**, 158104 (2013).

## BP 18: Complex Fluids and Soft Matter (joint DY/CPP/BP)

Time: Tuesday 9:30–11:30 Location: ZEU 118

BP 18.1 Tue 9:30 ZEU 118

**Microrheology of shear thinning solutions** — •Juan Ruben Gomez-Solano[1,2] and Clemens Bechinger[1,2] — [1]Universitaet Stuttgart, 2. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, 70569 Stuttgart, Germany

Colloidal probes embedded in complex fluids have been extensively employed to investigate their rheological response to small stress. However, this approach is not evident for fluids subjected to large stresses, where a variety of non-Newtonian behaviors can occur. One example of such systems are semi-dilute micellar solutions, which consist of surfactant molecules forming worm-like micelles entangled in aqueous solution. In this work, we study the motion of a colloidal probe dragged by an optical trap through a semi-dilute micellar solution of cetylpyridinium chloride. The motion of the probe creates a shear strain, which depends linearly on its mean velocity v. We measure the effective viscous drag on the probe and the fluctuations of its position as a function of v. We find that at small v, the system can be characterized by a constant viscosity, whereas the position fluctuations are statistically the same as in thermal equilibrium. However, above a certain value, the viscosity decreases as a function of v. The fluctuations of the particle position are also affected in the shear-thinning regime, and their power spectral density increases with increasing v. We find that the transition between both regimes typically occurs when the shear rate exceeds the inverse relaxation time of the entangled micelles.

BP 18.2 Tue 9:45 ZEU 118

**Shear driven instabilities in anisotropic colloidal mixtures** — •Rodrigo Lugo-Frias and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In recent years much attention has been paid in understanding the orientational order of anisotropic hard bodies in the presence of steady shear flow [1,2]. On the other hand, sheared systems of binary mixtures of hard disc and rodlike particles have also been examined [3].

We focus in the nonequilibrium dynamics of a binary mixture of rodlike nematic polymers under shear flow. To do so, we derive from density functional theory (DFT) a mesoscopic free energy in terms of the alignment tensor for each component. We proceed to investigate their dynamical behavior using the well known mesoscopic Doi–Hess theory, which lead to a set of nonlinear differential equations [4,5,6]. Finally, we examine the total alignment of each component and its dependencies with the physical properties of the system.

[1] S. H. L. Klapp and S. Hess, Phys. Rev. E **81**, 051711 (2010).
[2] D. Strehober, H. Engel and S. H. L. Klapp, Phys. Rev. E **88**, 012505 (2013).
[3] F. Tardani, L. Gentile, G. A. Ranieri and C. La Mesa, J. Phys. Chem. C, **117**, 8556 (2013).
[4] S. Hess, Z.Naturforsch. A **31a**, 1034 (1976).
[5] M. Doi, J.Polym. Sci., Polym. Phys. Ed. **19**, 229 (1981).
[6] S. Hess and M. Kröger, J.Phys.: Cond. Matter, **16**, S3835 (2004).

BP 18.3 Tue 10:00 ZEU 118

**Friction of Colloidal Crystals on Commensurate and Incommensurate Substrates** — •Aleksandar Mijailović and Michael Schmiedeberg — Theoretische Physik 2, Heinrich-Heine Universität, Düsseldorf, Germany

Among the fascinating properties of quasicrystals - structures that possess long range order but no translational symmetry - is the very low friction that was observed when a periodic crystal is moved over the surface of a quasicrystal [1]. Here we want to explore whether there are geometrical reasons for the small friction.

Using Brownian Dynamics simulations, the friction properties of 3D colloidal fcc-crystals on substrates with different geometries are studied. We measure the friction as a function of the drag force applied on the crystal, from which the friction coefficient is extracted. We repeat this analysis for commensurate, incommensurate perodic, and quasicrystalline substrates and investigate the effect of incommensurability as well as aperiodicity.

The (charged) colloidal particles are interacting via the Asakura-Oosawa Model, i.e., a superposition of the screened-Coulomb potential and an attractive term, which is due to the presence of non-adsorbing polymers (not treated explicitly). Finally, our results are compared to the 2D case (cf., e.g., [2].

1. J. Y. Park *et al.*, *Science* **309**, 1354 (2005).
2. T. Bohlein *et al.*, *Nat. Mat.* **11**, 126 (2012).

BP 18.4 Tue 10:15 ZEU 118

**Complex dynamics of a bilamellar vesicle as a simple model for leukocytes** — •Badr Kaoui — Theoretical Physics I, University of Bayreuth, 95440 Bayreuth, Germany — Department of Applied Physics, Eindhoven University of Technology, P. O. Box 513, 5600 MB Eindhoven, The Netherlands

The influence of the internal structure of a biological cell (e.g., a leukocyte) on its dynamics and rheology is not yet fully understood. By using 2D numerical simulations of a bilamellar vesicle (BLV) consisting of two vesicles as a cell model, we find that increasing the size of the inner vesicle (mimicking the nucleus) triggers a tank-treading-to-tumbling transition. A new dynamical state is observed, the undulating motion: the BLV inclination with respect to the imposed flow oscillates while the outer vesicle develops rotating lobes. The BLV exhibits a non-Newtonian behavior with a time-dependent apparent viscosity during its unsteady motion. Depending on its inclination and on its inner vesicle dynamical state, the BLV behaves like a solid or a liquid [Badr Kaoui, Timm Krüger and Jens Harting, Soft Matter 9, 8057 (2013)].

**15 min break**

BP 18.5 Tue 10:45 ZEU 118

**Random Organization and Jamming within a unifying model system** — •Lars Milz[1] and Michael Schmiedeberg[2] — [1]Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40204 Düsseldorf, Germany

We show that both random organization and jamming occur within the same model packing problem despite the obvious differences between these two transitions: The random organization transition describes the change from reversible to irreversible dynamics in a non-equilibrium system and the athermal jamming transition occurs when particles can no longer avoid overlaps if quenched from infinite to zero temperature.

In our unifying model system the particles are initially randomly distributed and then displaced in each step if they overlap. For random displacements we obtain a random organization transition while jamming occurs in case of deterministic shifts. For the random organization transition, we also determine the critical exponents. For the jamming transition we observe a divergence of the relaxation time of our method.

Within our model system, random organization and jamming are opposite limits of random sphere packings. In future, we want to study intermediate packing problems or mixtures or random organization and jamming that probably correspond to other equilibrium or non-equilibrium transitions.

BP 18.6 Tue 11:00 ZEU 118

**Foam morphology, frustration and topological defects in a Negatively curved Hele-Shaw geometry** — •Adil Mughal, Myfanwy Evans, and Gerd Schröder-Turk — Institut fur Theoretische Physik, Friedrich-Alexander Universitat Erlangen-Nurnberg, Staudtstr. 7, D-91058 Erlangen, Germany

We present preliminary simulations of foams and single bubbles confined in a narrow gap between parallel surfaces. Unlike previous work, in which the bounding surfaces are flat (the so called Hele-Shaw geometry), we consider surfaces with non-vanishing Gaussian curvature.

We demonstrate that the curvature of the bounding surfaces induce a geometric frustration in the preferred order of the foam. This frustration can be relieved by the introduction of topological defects (disclinations, dislocations and complex scar arrangements). We give a detailed analysis of these defects for foams confined in curved Hele-Shaw cells and compare our results with exotic honeycombs, built by bees on surfaces of varying Gaussian curvature.

Our simulations, while encompassing surfaces of constant Gaussian curvature (such as the sphere and the cylinder), focus on surfaces with negative Gaussian curvature and in particular triply periodic minimal surfaces (such as the Schwarz P-surface and the Schoen's Gyroid surface). We use the results from a sphere-packing algorithm to generate a Voronoi partition that forms the basis of a Surface Evolver simulation, which yields a realistic foam morphology.

BP 18.7 Tue 11:15 ZEU 118

**Molecular simulation methods to compute interfacial free energies** — •Ronald Benjamin and Juergen Horbach — Theoretical Physics II, Heinrich-Heine Universitaet, 40225 Duesseldorf, Germany

Knowledge of interfacial free energies are crucial to understanding physical phenomena such as wetting and nucleation. In this talk we discuss several ways to extract this quantity for wall-liquid and wall-crystal interfaces. Chiefly, we discuss a new thermodynamic integration scheme developed to determine the interfacial free energy and compare it to a non-equilibrium work method and a Gibb's-Duhem type of approach known as "Gibb's-Cahn integration".

We also extended our thermodynamic integration scheme to obtain the excess free energy of a supercooled liquid in contact with amorphous walls having the same structure as the liquid. Our results shed new light on the thermodynamic behavior of supercooled liquids and help explain their slowing down in the presence of such rough walls.

## BP 19: Focus Session: Dynamical Patterns in Neural Systems: From Brain Function to Dysfunction (joint DY/BP)

Pattern formation in biological systems is at the forefront of current cross-disciplinary research; scientists are striving across disciplines to understand detailed activity patterns in neural systems and their role in brain function.This focus session will outline the potential of modern imaging and network approaches for revealing collective mechanisms underlying normal and pathophysiological activity in the brain. (Organizers St. C. Müller and Th. Geisel)

Time: Tuesday 9:30–11:30 Location: HÜL 186

**Invited Talk** BP 19.1 Tue 9:30 HÜL 186

**From epilepsy to migraine to stroke: A unifying framework.** — •Markus A Dahlem — Department of Physics, Humboldt-Universität zu Berlin

We seek to understand in terms of quantitative mathematical models the dynamics of ion imbalances in three pathological conditions: epileptiform activity during seizures, cortical spreading depression in migraine, and anoxic depolarizations after stroke or traumatic brain injury. A family history of epilepsy increases the chances of having severe migraines and certain patients with migraine are at greater risk for stroke. The multiplicity of potential links include common genetic risk factors and indirect links like common triggers outside the brain. In the present approach, however, we will focus on basic electrophysiological mechanisms of neural excitability and the transitions between different activity forms related to ion imbalances in the brain. The change of both membrane potential and—due to reduced ion gradients—Nernst potentials together cause in varying degrees a release of Gibbs free energy, that is, the thermodynamic potential that measures the energy available to the neurons for normal functioning. We hence describe the three states related to epilepsy, migraine, and stroke in terms of their free energy starvation and stress. The mathematical description of such phenomena requires a broader thermodynamical perspective, as it goes beyond the original Hodgkin-Huxley description based on equivalent electrical circuits in membrane physiology.

**Invited Talk** BP 19.2 Tue 10:00 HÜL 186

**Non-standard Interactions in Networks: Synchrony and the Emergence of Neural Activity Patterns** — •Marc Timme[1], Sven Jahnke[1], Raoul-Martin Memmesheimer[2], Wen-Chuang Chou[1], and Christian Tetzlaff[1] — [1]Network Dynamics, MPI for Dynamics and Self-Organization — [2]Donders Institute for Neuroscience, University of Nijmegen

Patterns of spatio-temporally distributed neural activity have been experimentally observed in different systems and are intimately related

to network function. How spatial and temporal specificity emerge dynamically in neural circuits, however, remains unclear.

Here we demonstrate how non-standard interaction mechanisms such as non-additive coupling and inhibitory feedback co-acting with heterogeneities may generate apparently disordered patterns that yet are precise in space and time and selectively respond to specific inputs only. The results may contribute towards an explanation of sensory processing in olfactory systems and processes involved in memory consolidation.

References: PLoS Comput. Biol. 8:e1002384 (2012); Phys. Rev. X 2:041016 (2012); PLoS Comput. Biol. 9:e1003307 (2013); Chou et al., in prep.

**Invited Talk** BP 19.3 Tue 10:30 HÜL 186

**Towards a dynamic map of neuronal circuits** — •Alipasha Vaziri — Research Institute of Molecular Pathology (IMP), — Center for Molecular Biology, University of Vienna — Research Platform for Quantum Phenomena and Nanoscale Biological Systems, University of Vienna

Knowledge on structural connectivity in neuronal circuits is necessary for understanding information representation and processing in local circuits. Addressing this challenge has been hampered by lack of appropriate tools and methods that allow parallel and spatiotemporally specific application of excitation patterns onto neuronal populations while capturing the dynamic activity of the entire network at high spatial and temporal resolution. The combination of new optical excitation techniques, optogenetics and high speed functional imaging are providing new opportunities to address this question and move towards a dynamic map of neuronal circuits. Compared to standard two-photon microscopy exploiting the spectral properties of femtosecod lasers provide an additional degree of freedom whereby alternative spatial light distributions can be "sculpted" in a biological sample. We have developed such a two-photon technique for brain-wide calcium imaging in C. elegans. The combination of this microscope with a nuclear-localized, genetically encoded calcium indicator, NLS-GCaMP5K, has allowed us to capture the activity of individual neurons within the densely packed head ganglia of C. elegans. We demonstrate near-simultaneous recording of activity of up to 70% of all head neurons.

BP 19.4 Tue 11:00 HÜL 186

**Fast reconfiguration of high-frequency human brain networks in response to surprising changes in auditory input** — •Sandra Chapman[1,2,3], Ruth Nicol[4], Petra Vertes[5], Pradeep Nathan[5,6], Marie Smith[7], Yury Shtyrov[8], and Edward Bullmore[5,6] — [1]CFSA, Physics, Univ. of Warwick, UK — [2]MPIPKS, Dresden, Germany — [3]Mathematics and Statistics, UIT, Norway — [4]University Hospitals Coventry and Warwickshire NHS Trust, Coventry, UK — [5]Behavioral and Clinical Neuroscience Institute, Dept. of Psychiatry, Univ. of Cambridge, UK — [6]GSK Clinical Unit, Addenbrooke's Hospital, Cambridge, UK — [7]Dept. of Psychological Sciences, Birkbeck, Univ. of London, UK — [8]MRC Cognition and Brain Sciences Unit, Cambridge, UK

We measured rapid changes in functional brain network organization in response to brief, discrete, changes in auditori stimulii. We estimated network topology and distance parameters in the immediate response, $< 1$ s, following auditory presentation of standard, repeated tones interspersed with occasional 'surprising' tones, using MEG to measure synchronization of high frequency (gamma band 33-64 Hz) oscillations in healthy volunteers. We found that global small-world parameters of the networks were unchanged between the standard and surprising tones. However, auditory surprises were associated with local changes in clustering of connections between temporal and frontal cortical areas, and with increased interlobar, long-distance synchronization. This work maps the dynamic network response that corresponds to the well known evoked response to this mismatch-negativity paradigm.

BP 19.5 Tue 11:15 HÜL 186

**The Cerebral Cortex as an Excitable Medium: Spiral Dynamics in Cortical Models of Epilepsy** — •Kentaroh Takagaki — Leibniz Institut für Neurobiologie, Magdeburg, Germany

Epilepsy affects up to 50 million people worldwide, each year. Although much research has focused on the genetic and pharmacological aspects of this disorder, little is known about how the population activity patterns of neurons initiate and stabilize within the epileptic cortex. Our work in cortical slice models of epilepsy shows that spatially organized, dynamically stable spiral patterns may contribute to such epileptogenesis. We have also recently recorded such phenomena in vivo, in the Mongolian Gerbil.

We hypothesize that such spiral dynamics may serve a role similar to the well-known reentrant spirals in ventricular fibrillation of the heart. To explore this hypothesis and brain population dynamics in general, we have been applying transcranial DC stimulation to modulate the excitability of the cortex, and observing the resulting population dynamics via voltage-sensitive dye imaging.

## BP 20: Cell adhesion, mechanics and migration I

Time: Tuesday 13:00–16:00 Location: HÜL 386

**Topical Talk** BP 20.1 Tue 13:00 HÜL 386

**Catch bond interaction between glycosaminoglycans and cell surface sulfatase Sulf1** — Alexander Harder[1], Ann-Kristin Moeller[1], Fabian Milz[2], Phillipp Neuhaus[2], Volker Walhorn[1], Thomas Dierks[2], and •Dario Anselmetti[1] — [1]Experimental Biophysics, Physics Faculty, Bielefeld University, D-33615 Bielefeld, Germany. — [2]Biochemistry I, Faculty of Chemistry, Bielefeld University, D-33615 Bielefeld, Germany.

In biological adhesion, the biophysical mechanism of specific non-covalent biomolecular interaction can be divided in slip- and catch-bonds, respectively. Conceptually, slip bonds exhibit reduced bond lifetime under increased external loads whereas catch-bonds, in contrast, increased lifetime for a certain force interval. Since 2003, a handful of biological systems such as the adhesive proteins P-Selectin and FimH have been identified to display catch bond properties.

Upon investigating the specific interaction between the unique hydrophilic domain (HD) of human cell-surface sulfatase Sulf1 against the native glycosaminoglycan (GAG) target heparan sulfate (HS) by single molecule force spectroscopy (SMFS), we found clear evidence of catch-bond behavior in this system. The HD, about 320 amino acids long and strongly positive charged, and the GAG-polymers, composed of up to 200 disaccharide units, were quantitatively investigated with atomic force microscopy (AFM) based dynamic force spectroscopy (DFS) as well as force clamp spectroscopy (FCS). The observed catch bond character of HD against GAGs was found to be specifically related to the GAG 6-O-sulfation site. Therefore, this behavior can also be found in HS-related GAGs like heparin and (to a lesser extent) dermatan sulfate whereas in contrast, only slip bond binding can be observed in a GAG system where these sites are explicitly lacking. Our observed catch bond binding data can be interpreted within the theoretical framework of a force mediated transition between two slip bond regimes modelled by a switchover within a double-well energy landscape. Interestingly, the transition occurs in a force interval of only 5 Piconewtons while the life-time of the adhesion bond increases approximately 5-fold for heparan sulfate and heparin.

BP 20.2 Tue 13:30 HÜL 386

**Migration patterns of dendritic cells in response to chemokines** — •Veronika Bierbaum, Eva Kiermaier, Jan Schwarz, Michael Sixt, and Tobias Bollenbach — IST Austria, Am Campus 1, 3400 Klosterneuburg, Austria

Dendritic cells are decisive components of the adaptive immune system. They navigate through tissues by sensing two different chemokines, CCL19 and CCL21. We develop a predictive physical description of dendritic cell migration as a function of the surrounding chemokine concentration fields. We are particularly interested in the role of cell size and shape in sensing and migration. We gain quantitative information about the influence of these parameters on cellular motion from in vitro assays. In these assays, cells are exposed to specific well-controlled combinations of the two different chemokines. We quantify the dynamics of the chemokine profiles and cell motion using time-lapse microscopy. In this way, we obtain ensembles of cell trajectories, which we use to identify the key parameters that control cellular motion in varying environments. Our preliminary results indicate that

dendritic cells perform a random walk in the absence of any chemokine gradient. The observed trajectories are generally well captured by Langevin equations, enabling us to separate the stochastic and deterministic contributions to the directionality and velocity of the moving cells. We further find that dendritic cells show qualitatively different migration behaviors for the two types of chemokines. Our combined experimental-theoretical study will enable us to identify general principles of cellular responses to chemokines that ensure robust cell migration.

BP 20.3 Tue 13:45 HÜL 386

**Model-based Traction Force Microscopy Reveals Differential Tension in Stress Fibers** — •Christoph A. Brand[1,2], Jérôme R. D. Soiné[1,2], Jonathan Stricker[3], Patrick W. Oakes[3], Margaret L. Gardel[3], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University — [2]Bioquant, Heidelberg University — [3]Gordon Center for Integrative Science, University of Chicago, USA

Adherent tissue cells use self-generated mechanical forces to probe and adapt to their mechanical environment. Traction force microscopy (TFM) has been successfully employed to obtain cellular forces transmitted to elastic substrates via cell-matrix adhesions. However, traction reconstruction represents an ill-posed problem and requires regularization to estimate optimal solutions. Here we introduce a novel technique termed model-based traction force microscopy (MB-TFM) to increase the predictive power of TFM and to reduce the effect of noise. In a first step, image processing of fluorescence microscopy data for focal adhesions and the actin cytoskeleton is used to identify contractile structures and attachement points. In a second step, these data are converted into a mechanical model of the cell using recent advances in modeling whole cell contractility with an actively contracting cable network. In a third step, we optimize the intracellular tension configuration for the best agreement between measured and simulated substrate displacement fields. As a first application, we show that different types of stress fibers are characterized by different tension levels.

BP 20.4 Tue 14:00 HÜL 386

**Directional Motors Move on Cell Surface and Give Rise to Gliding Motility and Sporulation in M. xanthus** — •Fabian Czerwinski[1], Morgane Wartel[2], Adrien Ducret[2,3], Shashi Thutupalli[1], Anne-Valerie Le Gall[2], Emilia Mauriello[2], Ptissam Bergam[2], Yves Brun[3], Joshua Shaevitz[1], and Tam Mignot[2] — [1]Institute for Integrative Genomics, Princeton University — [2]Institut de Microbiologie de la Méditerranée, CNRS Marseille — [3]Department of Biology, Indiana University, Bloomington

Eukaryotic cells utilize an arsenal of processive transport systems to deliver macromolecules to specific subcellular sites. In prokaryotes, such transport mechanisms have only been shown to mediate gliding motility, a form of microbial surface translocation. Here, we show that the motility function of the Myxococcus xanthus Agl-Glt machinery results from the specialization of a versatile class of bacterial transporters.

Specifically, we used fluorescence microscopy and optical traps to demonstrate that the Agl motility motor is modular and dissociates from the rest of the gliding machinery (the Glt complex) to bind the newly expressed Nfs complex, a close Glt paralogue, during sporulation. Following this association, the Agl system transports Nfs proteins directionally around the spore surface. Since the main spore coat polymer is secreted at discrete sites around the spore surface, its transport by Agl-Nfs ensures its distribution around the spore. Thus, the Agl-Glt/Nfs machineries may constitute a novel class of directional bacterial surface transporters that can be diversified to specific tasks depending on the cognate cargo and machinery-specific accessories.

BP 20.5 Tue 14:15 HÜL 386

**Magneto-aerotaxis in different strains of Magnetotactic bacteria** — •Livnat Landau[1,2], Christopher T. Lefèvre[1], Mathieu Benneta[1], Peter Vach[1], Dennis A. Bazylinski[3], Richard B. Frankel[4], Stefan Klumpp[2], and Damien Faivre[1] — [1]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany — [2]Department of Theory and Bio-Systems, Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany — [3]University of Nevada at Las Vegas, School of Life Sciences, Las Vegas, Nevada 89154-4004 USA — [4]Department of Physics, California Polytechnic State University, San Luis Obispo, California 93407, USA

Magnetotactic bacteria align and swim along magnetic field lines in order to facilitate positioning at an optimal oxygen concentration. Magnetic navigation is accomplished through special magnetic organelles, the magnetosomes, biomineralized, membrane-coated magnetic nanoparticles. We have characterized the magneto-aerotactic behavior of twelve magnetotactic bacteria with various morphologies, phylogenies, physiologies and flagellar apparatus. We have observed five different magneto-aerotactic behaviors that can be described as a combination of distinct mechanisms. Finally, we adapted a model for bacterial aerotaxis to describe magneto-aerotaxis with several different sensing mechanisms. Different sensing mechanisms lead to different behaviors in the presence of conflicting information, i.e. when the magnetic field points in a different direction relative to the oxygen gradient than in the natural environment.

**15 min. break**

**Invited Talk** BP 20.6 Tue 14:45 HÜL 386

**Synthetic mechanobiology: Dissecting and rewiring force-based signaling** — •Sanjay Kumar — University of California, Berkeley, USA

Living cells encounter a variety of mechanical signals encoded within their microenvironment, and these inputs can strongly regulate many fundamental cell and tissue behaviors. Here we present two complementary approaches we have recently created and applied to dissect and genetically manipulate this force-based signaling in living cells. First, we have used laser nanosurgery to spatially map the nanomechanical properties of actomyosin stress fibers. We have combined this approach with advanced molecular imaging tools (FRAP, FRET) to relate intracellular tensile forces to the conformational activation of mechanosensory proteins at the cell-extracellular matrix interface and the activities of specific myosin activators and isoforms. Second, we have used the tools of synthetic biology to precisely control the expression and activation of mechanoregulatory proteins in single cells using multiple mutually orthogonal inducer/repressor systems. This capability has enabled us to quantitatively elucidate relationships between signal activation and phenotype and to deconstruct complex signaling networks. In addition to improving our understanding of force-based signaling, these approaches are enabling us to "rewire" how cells communicate with their physical microenvironment, which we view as an important first step towards instructing cell behavior at interfaces between living and nonliving systems.

BP 20.7 Tue 15:15 HÜL 386

**Blood platelet dynamics on structuredsubstrates** — •Rabea Sandmann and Sarah Köster — University of Göttingen, Institut for X-Ray Physics, Friedrich-Hund Platz 1, 37077 Göttingen, Germany

Blood platelets are the first cells to interact with implants and build a scaffold into which other cells are embedded. The implant's surface texture plays an important role for platelet behavior and thus for the correct incorporation of implants into the body. We investigate the reaction of platelets to microstructured surfaces by studying their spreading dynamics as well as the formation of cell protrusions (filopodia and lamellipodia). We observe, that on structured substrates, spreading takes more time than on flat substrates. This may be attributed to the decreased number of filopodia and the preference of these filopodia for certain directions. The spread area over time shows a sigmoidal shape and its turning point coincides with the transition from filopodia to lamellipodia. The phase of cellular retraction that follows spreading starts primarily over the holes. This behavior can be explained, since the parts of the cell that span over the holes are probably the mechanically most instable parts. When the spread area has decreased to values close to those at the turning point, new filopodia are formed. This leads us to the conclusion that platelets can detect their area and react to an area decrease by formation of filopodia to start the spreading process anew.

BP 20.8 Tue 15:30 HÜL 386

**modulation of t-lymphocyte adhesion forces by activation with tnf** — •qian li[1], constanze lamprecht[1], dieter adam[2], and christine selhuber-unkel[1] — [1]Biocompatible Nanomaterials, Institute for Materials Science, University of Kiel, Germany — [2]Institute of Immunology, University of Kiel, Germany

Integrin-mediated T-lymphocyte adhesion to endothelial cells is a crucial step in the mammalian inflammatory response and the elimination of pathogens. In recent years, the outside-in signalling pathway of integrins in response to the proinflammatory cytokine tumor necrosis factor (TNF) was thoroughly studied. In addition, also an inside-out

signalling pathway of integrins in lymphocyte activation by TNF has been reported. How this activation modulates T-lymphocyte adhesion strength and dynamics is still not understood at all. We have chosen a biophysical approach to address this question and applied single-cell force spectroscopy (SCFS) to investigate T-lymphocyte (Jurkat E6-1) cell adhesion to fibronectin, which is naturally present on top of endothelial cell layers. In detail, we approached single Jurkat E6-1 cells to fibronectin-coated surfaces and analyzed cell detachment forces. We found that the addition of TNF significantly increased the maximum adhesion force and detachment energy of the cells, even at sub-second timescales.

BP 20.9 Tue 15:45 HÜL 386

**Modeling ring formation in cell adhesion** — •Daniel Schmidt[1,2], Timo Bihr[1,2], Udo Seifert[2], and Ana-Sunčana Smith[1] — [1]Inst. f. Theor. Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg — [2]II. Inst. f. Theor. Physik, Universität Stuttgart

Cellular adhesion is mediated by pairs of adhesion molecules which form bonds. A famous example is the immune synapse where the adhesion of membranes of antigen presenting cells and different cells of the immune system takes place. The key step in this process involves two pairs of binding partners which upon recognition form a ring pattern, in a process that has not yet been fully understood. We study necessary conditions for the formation of rings in a minimal model within a newly developed Monte Carlo scheme. This simulation framework allows us to simulate the entire adhesion process on experimentally observed time and length scales while maintaining the full information about membrane transmitted cooperative effects between individual adhesion molecules. We show that the competition between the recruitment of adhesion molecules into the zone of contact between two cells and the binding kinetics between pairs of binders is sufficient to trigger this particular pattern formation. We find that the ring is transient if one of the binders is immobilized before molecular recognition takes place. However, if both adhesion molecules are mobile, the ring is stabilized through by membrane induced correlations and the ring becomes meta-stable. We compare our results to alternative theoretical models and to experiments in cell-mimetic systems.

## BP 21: Membranes and Vesicles II

Time: Tuesday 14:00–16:00 Location: ZEU 250

BP 21.1 Tue 14:00 ZEU 250

**Interactions of Radical Oxygen Species with Phosphatidylcholine Monolayers and Liposomes** — •Andreas Gröning[1], Heiko Ahrens[1], Frank Lawrenz[1], Thomas Ortmann[1], Gerald Brezesinski[2], Fritz Scholz[3], Doris Vollmer[4], and Christiane A. Helm[1] — [1]Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany — [2]MPI KGF, 14476 Potsdam, Germany — [3]Inst. f. Biochemie, Uni Greifswald, 17487 Greifswald — [4]MPIP, 55128 Mainz, Germany

During times of environmental stress (e.g., UV or heat exposure), levels of reactive oxygen species (ROS) can increase. This may result in significant damage to cell structures. Here we focus on the effect of hydroxyl radicals (produced by Fenton reaction) on model membranes.

For DPPC monolayers at the air/water interface a decrease in the lateral pressure is used as a measure of the efficiency of the radical attack. Combining isotherms, X-ray diffraction and IRRAS we find a partial cleavage of the head group leading to a reduced head group size with negative charge. X-ray reflectivity demonstrates $Fe^{2+}$ binding to the head group, fluorescence microscopy immediate nucleation of new domains in the condensed phase.

The radicals destroy DMPC liposomes, only fragments remain as is observed with confocal microscopy. Differential scanning calorimetry shows that an increasing radical concentration causes a shift of the alkyl chain melting transition to higher temperatures.

Summarising, both monolayers and liposomes solidify on exposure to ROS, consistent with a common molecular mechanism.

BP 21.2 Tue 14:15 ZEU 250

**The complexity of membrane domain formation.** — •Djurre H de Jong[1], Siewert J Marrink[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, Germany — [2]Molecular Dynamics Group, University of Groningen, The Netherlands

Living cells are enveloped by the plasma membrane (PM): a thin layer consisting of a complex mixture of lipids and proteins. Rather than being a "shopping bag" keeping together the cell content, the PM plays an active and diverse role in the functioning of the cell. A fascinating aspect of the PM is the formation of transient, lateral domains, consisting of both lipids and proteins.

The time and length scales at which these membrane domains occur make them difficult to study, both experimentally (too small, too transient) or with simulations of full atomistic detail (too large, too long timescales). Here we use coarse grain molecular dynamics (CGMD) simulations, applying the Martini force field, to gain insight in the dynamics involved. Previously we have used this model to study the partitioning of membrane proteins between different domains in model bilayers and the influence of specific proteins and minor lipid species on the formation of domains. Here we quantify the energetic contributions to phase separation that different variation in system composition have. To this aim we combined the long timescales achieved with the Martini force field with the ability to sample non-physical states using sophisticated free energy sampling methods implemented in the software packages PLUMED and Gromacs.

BP 21.3 Tue 14:30 ZEU 250

**Molecular Requirements for Raft Formation in a Lipid/Cholesterol System** — •Davit Hakobyan and Andreas Heuer — WWU Münster, Institut für Physikalische Chemie, Münster, Germany

Recent comparison of the MARTINI coarse-grained (CG) bilayer system with an equivalent atomistic system comprised of DPPC, unsaturated dilinoleyl phosphatidylcholine (DUPC) lipids and cholesterol (CHOL) showed very good agreement on the phase separation phenomena [1]. Here the properties of CG lipids and CHOL are systematically varied to study the molecular requirements for the raft formation. The DUPC lipid is assimilated to DPPC lipid by modifying the angles, the angle force constants as well as the bead types of the chains. It turns out that the unmixing is largely driven by van der Waals interactions between DPPC - CHOL/DPPC pairs and is nearly independent of the entropy of the DUPC chains. On the other hand reduction of the angle force constant of DPPC chains by 60 % keeps the system mixed suggesting that the entropic contribution of DPPC chains is important for the unmixing. By substituting the CHOL with shorter and stiffer DPPC-like molecules one observes unmixing similar to DPPC/DUPC/CHOL system which suggests the rigid and flat structure of CHOL to play a key role in raft formation. With a stiffened last bead of CHOL the order of DPPC/CHOL domain significantly increases indicating that the conformational entropy of CHOL is important to prohibit the gelation [2]. 1. Hakobyan, Heuer, J. Phys. Chem. B, 2013, 117, 3841. 2. Hakobyan, Heuer, PLOS ONE, In Press.

BP 21.4 Tue 14:45 ZEU 250

**Domain formation in a membrane coupled to an actin network** — •Sina Sadeghi[1], Alf Honigmann[2], Christian Eggeling[2], and Richard Vink[1] — [1]Institute of Theoretical Physics, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Max Planck Institute for Biophysical Chemistry, Department of NanoBiophotonics, Göttingen, Germany

Lateral heterogeneity of the plasma membrane is receiving much attention. In contrast to model membranes which exhibit phase separation below a certain temperature, biological membranes typically do not phase separate. One hypothesis is that the cytoskeleton network on the cytoplasmic side of the cell membrane prevents phase separation. This motivates the study of pattern formation in membranes in the presence of an actin network. To this end, a series of experiments were performed on a supported membrane that was bound to an actin network via certain cross linker lipids (pinning sites). These experiments show that the lipid domain pattern that arises is strongly affected by the interaction of the pinning site with the surrounding diffusing lipids. In the present work, we propose an extended (Ising) model to rationalize these findings. Our model includes the effects of the membrane curvature on the lipid organization. To be precise, we modelled the

elastic properties of the membrane using the Helfrich expansion, and assumed a coupling between the lipid domains and the local membrane curvature. Using computer simulation, we find that this coupling is crucial in order to reproduce the experimental results, especially for the case where the pinning sites have a small affinity for saturated lipids.

BP 21.5 Tue 15:00 ZEU 250

**Probing the influence of soluble domains on the diffusion of peripheral membrane proteins** — •Gernot Guigas and Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Diffusion coefficients of membrane proteins are commonly assumed to be well predicted by the Saffman-Delbrück relation. The latter describes proteins as single membrane-spanning cylinders, i.e. effects of bulky extra-membrane domains and spatial protein interactions at crowded conditions are neglected. However, these quantities potentially play an important role for the survival of parasites of the trypanosome family in the bloodstream of mammals. To evade antibody recognition by the host's immune system, trypanosomes exchange their complete, very dense surface coat of bulky GPI-anchored glycoprotein VSG by a genetic variant within few minutes. Diffusion plays a crucial role for an efficient exchange of the dense VSG coat. We have used coarse-grained membrane simulations to study the diffusion properties of VSG and similar peripheral membrane proteins at crowded conditions. Both protein packing density and the size of the soluble domain have a strong influence on protein mobility. Diffusion coefficients are reduced by almost an order of magnitude when the VSG surface area fraction reaches physiological values of 30% and more. Enlarging the extra-membrane domain results in a similar reduction of VSG's diffusional mobility.

BP 21.6 Tue 15:15 ZEU 250

**Translocation of amphiphilic polymers through lipid bilayer membranes - balanced hydrophobicity versus polarization** — •Marco Werner[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

We discuss adsorption and passive translocation of amphiphilic polymers such as random copolymers [1] through a self-assembled lipid bilayer membrane. By using the bond fluctuation model with explicit solvent [2] we consider copolymers of hydrophilic and hydrophobic sites under variation of the fraction, H, of hydrophobic sites and chain length. Our results indicate a point of balanced hydrophobicity, $H_L = 0.6$, where a slight excess of hydrophobic monomers compensates an additional insertion barrier due to the self-organized packing of the bilayer. Translocation events of shorter polymers through the membrane can be observed close to the balanced condition $H = H_L$. For longer chains, translocations are suppressed due to the "polarization" of the amphiphilic molecules with respect to the interface. Close to the point of balanced hydrophobicity, the polymer induces dynamic and static perturbations in the bilayer and increased permeability with respect to solvent. We give a more general outlook on how to design membrane active polymers with a desired emphasis on either translocation or permeabilization on the onset of balanced hydrophobicity.

[1] T. Goda, Y. Goto, und K. Ishihara, Biomaterials, 31, 2380 (2010).
[2] J.-U. Sommer, M. Werner, und V. A. Baulin, Europhys. Lett., 98, 18003 (2012)

BP 21.7 Tue 15:30 ZEU 250

**Asymmetric phospholipid: lipopolysaccharide bilayers; a Gram-negative bacterial outer membrane mimic** — •Maximilian Skoda[1], Luke Clifton[1], Emma Daulton[1], Arwel Hughes[1], Anton Le Brun[2], Jeremy Lakey[3], and Stephen Holt[2] — [1]ISIS, STFC, Harwell, UK — [2]Bragg Institute, ANSTO, Kirrawee DC,Australia — [3]Institute for Cell and Molecular Biosciences, Newcastle University, Newcastle upon Tyne, UK

The Gram-negative bacterial outer membrane (OM) is a complex and highly asymmetric biological barrier but the small size of bacteria has hindered advances in in-vivo examination of membrane dynamics. Thus, model OMs, amenable to physical study, are important sources of data. Here, we present data from asymmetric bilayers which emulate the OM and are formed by a simple two-step approach. LB deposition of phosphatidylcholine on an SiO2 surface formed the inner leaflet and Langmuir-Schaefer deposition of either Lipid A or Escherichia coli rough lipopolysaccharides (LPS) the outer one. The membranes were examined using neutron reflectometry (NR). NR data showed that in all cases the initial deposition asymmetry was mostly maintained for more than 16 h. This stability enabled the sizes of the headgroups and bilayer roughness of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine and Lipid A, Rc- and Ra-LPS to be clearly resolved. This shows that rough LPS can be manipulated like phospholipids and used to fabricate advanced asymmetric bacterial membrane models using well-known bilayer deposition techniques. Such models will enable OM dynamics and interactions to be studied under in-vivo like conditions.

BP 21.8 Tue 15:45 ZEU 250

**Water-mediated forces at hydrophilic and hydrophobic surfaces** — •Matej Kanduc[1], Emanuel Schneck[2], and Roland Netz[1] — [1]Free University Berlin, D-14195 Berlin, Germany — [2]Institut Laue-Langevin, Grenoble, France

Using all-atom molecular dynamics simulations, we study water-mediated interactions between surfaces of various polarities in order to elucidate the relation between the repulsive hydration and attractive hydrophobic forces. We find that the hydration forces are oscillatory in the stiffer membranes, whereas monotonically-decaying in softer ones and they correlate with oscillations in density profiles. Based on the simulations at prescribed chemical potential and the free energy analysis, we determine the "Berg limit" crossover, which delimits the repulsive and attractive regimes. The surface attraction appears as a result of water cavitation, since the liquid water between the membranes becomes metastable with respect to vapor phase. We also show that the attraction repulsion regimes highly correlate with the formation and breaking of overall hydrogen bonds upon bringing the surfaces in close-contact state.

## BP 22: Networks, From Topology to Dynamics I (joint SOE/DY/BP)

Time: Tuesday 15:00–16:00 Location: GÖR 226

BP 22.1 Tue 15:00 GÖR 226

**The Hidden Geometry of Complex, Network-Driven Contagion Phenomena** — •Dirk Brockmann[1,2] and Dirk Helbing[3] — [1]Humboldt University, Berlin — [2]Robert Koch Institute, Berlin — [3]ETH Zurich

The global spread of epidemics, rumors, opinions, and innovations are complex, network-driven dynamic processes. The combined multiscale nature and intrinsic heterogeneity of the underlying networks make it difficult to develop an intuitive understanding of these processes, to distinguish relevant from peripheral factors, to predict their time course, and to locate their origin. We show that complex spatiotemporal patterns can be reduced to surprisingly simple, homogeneous wave propagation patterns, if conventional geographic distance is replaced by a probabilistically motivated effective distance[1]. In the context of global, air-traffic-mediated epidemics, we show that effective distance reliably predicts disease arrival times. Even if epidemiological parameters are unknown, the method can still deliver relative arrival times. The approach can also identify the spatial origin of spreading processes. We validate the approach by application to data on the worldwide 2009 H1N1 influenza pandemic, the 2003 SARS epidemics and the 2011 outbreak of EHEC/HUS in Germany.

D. Brockmann, D. Helbing, Science (2013)

BP 22.2 Tue 15:15 GÖR 226

**Spread of Infectious Diseases with Finite Infectious Period on Temporal Networks** — •Andreas Koher, Lucian Willareth, Hartmut Lentz, and Igor M. Sokolov — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Traversal in temporal networks is only possible, if paths are formed by a causal sequence of edges. Recently, a matrix formalism has been introduced in order to compute the causal path structure of temporal

networks [1]. This formalism describes the spread of infectious diseases that can traverse the network even after arbitrary waiting times, i.e. a SI-model (susceptible-infected-model). Many infectious diseases however possess a finite infectious period, i.e. the time period after which the infection dies out, if it is not passed on. This can be implemented as an SIS or SIR (susceptible-infected-recovered) model, respectively. In this work, we introduce a novel matrix formalism that allows for an explicit consideration of finite infectious periods, which gives a more realistic model of outbreak scenarios. As a central result, we compute the critical infectious period necessary in order to allow for percolation on a given temporal network. The introduced methods can be implemented efficiently and we demonstrate their capability on different datasets.

[1] Lentz et al., Unfolding Accessibility Provides a Macroscopic Approach to Temporal Networks, Phys. Rev. Lett. (2013)

BP 22.3 Tue 15:30 GÖR 226

**Dynamics of Manufacturing Supply Networks** — •Thilo Gross — University of Bristol

High-value manufacturing builds on increasingly complex supply networks. In contrast to classical supply chains these networks have a high connectivity and can contain loops and hubs. Failure of the supply network can cause business disruptions associated with high financial losses. Presently, already more than 30% of such losses are caused by cascading effects that propagate through the system. In the face of this threat mathematical tools are needed to assess the robustness and resilience of supply networks and identify vulnerabilities. In this talk I present modelling approaches and results on the stability of dynamical manufacturing supply networks. In particular, I identify potential bifurcations of the network and propose a method to identify the most critical suppliers in large networks.

BP 22.4 Tue 15:45 GÖR 226

**Automatic discovery of plausible network models** — Telmo Menezes[1,2] and •Camille Roth[1] — [1]Centre Marc Bloch Berlin, CNRS — [2]Centre d'Analyse et de Mathématique Sociales, CNRS/EHESS

A methodology is proposed to discover plausible network generators for complex networks. Generators are defined as computer programs that define local morphogenetic behaviors. We employ a machine learning technique inspired by biological Darwinism to look for generators that produce synthetic networks which match a number of metrics on target real networks. We use a number of metrics that capture both global and fine-grained structural characteristics of networks. Remarkably, when applied on networks stemming from prototypical models of the Erdös-Rényi or Barabási-Albert sort, our approach generally discovers the exact original generator. Empirical validation of our methodology is then presented in the form of a number of plausible generators for a series of five real networks, including a simple brain and a social network.

## BP 23: Cytoskeleton (joint BP/CPP)

Time: Wednesday 9:30–13:00 Location: HÜL 386

**Topical Talk** BP 23.1 Wed 9:30 HÜL 386

**Intermediate filaments - mechanical building blocks and dynamic elements of the cell** — •Sarah Köster — Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, Germany

Intermediate filaments (IFs) are a major component of the eukaryotic cytoskeleton. By contrast to actin filaments and microtubules, which are highly conserved throughout cell types and organisms, IFs are divers and are believed to define cellular mechanics to a considerable degree. In the cell, IFs form complex hierarchical networks and bundles that are linked to other cytoskeletal proteins. In vitro experiments on purified proteins in combination with cell experiments thus provide insight into the mechanical and dynamic properties of IFs. Following this concept, we investigate the mechanical characteristics of individual purified IFs in confinement and inter-filament interactions mediated by multivalent cations. In the cell, bundling of IFs is more complex as various regulatory proteins are involved. Despite this complexity, direct observation of the bundle-and network-dynamics sheds light onto the mechanical and structural properties of the bundles themselves as well as of the surrounding cytoplasm.

BP 23.2 Wed 10:00 HÜL 386

**Keratin 8/18 Networks and their Interplay with Different Crosslinkers** — •Ines Martin[1], Tobias Neckernuss[1], Tobias Paust[1], Michael Beil[2], Harald Herrmann[3], and Othmar Marti[1] — [1]Department of Experimental Physics, Ulm University, Ulm, Germany — [2]Clinic of Internal Medicine I, Ulm University, Ulm, Germany — [3]Division of Molecular Genetics, German Cancer Research Center (DKFZ), Heidelberg, Germany

The keratin 8/18 dimer is a structural building block of intermediate filaments (IFs), which are basic constituents of the cytoskeleton in epithelial cells. They are responsible for the stiffness of cells and responses to mechanical stimuli. The understanding of the cytoskeleton is for example important for the characterization of the movement of metastasizing cells.

Keratin filaments can be crosslinked by proteins like plectin, which also link IFs to hemidesmosomes as well as to different constituents of the cytoskeleton. Additionally Keratins can be bundled by ions like $MgCl_2$ or KCl. In this work we assembled keratin 8/18 together with plectin, KCl and $MgCl_2$ *in vitro* to form crosslinked networks. We checked the resulting networks with Scanning Electron Microscopy (SEM) and Immuno-Gold-Labeling. With this we were able to identify the position of plectin molecules. The viscoelastic network properties were measured by passive microrheology and we compared *in vitro* assembled networks without crosslinker and with KCl, $MgCl_2$ and plectin.

BP 23.3 Wed 10:15 HÜL 386

**The role of keratins for the mechanical properties of keratinocytes** — •Gloria Fabris[1], Ronald Springer[1], Lena Ramms[1], Reinhard Windoffer[2], Nicole Schwarz[2], Simone Stiefel[1], Nils Hersch[1], Thomas Magin[3], Rudolf Leube[2], Bernd Hoffmann[1], and Rudolf Merkel[1] — [1]ICS-7, Forschungszentrum Jülich, Germany — [2]Institute of Molecular and Cellular Anatomy, RWTH Aachen, Germany — [3]Translational Centre for Regenerative Medicine and Institute of Biology, University of Leipzig, Germany

Keratin intermediate filaments contribute forming the cytoskeleton of many epithelial cell types: in keratinocytes, for example, type I and type II keratins form a stable network which is supposedly crucial to the mechanical integrity at the cellular and tissue level.

Owing to compensatory keratin expression, the overall contribution of keratin proteins to cell mechanics is difficult to examine in vivo upon deletion of single genes. In our study, we compared wild type mouse epidermal keratinocytes with mutant cells (KO) in which the whole gene cluster expressing members of the keratin family was deleted [1].

Atomic force microscopy indentation experiments showed a highly significant softening of KO keratinocytes when compared with the wild type, which could not be attributed to modifications of other cytoskeletal structures (i.e. microfilaments/microtubules).

Data clearly indicated that the keratin cytoskeleton plays a vital role in conferring stiffness and structural stability to keratinocytes.

[1] Ramms L, et al., PNAS 110(46):18513-18518 (2013).

BP 23.4 Wed 10:30 HÜL 386

**Correlations in the random hydrolysis model of actin filaments and microtubules** — •Thomas Niedermayer and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The polymerization (assembly) and depolymerization (disassembly) of actin filaments and microtubules are pivotal for cell motility, cell adhesion, and cell division. These dynamic processes are controlled by analogous mechanisms: Actin monomers can bind ATP or ADP, whereas tubulin dimers bind either GTP or GDP. In both cases, the hydrolysis of the bound ATP/GTP within the filaments increases the subunit dissociation rate and thereby couples to the stochastic dynamics of filament growth and shrinkage. In the widely discussed random hydrolysis model, which appropriately describes actin and microtubule dynamics in vitro, the hydrolysis rate is identical at each filament subunit. We studied this model by a novel theoretical approach and stochastic

simulations. While mean field solutions, which are considered in the recent literature, fail to describe the filament dynamics in physiologically relevant cases, our analytical approach matches the simulations, as it accounts for correlation effects.

BP 23.5 Wed 10:45 HÜL 386

**Nematic microstructure in biopolymer solutions** — •Marc Lämmel and Klaus Kroy — Institut für Theoretische Physik, Leipzig, Germany

Alignment of polymers is a major mechanism employed by cells to adapt their mechanical strength. Since it is easily induced by steric and energetic interactions, as well as by shear ordering, it is also ubiquitious in biopolymer solutions and gels. Here, we address the influence of such nematic order on the packing structure of semiflexible polymer networks, based on the wormlike chain model. The complicated many-body problem is approached utilizing the concept of the tube [1], which accounts for caging of a test polymer by surrounding filaments. As recently elucidated [2], this cage, rather than being homogeneous, features characteristic variations along the polymer contour. In our approach, the tube is represented through of harmonic confinement potential that is self-consistently determined. In particular, we analyze the effect of local nematic order on the microstructure in terms of the mean tube radius and its distribution [3], for which we observe a remarkable agreement between the analytical predictions and results of hybrid Brownian dynamics/Monte Carlo simulations [4].

[1] Morse, Phys. Rev. E 63, 031502 (2001)
[2] Glaser and Kroy, Phys. Rev. E 84, 051801 (2011)
[3] Glaser *et al.*, Phys. Rev. Lett. 105, 037801 (2010)
[4] Ramanathana and Morse, J. Chem. Phys. 126, 094906 (2007)

BP 23.6 Wed 11:00 HÜL 386

**Elasto-plastic response of reversibly crosslinked biopolymer bundles** — •Poulomi Sadhukhan and Claus Heussinger — Institute for theoretical Physics, University of Goettingen, Friedrich Hund Platz 1, 37077 Goettingen, Germany.

We model cytoskeletal actin bundles under stress in order to explain the elasto-plastic response observed in recent experiments (D. Strehle et al 2011). In doing so, we allow crosslinks to reversibly un- and rebind to the actin filaments. Cross-link reorganization leads to defect formation, which we speculate to be the underlying mechanism responsible for the residual ("plastic") deformation observed in the experiments. The problem is studied for two cases related by the Legendre transformation - under given force and under given deflection of the bundle. Our main result is in agreement with the experiment. We show that a small bending stress can deform the bundle for soft crosslinks, and shows plastic-like behaviour. On the other hand, bundles with stiff crosslinks show elastic behaviour. Along with this, we also observe how the defect position is related to the applied stress and crosslink stiffness and how the required stress to create a residual deformation of the bundle varies with the crosslink stiffness.

**15 min. break**

BP 23.7 Wed 11:30 HÜL 386

**Physical basis of spindle self-organization** — •Jan Brugues[1] and Daniel Needleman[2] — [1]MPI for Physics of Complex Systems/MPI of the Molecular Cell Biology and Genetics. Dresden. Germany — [2]Center for Systems Biology, Harvard University. Cambridge. USA

The spindle, which segregates chromosomes during cell division, is known to be composed of microtubules and hundreds of other proteins, but the manner in which these molecular constituents self-organize to form the spindle remains unclear. Here we use a holistic approach, based on quantitative measurements in spindles of the spatio-temporal correlation functions of microtubule density, orientation and stresses, to identify the key processes responsible for spindle self-organization. We show that microtubule turnover and the collective effects of local microtubule interactions, mediated via motor proteins and crosslinkers, can quantitatively account for the dynamics and the structure of the spindle. We thus reveal the physical basis of spindle self-organization and provide a framework that may be more generally useful for understanding cytoskeletal function in vivo.

BP 23.8 Wed 11:45 HÜL 386

**Structural and mechanical properties of the kinetochore: a biophysical approach.** — •Gheorghe Cojoc[1], Emanuele Roscioli[2], Lijuan Zhang[3], Iva M. Tolić-Nørrelykke[1], Daniela Cimini[2], and Juraj Gregan[3] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Dept. Biological Sciences, Virginia Tech, Blacksburg, VA, USA — [3]Max F. Perutz Laboratories, University of Vienna, Vienna, Austria

The equal partitioning of replicated sister chromatids during cell division depends on proper attachment of kinetochores (KTs) to the microtubules (MTs) emanating from opposite poles. The KT is a multidomain structure that assembles during mitosis to create the MT-binding sites on the centromere. Although mounting evidence suggests that the mechanical properties of KTs may contribute to faithful chromosome segregation, an in-depth characterization of such properties is still lacking. Here, we used merotelic KTs as a model to characterize the mechanical properties of different KT subdomains. Merotelic KT attachment is an error in which MTs nucleating from both poles attach to the same KT. Merotelic KTs persisting into anaphase become significantly stretched, which makes them an ideal model to study KT mechanical properties. We developed an in vivo assay to investigate KT mechanics by releasing the forces acting on the merotelic KT and performing live cell imaging at high spatial and temporal resolution. In our assay, the forces on the KT are released by severing (using laser microsurgery) one of the two MT bundles attached to the stretched merotelic KT.

BP 23.9 Wed 12:00 HÜL 386

**Network elasticity of microtubules cross-linked with ds DNA** — •Meenakshi Prabhune[1], Knut Heidemann[2], Max Wardetzky[2], Christoph F. Schmidt[1], and Florian Rehfeldt[1] — [1]Third Institute of Physics-Biophysics, Georg August University, Göttingen — [2]Department for Numerical and Applied Mathematics, Georg August University, Göttingen

The cytoskeleton is a composite polymer network of cytoskeletal filaments ranging from rod-like microtubules and actin bundles to softer semi-flexible intermediate filaments and actin filaments. Studying the interactions between these heterogeneous filaments is an important step in understanding cell mechanics. Single-component in vitro networks have been studied, but well defined composites are more difficult to construct and are not yet well understood. Here, we have generated heterogeneous networks in vitro by cross-linking microtubules using ds DNA via a hetero-bifunctional cross-linker (sulpho SMCC). DNA as a cross-linker has the unique advantage of having a monodisperse well-defined length, which we vary in our experiments. We have measured the linear and nonlinear shear-elastic response in these networks by macrorheology experiments. Simultaneously, we also compare the experimental data to numerical simulations that we have developed for networks of stiff slender rods connected by semi-flexible linkers.

BP 23.10 Wed 12:15 HÜL 386

**Fluorescent beads disintegrate actin networks** — •Tom Golde, Carsten Schuldt, Jörg Schnauss, Dan Strehle, Martin Glaser, and Josef Käs — Institut für Experimentalphysik 1, Universität Leipzig, Leipzig, Deutschland

We studied the influence of fluorescent polystyrene beads on both entangled and cross-linked actin networks. Thermal bead fluctuations were observed via video particle tracking and analyzed with one-point microrheology. Illumination of fluorescent beads with their appropriate excitation wavelength leads to a drastic softening of actin gels. Other wavelengths and bright field microscopy do not increase thermal bead fluctuations. This effect cannot be significantly reduced by adding common oxygen scavengers. We conclude that the usage of fluorescent beads impairs results when studying the microrheology of actin networks [1].

[1] Golde et al., Physical Review E 88, 044601 (2013)

BP 23.11 Wed 12:30 HÜL 386

**Circular Dorsal Ruffles** — •Erik Bernitt and Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen, 28334 Bremen

Circular Dorsal Ruffles (CDRs) are actin-based structures that form at the dorsal side of adherent cells like, e.g., fibroblasts. CDRs are usually of a ring-like morphology and exhibit a soliton-like propagation. We are interested in the underlying mechanism that leads to CDR formation and propagation. We observe a rich set of phenomena that allows to draw conclusions on the underlying processes. Among them are periodic formations of CDRs at the same location, fusion and

fission dynamics, stationary behavior, and reflection of CDRs.

Apparently, cell morphology plays a key role for CDR dynamics. Despite the typically inhomogeneous shape of adherent fibroblasts we find a universal trajectory in phase space that seems to govern CDR dynamics.

To simplify the constraints set by the morphology, we plate cells on circular fibronectin patterns. This system allows us to compare data acquired on different cells. We find waves that propagate in angular direction with a remarkably conserved velocity.

BP 23.12 Wed 12:45 HÜL 386

**FtsZ rings and helices: physical mechanisms for the dynamic alignment of biopolymers in rod-shaped bacteria** — •Elisabeth Fischer-Friedrich, Benjamin M. Friedrich, and Nir S. Gov — Weizmann Institute of Science, Rehovot, Israel

In many bacterial species, the protein FtsZ forms a cytoskeletal ring that marks the future division site and scaffolds the division machinery. In rod-shaped bacteria, most frequently membrane-attached FtsZ rings or ring fragments are reported and occasionally helices. By contrast, axial FtsZ clusters have never been reported. In this paper, we investigate theoretically how dynamic FtsZ aggregates align in rod-shaped bacteria. We study systematically different physical mechanisms that affect the alignment of FtsZ polymers using a computational model that relies on autocatalytic aggregation of FtsZ filaments at the membrane. Our study identifies a general tool kit of physical and geometrical mechanisms by which rod-shaped cells align biopolymer aggregates. Our analysis compares the relative impact of each mechanism on the circumferential alignment of FtsZ as observed in rod-shaped bacteria. We determine spontaneous curvature of FtsZ polymers and axial confinement of FtsZ on the membrane as the strongest factors. Including Min oscillations in our model, we find that these stabilize axial and helical clusters on short time scales, but promote the formation of an FtsZ ring at the cell middle at longer times. This effect could provide an explanation to the long standing puzzle of transiently observed oscillating FtsZ helices in Escherichia coli cells prior to cell division.

## BP 24: Systems biology

Time: Wednesday 9:30–11:15 Location: ZEU 250

**Topical Talk** BP 24.1 Wed 9:30 ZEU 250

**Collaboration between biomolecules: A physical analysis** — •Ulrich Gerland — Ludwig Maximilians Universität, München, Germany

In biology, different molecules often collaborate on a common task, creating functionalities far beyond what a single type of molecule could accomplish. The physical principles underlying this synergism are only beginning to be understood and exploited in engineered systems. I will present a theoretical study that focuses on enzymes which collaborate to catalyze multi-step biochemical reactions. Cells often coordinate the spatial arrangement of such enzyme teams, into intra- or extracellular clusters, or co-localize them on the cell membrane. We study the impact of the spatial arrangement on the reaction efficiency within reaction-diffusion models [1,2]. Remarkably, although the study of reaction-diffusion systems has a long history, many questions about systems with localized reaction centers remain largely unexplored.

[1] A. Buchner, F. Tostevin, and U. Gerland (2013) Clustering and optimal arrangement of enzymes in reaction-diffusion systems. *Phys. Rev. Lett.* 110, 208104.

[2] A. Buchner, F. Tostevin, F. Hinzpeter, and U. Gerland (2013) Optimization of collective enzyme activity via spatial localization. *J. Chem. Phys.* 139, 135101.

BP 24.2 Wed 10:00 ZEU 250

**A model for sigma factor competition in bacterial cells** — •Marco Mauri and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Bacteria respond to changing environment conditions by switching the global pattern of transcribed genes, making only those products essential for their survival. In response to specific environmental stresses, the cell activates several stress-specific molecules called sigma factors. They bind the core RNA polymerase and direct it towards the appropriate stress response genes. Since more than one sigma species could be present in the cell at the same time, it is believed that the modulation of their availability and competition among them for core RNAP provide important mechanisms for the global switch of the transcriptional program. To analyze this competition, we developed a theoretical model based on earlier work from the Gross lab. Within this framework, we inspect the effects of some factors that modulate the competition such as anti-sigma factors, small RNA, active transcription and non-specific binding. The model shows that a passive regulation of the transcription of the alternative sigma cognate genes is feasible and a more effective upregulation is achieved in competition regime. We also examine under which conditions a stop of transcription of ribosomal RNA as in the stringent response can passively up-regulate transcription driven by alternative sigmas. Our model matches well to in vitro and in vivo measurements here analyzed. The theory supports evidence for a passive global switch of the transcriptional program and gives new insights into RNAP partitioning in the cell.

BP 24.3 Wed 10:15 ZEU 250

**Centrosomes are autocatalytic droplets of pericentriolar material organized by centrioles** — •David Zwicker[1], Markus Decker[2], Steffen Jaensch[2], Anthony A. Hyman[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

During cell division, the mitotic spindle is organized with the help of two centrosomes located at the spindle poles. Centrosomes consist of centrioles that are surrounded by pericentriolar material. The physical nature of centrosomes and in particular of the pericentriolar material remain unclear. We describe centrosomes as liquid-like droplets and study their assembly using a general theoretical description. Our model is based on two forms of the centrosome components: A soluble form in the cytoplasm and a form that tends to phase separate and forms droplets. We show that an autocatalytic chemical transition between these forms can account for the experimentally observed growth dynamics of centrosomes. Such autocatalytic growth requires an initial trigger, which we propose is provides by a catalytic activity of the centrioles. This activity provides a nucleation mechanism that puts centrosome formation under the reliable control by centrioles. Spontaneous homogeneous or heterogeneous nucleation is strongly suppressed in this scenario. Autocatalytic growth can explain rapid centrosome assembly from material provided in the cytoplasm while the control of nucleation by centrioles is reliable. Our theory highlights the role of phase separation in the spatial organization of cells.

BP 24.4 Wed 10:30 ZEU 250

**A Biophysical Taxonomy of Quorum Sensing Networks** — •Bastian Drees and Ilka Bischofs — BioQuant, Center for Quantitative Analysis of Molecular and Cellular Biosystems at Heidelberg University, Heidelberg

Bacteria control their collective behavior in response to population size by encoding information about cell density into a concentration of signaling molecules. To carry out this process, called quorum sensing (QS), bacteria use signaling networks that vary in their organization between different organisms. This diversity in the physical organization (transport mechanism, receptor location, etc.), potentially gives rise to classes of different QS architectures. To introduce a classification scheme we systematically studied the encoding properties of a comprehensive set of 116 generic signal generating network topologies focusing on their sensitivity and noise characteristics. Intimate relationships between architecture and encoder function can be employed to rationalize a hierarchical network classification scheme. Our model shows that almost all signal generating architectures are able to mediate QS. The resulting taxonomic scheme consists of two layers: One layer containing three basic encoder classes that are defined by a characteristic "core network motif" and that share the same qualitative noise and sensitivity behavior, independent of system parameters. The second layer contains five classes of architectures that are composed out of two core motifs and as a result can express complex and counter-intuitive encoding behaviors. Our analysis indicates that different QS systems might enable bacteria to conduct different types of

QS.

**Invited Talk** BP 24.5 Wed 10:45 ZEU 250

**Gene expression in embryos: from single molecules to network dynamics** — •Thomas Gregor — Joseph Henry Laboratories of Physics and Lewis Sigler Institute for Integrative Genomics, Princeton University, Princeton, USA

The nodes of the pattern forming segmentation network in the early fly embryo are transcription factors, i.e. proteins that cross-regulate each other via activating or repressive interactions. Hence, in order to answer questions about the physical underpinnings of this network, obtaining quantitative access to the transcription processes is key. In particular, in addition to proteins, quantitative handles to other molecular species such as RNA-polymerases and mRNA molecules are crucial to understand the transition from one network node to the next. I will report on our recent progress in developing methods to count individual molecules of mRNA in intact embryos, and to monitor the transcriptional activity of nascent mRNA at their site of production on the DNA in living fly embryos. Initial results using these methods will be discussed.

## BP 25: Statistical Physics in Biological Systems (joint DY/BP)

Time: Wednesday 9:30–12:00 Location: ZEU 160

BP 25.1 Wed 9:30 ZEU 160

**Statistics of local multiple sequence alignments** — •Pascal Fieth and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

To assess the significance of alignment scores obtained by comparing DNA or amino acid sequences using sequence alignment, knowledge of the score distribution in the biologically relevant high-scoring region is necessary. The score distribution can analytically be shown to follow a Gumbel extreme value distribution for gapless local alignments. For gapped alignments, however, the distribution can only be obtained numerically. To cover the rare-event region of the distribution, studies of the score distribution of pairwise local alignments were done utilising parallel tempering[1]. They showed that, unlike predicted by previous simple sampling approaches, a Gaussian correction to the Gumbel distribution is necessary in case of finite sequence lengths. Here, this study is expanded to sum-of-pair scores of multiple sequence alignments, i.e. the alignments of more than two sequences, with gaps. Results will be shown for the score distributions of local multiple alignments and compared to previous results for global multiple alignments, where regions with probabilities smaller than $10^{-70}$ could be obtained.

[1] S. Wolfsheimer, B. Burghardt, A.K. Hartmann, *Local sequence alignment statistics: deviations from Gumbel statistics in the rare-event tail*, Algorithms for Molecular Biology (2007)

BP 25.2 Wed 9:45 ZEU 160

**Optimising the spatial structure of BLN protein models by means of "partial distortion"-quench cycles** — •Florian Günther[1,2,3], Arnulf Möbius[2], and Michael Schreiber[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Institute of Physics, Technical University Chemnitz, Germany

The prediction of the spatial structure of a protein based on its amino acid sequence is a challenging problem. Corresponding theoretical studies of the protein folding require highly efficient structure optimisation tools. Here we investigate whether and to what extent the thermal cycling (TC) algorithm [1] is appropriate for determining low energy structures of the BLN protein model by J.D. Honeycutt and D. Thirumalai [2]. In our simulations for 46-, 58-, and 69-bead sequences, the TC algorithm reliably finds the global minimum within reasonable computing time. In comparison to the multi-start local search and simulated annealing approaches, TC turns out to be far more efficient.

In the present work, the BLN model with rigid bonds is studied in detail for the first time. Comparing these results to data for the extended model by Berry *et al.* [3], where stiff springs are substituted for the rigid bonds, we observe several level crossings when varying the spring constant, even for quite hard springs.

[1] A. Möbius *et al.*, Phys. Rev. Lett. **79** (1997) 4297.
[2] J.D. Honeycutt and D. Thirumalai, Biopolymers **32** (1992) 695.
[3] R.S. Berry *et al.*, Proc. Natl. Acad. Sci. USA **94** (1997) 9520.

BP 25.3 Wed 10:00 ZEU 160

**Stochastic Processes with Delays and Their Application to Gene Regulation and Epidemics** — •Tobias Brett and Tobias Galla — The University of Manchester, Manchester, United Kingdom

Many of the systems modeled in biology have memory: not all of the effects of interactions can be well approximated as occurring instantaneously. Examples are transcriptional and translational delays in gene regulation, or recovery periods in the context of infectious diseases. We focus on chemical reaction models with delays. For such processes it is not straightforward to formulate Master equations, and it is not clear how to derive systematic Gaussian approximations. We demonstrate that progress can be made using a path-focused view, based on generating functionals. These do not describe the time-evolution of one-time probability distributions, instead they capture the probabilities of entire paths. We derive analytical expressions for Gaussian approximations for a wide class of delay systems, and apply these to two biological problems in which delay is relevant. One is the susceptible-infective-recovered model in epidemiology and the other a model of delayed autoinhibition in gene regulation. This allows us to characterise the phenomena arising from the combination of intrinsic noise and delayed dynamics.

Reference: T. Brett, T. Galla, Phys. Rev. Lett. **110**, 250601 (2013)

BP 25.4 Wed 10:15 ZEU 160

**Environmental effects on DNA denaturation** — •Christian von Ferber[1] and Yurij Holovatch[2] — [1]AMRC, Coventry University, Coventry, UK — [2]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, Ukraine

We re-consider the Poland and Scheraga model for the DNA denaturation transition where the double DNA strands locally and then globally detach as the transition temperature is attained. Applying a polymer field theory approach we discuss in particular variants of this transition that may occur due to the properties of the environment. We show that different environments may shift the transition further or less towards a first order transition. Effects we discuss are: the presence of (1) uncorrelated and (2) power-law long-range correlated disorder where the latter influences the transition as function of the power law exponent,(3) quality of the solution which may affect the self- and mutual interaction of both single and double strands, and (4) combinations of these effects. We find that the effects studied significantly influence the transition.

**15 min break**

BP 25.5 Wed 10:45 ZEU 160

**Pattern formation in individual-based systems with time-varying parameters** — •Peter Ashcroft and Tobias Galla — The University of Manchester, Manchester, UK

We study the patterns generated in finite-time sweeps across symmetry-breaking bifurcations in individual-based models of evolutionary dynamics and cell differentiation. Similar to the well-known Kibble-Zurek scenario of defect formation, large-scale patterns are generated when model parameters are varied slowly, whereas fast sweeps produce a large number of small domains. The symmetry breaking is triggered by intrinsic noise, originating from the discrete dynamics at the microlevel. Based on a linear-noise approximation, we calculate the characteristic length scale of these patterns. We demonstrate the applicability of this approach in a model of evolutionary game theory with a time-dependent fitness structure, and in a model of cell differentiation, which we relate to Waddington's epigenetic landscape. Our theoretical estimates are confirmed in simulations. In further numerical work, we observe a similar phenomenon when the symmetry-breaking bifurcation is triggered by population growth.

Reference: P. Ashcroft and T. Galla, Phys. Rev. E 88, 062104 (2013)

BP 25.6 Wed 11:00 ZEU 160

**A time-continuous model for E. coli's motion using shot noise** — •Oliver Pohl[1], Marius Hintsche[2], Carsten Beta[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam, Germany

The bacterium Escherichia coli moves with alternating runs and tumbles that occur with a mean tumble rate. In the presence of gradients of a chemoattractant, E. coli performs chemotaxis [1]. It adjusts the tumble rate in response to the time-integrated concentration in order to increase the uptake of the chemical.

We set up a time-continuous model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed. The swimming direction updates according to rotational Brownian motion and additional shot noise, which initiates tumbling events. The speed is not constant as in previous models but is determined by the random shots as well. By analyzing experimental data on swimming trajectories, we adjust the parameters of our model. First, we determine the shot noise from higher moments of the experimental trajectories. Second, we present a novel approach to determine the chemotactic response function, which E.Coli uses to integrate the chemical concentration in time. Finally, we want to use our model to explore the behavior of E. Coli in different chemical concentration profiles.

[1] H.C. Berg, "E.Coli in motion", Springer, New York, (2003)

BP 25.7 Wed 11:15 ZEU 160

**Self-propelled particles with alignment and anti-alignment** — •Robert Grossmann[1], Pawel Romanczuk[1], Markus Bär[1], and Lutz Schimansky-Geier[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Department of Physics, Humboldt-Universität zu Berlin, Germany

It was recently suggested that the observations of vortex structures in the local polarization of dense bacterial suspensions can be explained by a negative viscosity in the hydrodynamic equation for the polar order parameter [1]. Here, we propose a simple model of self-propelled particles interacting via a short-ranged alignment and a long-ranged anti-alignment, which may exhibit negative viscosity. This simple model allows us to systematically derive a coarse-grained description via a one-particle Fokker-Planck equation [2], and to analyze the relation of hydrodynamic transport coefficients on the microscopic parameters of the model. We explore the impact of different approximations required in the derivation of the coarse-grained theory on the validity of the linearized equations. Furthermore, we verify our results by comparing numerical simulations of the microscopic model with predictions of the coarse-grained theory.

[1] Dunkel, J. et al., New J. Phys., 15, 045016 (2013)
[2] Grossmann, R. et. al, New J. Phys., 15, 085014 (2013)

BP 25.8 Wed 11:30 ZEU 160

**Constructing a Stochastic Model of Bumblebee Flights from Experimental Data** — Friedrich Lenz[1], Aleksei V. Chechkin[2], and •Rainer Klages[1] — [1]Queen Mary U. of London, School of Math. Sci., UK — [2]Inst. f. Theor. Physics, NSC KIPT, Kharkov, Ukraine

The movement of organisms is subject to a multitude of influences of widely varying character: from the bio-mechanics of the individual, over the interaction with the complex environment many animals live in, to evolutionary pressure and energy constraints. As the number of factors is large, it is very hard to build comprehensive movement models. Even when movement patterns in simple environments are analysed, the organisms can display very complex behaviours. While for largely undirected motion or long observation times the dynamics can sometimes be described by isotropic random walks, usually the directional persistence due to a preference to move forward has to be accounted for, e.g., by a correlated random walk. We generalise these descriptions to a model in terms of stochastic differential equations of Langevin type, which we use to analyse experimental search flight data of foraging bumblebees [1]. Using parameter estimates we discuss the differences and similarities to correlated random walks. From simulations we generate artificial bumblebee trajectories which we use as a validation by comparing the generated ones to the experimental data [2]

[1] T.C.Ings, L.Chittka, Curr. Biol. **18**, 1520 (2008)
[2] F.Lenz, A.V.Chechkin, R.Klages, PLoS ONE **8**, e59036 (2013)

BP 25.9 Wed 11:45 ZEU 160

**Swarming of self-propelled agents with selective attraction-repulsion interaction - From microscopic dynamics to coarse-grained theories** — •Pawel Romanczuk[1], Robert Grossmann[1], and Lutz Schimansky-Geier[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin — [2]Department of Physics, Humboldt Universität zu Berlin

We propose a model of stochastic self-propelled agents interacting via selective attraction-repulsion interaction, where individuals respond differently to their neighbours depending on their relative state of motion (approach versus movement away) [1]. This kind of social response is directly motivated by visual sensory information available to individuals (e.g. looming stimuli). We show that the model exhibits various modes and collective behaviour and derive a coarse-grained description via a non-linear Fokker-Planck equation, which allows us to formulate hydrodynamic equations for the density and velocity fields of the Toner-Tu type [2]. Finally, we compare the predictions on the linear stability from our coarse-grained theory with the results of individual-based simulations of the microscopic model, and discuss the limitations of the hydrodynamic theory and its region of validity.

[1] Romanczuk P. and Schimansky-Geier L., Interface Focus 2, 746-756 (2012)
[2] Grossmann R., Schimansky-Geier L., Romanczuk P., New J Phys 15, 085014, (2013)

## BP 26: Multi-cellular systems and Physics of Cancer

Time: Wednesday 11:45–13:30 Location: ZEU 250

BP 26.1 Wed 11:45 ZEU 250

**Modeling the electrical excitation in a cross section of the human heart with simultaneous consideration of varied cell-type distribution, fiber-angle rotation and stimulation protocol.** — •Maximilian Eisbach[1], Stefan Fruhner[2], Harald Engel[1], and Markus Bär[2] — [1]TU Berlin — [2]PTB Berlin

The anisotropy of the electrical conduction system in a human heart is believed to play a critical role in the electrical wavefront dynamics. Yet, the validity of rule based approaches for embedding fibre orientation and cell-type distribution remains unclear. We investigated the influence of different fibre assignments and cell type distribution on the propagation of the electrical excitation in a 2D slice obtained from MRI measurements of a human heart. Since a cross section is a radical simplification of the 3D structure of the human heart, we additionally studied the impact of varying stimulation protocols. We conclude that the stimulation position has a greater influence on the shape of the excitation wave in a cross section of the heart, than differing anisotropy of the electrical conduction system.

BP 26.2 Wed 12:00 ZEU 250

**Osmotic effects in MDCK model tissues** — •Damir Vurnek[1], Sara Kaliman[1], Matthias Gebhardt[2], Florian Rehfeldt[3], Katrina Binger[2], and Ana-Sunčana Smith[1] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg — [2]Max-Delbrück Center for Molecular Medicine, Berlin — [3]$3^{rd}$ Institute of Physics-Biophysics, University of Göttingen

The capacity to respond and adapt to changes in the environmental osmotic conditions is vitally important for the functioning of epithelial tissues. We study this response by growing MDCK II model tissues in environments with an increased concentration of mannitol, urea or NaCl. The phase space of tissue viability is established and characterized from isotonic to elevated toxic conditions. Furthermore, we identify the time scales on which the survival, growth and the internal organization of the colony is affected. In young colonies, elevated osmotic conditions suppress the growth. As the age of the colony increases, adaptation takes place, and the colony develops the same morphology as the controls, with the edge at the low and the center at relatively high densities. We show that the appearance of this internal organization is independent of the initial configuration of seeded cells. Apart from the general trends, example of which is the quadratic

growth of the area observed in the young colonies, we characterize the osmolyte-and concentration-specific proliferation rates, growth rates and absolute colony sizes, as well as the steady state cell densities. Finally, we analyze the internal structure of cells within the colony and characterize the changes in their nuclei shape and the evident DNA damage.

BP 26.3 Wed 12:15 ZEU 250

**Size control on the fly ocellar complex pattern** — •Daniel Aguilar-Hidalgo[1], David Becerra-Alonso[2], María Carmen Lemos[3], Antonio Córdoba[3], and Fernando Casares[4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany. — [2]Dept. Engineering and Mathematics - Univ. Loyola Andalucía, Sevilla, Spain. — [3]Dept. Condense Matter Physics - Univ. de Sevilla, Sevilla, Spain. — [4]CABD (CSIC-UPO), Sevilla, Spain.

During development, organs grow until reaching a specific size. Different species show distinct organ sizes maintaining functionality. We are studying the organ growth scalability in the *D. melanogaster* ocellar complex. It comprises three simple eyes, or ocelli, located at the vertices of a triangular patch of cuticle on the fly's forehead. This pattern sets the specification of two mutually alternative cell fates: (1) interocellar cuticle flanked by two (2) ocelli. We developed a mathematical and computational model as a gene regulatory network (GRN) that describe the qualitative aspects of the patterning and predicts several of its properties [1]. In nature, different fly species show different size distribution of the ocellar complex constituents. Is the same GRN able to generate different size distributions? We found that randomized parametric sets show not random but structured size distributions. A study of this distribution on several fly species show the same structure as predicted by the model. This suggests that the same GRN defines different sizes for the ocellar complex, and that the system constrains the possible distribution results, avoiding non-functional structures.

[1] Aguilar-Hidalgo *et al.* Development, (2013) 140 (1), 82-92.

BP 26.4 Wed 12:30 ZEU 250

**Physical Principles of Body Plan Scaling in Planarians** — •Steffen Werner[1], Manuel Beirán Amigo[1], Jochen Rink[2], Frank Jülicher[1], and Benjamin M. Friedrich[1] — [1]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany

In many biological systems, body plan patterning operates at variable length scales during development and regeneration. The flatworm Planarian is a master of regeneration and body plan scaling, inspiring our theoretical work on fundamental principles of scalable pattern formation.

Planarians can grow and actively degrow by more than an order of magnitude in size, depending on feeding conditions, while maintaining shape and function of all parts of the body. Moreover, Planarians can rebuild its entire body plan from a tiny amputation fragment, prompting for size-independent mechanisms of self-organized body patterning.

We are interested in general principles underlying scalable pattern formation that go beyond classical Turing mechanisms. Turing mechanisms provide a means of self-organized patterning that is characterized by an intrinsic length scale, which eventually precludes scaling. We discuss feedback mechanisms that adjust this length-scale to the system size in an autonomous manner, resulting in a minimal model for robust pattern-formation that scales with system size. We are closely collaborating with the experimental lab of Jochen Rink at the MPI CBG (Dresden) to apply our theoretical framework to Planarians.

BP 26.5 Wed 12:45 ZEU 250

**A Distinct Intermolecular FasL Distance Triggers Either Apoptosis or Proliferation in Glioma and Pancreatic Cancer Cells** — •Cornelia Monzel[1], Thomas Kaindl[1], Joel Beaudouin[2,3], Susanne Kleber[2], Marcin Teodorczyk[2,4], Motomu Tanaka[1,5], and Ana Martin-Villalba[2] — [1]Dept. of Physical Chemistry of Biosystems, Heidelberg University, Germany — [2]Dept. of Molecular Neurobiology, DKFZ, Heidelberg, Germany — [3]Dept. of Signal Transduction Biophysics, BioQuant, Heidelberg, Germany — [4]Inst. for Microscopic Anatomy and Neurobiology, Mainz University, Germany — [5]Inst. for Integrated Cell Materials Science, Kyoto University, Japan

The trimerized Fas receptor-ligand (Fas-FasL) interaction has long been described as inducer of apoptosis, but recent studies also suggest its critical role in proliferation or metastasis. In order to elucidate the mechanisms inducing cell death we designed quantitative cell surface models of supported lipid membranes displaying FasL at defined intermolecular distances (6-17 nm). Utilizing live cell imaging, we evaluated the reaction kinetics of cancer apoptosis. Intriguingly, in both glioma and pancreatic cancers an optimal ligand distance for the most effective apoptosis was found, which was accompanied by increased Fas-FasL aggregate formation. In contrast, when we transferred this membrane on microbeads injected into 3D tumors, pronounced proliferation and self-renewal in vivo and in vitro was observed. These findings demonstrate the significant impact of a distinct FasL distance, which results in opposite consequences in single- and multicellular sytems.

BP 26.6 Wed 13:00 ZEU 250

**Multiple mutations in hierarchically organized tissues.** — •Benjamin Werner[1], David Dingli[2], and Arne Traulsen[1] — [1]Max Planck Institute for Evolutionary Biology, Plön Germany — [2]Mayo Clinic, Rochester USA

Cancers are rarely caused by single mutations, but often develop based on the combined effects of multiple mutations. For most cells, the number of possible cell divisions is limited due to various biological constrains, as for example progressive telomere shortening or a hierarchically organized tissue structure. Thus, the risk of accumulating cells carrying multiple mutations is low. Nonetheless, many diseases are based on the accumulation of such multiple mutations. We model a general, hierarchically organized tissue by a multi compartment approach, allowing any number of mutations within a cell. I present closed solutions for the deterministic clonal dynamics and the reproductive capacity of single clones. I show that hierarchically organized tissues strongly suppress cells carrying multiple mutations and derive closed solutions for the expected size and diversity of clonal populations founded by a single mutant within the hierarchy.

References:

Werner B., Dingli D., Lenaerts T., Pacheco J. M., and Traulsen A. Dynamics of mutant cells in hierarchical organized tissues. PLoS Computational Biology 2011(e1002290)

Werner B., Dingli D. and Traulsen A. A deterministic model for the occurrence and dynamics of multiple mutations in hierarchically organized tissues. Journal of the Royal Society Interface 2013 (10)

BP 26.7 Wed 13:15 ZEU 250

**Computer Simulation of the Metastatic Progression and Treatment Interventions** — •Anja Bethge[1], Udo Schumacher[2], and Gero Wedemann[1] — [1]CC Bioinformatics, University of Applied Sciences Stralsund, Germany — [2]Institute for Anatomy and Experimental Morphology, University Medical Center Hamburg-Eppendorf, Germany

The process of metastasis formation is still subject of discussion and even established models differ considerably in several basic details and conclusions drawn from them. A computer model was developed which permits comparison of different models quantitatively with clinical data and which additionally predicts the outcome of treatment interventions. It is based on a discrete event simulation protocol. The growth of the primary tumour is described via analytical functions, while a rate function models the intravasation events of the primary tumour and its metastases. Events describe the behaviour of the emitted malignant cells until the formation of new metastases. Using the computer model we investigated different questions: Are metastases able to metastasize? Is metastasis an early or a late event? Do metastases undergo a dormancy phase before they start to grow out into a macro metastasis? (Bethge et al. PLoS ONE 7(4): e35689, 2012) We studied the effects of different treatments, such as the resection of the primary tumour, radionuclide therapy, radioembolization and chemotherapy in the model.

# BP 27: Modelling of non-linear dynamics in biological movement (focus session, joint BP/DY)

Time: Wednesday 14:00–16:30 Location: ZEU 250

**Topical Talk** BP 27.1 Wed 14:00 ZEU 250

**Legged locomotion. - From biology to mechanics and return.** — •Reinhard Blickhan — Science of Motion, Jena, Germany

The locomotory system of animals has to cope with external and internal physical conditions confining and shaping the evolutionary space. This space can be probed by combining experimental observations with modelling supported by numerical simulations. To sustain locomotion animals are enforced to use oscillatory modes. In terrestrial locomotion this led to the development of legs in arthropods and vertebrates. Physical suitability combined with the requirement to enhance power and/or efficiency and to reduce or facilitate the control effort shape the space of solutions. We can show that gaits such as bipedal walking, grounded running, and running do represent an outcome of a compliant system being operated under different initial conditions. As nonlinear systems these systems inherit the property of attractive modes of operation which are used to reduce the control effort. During locomotion the legs as structural elements must fulfil their prescribed task efficiently. Segmentation of legs must prove itself with respect to this demand. The muscle as a common actuator is traded through evolution. Nevertheless, we start to understand that muscles seem to aggregate properties such as compliance, damping, and a geared output in a rather suitable and adaptable way. An integrative view covering the different levels of organization and the vast range of designs may help us to deduce general principles.

BP 27.2 Wed 14:30 ZEU 250

**Learning Motor Skills with Information-Theoretic Approaches** — •Jan Peters[1,2], Christian Daniel[1], and Gerhard Neumann[1] — [1]Technische Universität Darmstadt — [2]Max Planck Institut für Intelligente Systeme

Synthesizing new motor skills from data has been a long standing vision of robotics, artificial intelligence, and the cognitive sciences. A first step towards this goal is to create approaches that can learn tasks triggered by environmental context or higher level instruction. However, learning techniques have yet to live up to this promise as only few methods manage to scale to high-dimensionality of humans and anthropomorphic robots. In this talk, we investigate a general framework suitable for learning motor skills in robotics and for explaining human movement learning which is based on the information-theoretic principles, such as movement organization, representation and acquisition by information entropy. As a result, the framework involves generating a representation of motor skills by parameterized motor primitive policies acting as building blocks of movement generation, and a learned task execution module that transforms these movements into motor commands. We discuss task-appropriate information-theoretic learning approaches for movements and illustrate their effectiveness on human movement data and in robot motor skill learning on both toy examples (e.g., paddling a ball, ball-in-a-cup) and on playing robot table tennis.

BP 27.3 Wed 14:45 ZEU 250

**Humans run like pogosticks - with ankles** — •Horst-Moritz Maus[1], Shai Revzen[2], John Guckenheimer[3], Christian Ludwig[1], Johann Reger[4], and Andre Seyfarth[1] — [1]TU Darmstadt, Deutschland — [2]University of Michigan, Ann Arbor, USA — [3]Cornell University, Ithaca, USA — [4]TU Ilmenau, Deutschland

Running is an essential mode of human locomotion. Its large number of biomechanical and neural degrees of freedom are often modeled as a simple Spring Loaded Inverted Pendulum (SLIP). The SLIP body bounces as if on a pogo stick, pivoting on its spring leg and then jumping through a ballistic aerial phase. Updating SLIP model parameters to fit each step can result in trajectories that follow an observed path much more closely. These parameter updates represent a control input modulating the uncontrolled SLIP dynamics to obtain human-like movement and stability. Here we systematically construct a minimalistic *ankle-SLIP* model from measurements of humans running on a treadmill. Using Data Driven Floquet Analysis we identify candidate predictors for the parameter changes. Selecting a predictor related to ankle state allows us to predict running motion stride to stride and mimic rates of recovery from perturbation. We reveal inherent limitations in predictions made by other SLIP variants. Our methods produce a systematic means to search for prediction enhancing, yet low dimensional models of rhythmic processes in the physical sciences. More directly the "ankle-SLIP" models may impact gait assessment in sports and in clinical contexts and suggest control strategies for humanoid robots and prosthetic limbs.

BP 27.4 Wed 15:00 ZEU 250

**Quantifying control effort of biological and technical movements: an information entropy based approach** — •Daniel Häufle[1,2], Michael Günther[1], Günter Wunner[2], and Syn Schmitt[1,3] — [1]Institut für Sport- und Bewegungswissenschaft, Universität Stuttgart, Germany — [2]Institut für Theoretische Physik 1, Universität Stuttgart, Germany — [3]Stuttgart Research Centre for Simulation Technology, Universität Stuttgart, Germany

In biomechanics and biorobotics muscles are often associated with reduced movement control effort compared to technical actuators. This is based on the notion that the muscle properties positively influence movement control and allow for simpler controllers. Other physical measures, such as energy consumption, stability, or jerk, have already be applied to compare such systems. However, previous definitions of control effort were based on system specific measures, such as voltages, forces, muscle activity, etc., which made it impossible to quantitatively compare the control effort of different actuation systems. Here, a system independent measure of control effort based on information entropy is presented. By calculating the Shannon information entropy of all sensor signals required for control, models of biological and technical control systems can be compared. Exemplarily applied to (biomechanical) models of hopping it reveals that the required information for controlling hopping is only $I = 32$bit with a muscle vs. $I = 660$bit with a DC-motor. This approach to control effort is thus applicable to and comparable across completely different actuators and control approaches.

BP 27.5 Wed 15:15 ZEU 250

**COMPUTATIONAL MODEL FOR A FLEXIBLE SENSORIMOTOR MEMORY BASED ON A RECURRENT NEURAL NETWORK** — •Kim Joris Boström and Heiko Wagner — Motion Science, University of Münster, Germany

The motor system has the unique capacity to learn complex movements in a flexible manner. Using recent recurrent network architecture based on the reservoir computing approach, we propose a computational model of a flexible sensorimotor memory for the storage of motor commands and sensory feedback into the synaptic weights of a neural network. The stored patterns can be retrieved, modulated, interpolated, and extrapolated by simple static commands. The network is trained in a manner that corresponds to a realistic exercising scenario, with experimentally measured muscular activations and with kinetic data representing proprioceptive feedback. The model may help to explain how complex movement patterns can be learned and then executed in a fluent and flexible manner without the need for detailed attention. Furthermore, it may help to understand the reafference principle in a new way, as an internal feedforward model for the prediction of expected sensory reafference would no longer be necessary. Instead, the reafference would be learned together with the motor commands by one and the same network, so that neural resources were exploited in a highly efficient way.

BP 27.6 Wed 15:30 ZEU 250

**A COMPUTATIONAL MODEL EXPLAINS THE RELATIONSHIP BETWEEN MUSCULAR CO-ACTIVATION, REFLEXIVE CONTROL AND SELF-STABILITY** — •Heiko Wagner and Kim Joris Boström — Motion Science, University of Münster, Germany

Sustaining stability during bipedal locomotion poses a challenge to the neuro-muscular-skeletal system, not only for the extremities but also for the spine. Commonly, a major role in maintaining stability is attributed to the reflex control system, which, however, is limited by the neural conduction velocity. For this reason, the concept of self-stability has been introduced, which claims that the mechanical properties of the muscular-skeletal system are exploited to maintain stability via muscular co-activation. Based on a computational model, we analyze the relationship between muscular co-activation, reflexive control and self-stability. The model includes pelvis, rib cage, and

lumbar spine, as well as 90 Hill-type muscles, each endowed with a delayed monosynaptic reflex based on the lambda model. We show that muscular co-contraction not always increases the stability of the system, but rather that for a given reflex delay time there exists an optimal amount of co-contraction. These results may have an impact on the understanding of the motor control system in general, and in particular of the pathological reflex delay found in patients with low back pain.

BP 27.7 Wed 15:45 ZEU 250

**How to turn the non-linear muscle into a linear all-purpose tool** — •Karl Theodor Kalveram — Heinrich Heine Universität Düsseldorf, Germany — Technische Universität Darmstadt, Germany

The three basic categories of biologically motivated tasks that we discriminate we call "reaching", "cycling" and "enforcing". Because in all these activities the physical environment has to be influenced in a scaled manner, the organism must provide appropriately scaled forces. Our muscular-skeletal system solves those problems. We ascribe this to the organism's property to generate forces by muscular activation, and to generate this activation through neural stimulation. It remains, however, the open question, how to specify that stimulation, which exactly produces that forces, which are necessary to complete the respective task correctly?

Here we propose a control schema, which makes the non-linear Hill-type muscle a multiple-purpose tool for solving the biologically imposed motor tasks mentioned above. We achieve this by training an artificial neural network by a two-step auto-imitative learning algorithm (a special type of learning by regression), which makes the network an adaptive inverse controller of the physical environment to be controlled.

BP 27.8 Wed 16:00 ZEU 250

**Computer simulation in biomechanics – past, present, future** — •Hanns Ruder[1] and Syn Schmitt[2] — [1]Theoretische Astrophysik, Universität Tübingen — [2]Human Movement Simulation Lab, Universität Stuttgart

Since the beginning of science, humans wonder about, observe, and try to understand Nature. They do so by using the available tools and methods of their time to the best of their knowledge. In classical physics, over a century ago, research on the phenomena of life was common and driven by the desire to test the universality of physical laws. Already in 1906, Otto Fischer published theoretical considerations on studying the mechanics of human movement. Later, with the invention of computers, numerics helped researchers to solve more complex problems. It is now possible to study the birth and death of stars and the history of our universe. These new possibilities that come with Simulation technology are said to be the scientific paradigm of our age encouraging researchers from all disciplines to use these new methods. As physicists, we use reduced models to explore Nature and, for example in biomechanics, seek principles of human movement. We share the understanding that the very same forces which move the stars in the universe move the hips to let humans walk. Thus, computer simulations can help to understand the phenomena of human movement.

In this talk, we will discuss the organisation of biological material fulfilling the known principles of physics to walk, run, or jump. In short: from wobbling masses to intervertebral discs.

## BP 28: Protein structure and dynamics II

Time: Wednesday 15:00–18:30 Location: HÜL 386

**Topical Talk** BP 28.1 Wed 15:00 HÜL 386

**Single Molecule Mechanics of Proteins** — •Matthias Rief — Physikdepartment der TUM, James-Franck-Str., 85748 Garching, Germany

The development of nano-mechanical tools like Atomic Force Microscopy and optical traps has made it possible to address individual biomolecules and study their response to mechanical forces. In my talk, I will show how single molecule mechanical methods can be used to study the folding and interaction of proteins. Examples include the folding of calmodulin as well as the interaction of the cytoskeletal protein filamin with transmembrane proteins.

BP 28.2 Wed 15:30 HÜL 386

**Variable Temperature Single Molecule Force Spectroscopy of an Extremophilic Protein** — •Katarzyna Tych[1,2], Toni Hoffmann[1,2], David Brockwell[2], and Lorna Dougan[1,2] — [1]Molecular and Nanoscale Physics Group, School of Physics and Astronomy, University of Leeds, LS2 9JT, UK — [2]Astbury Centre for Structural Molecular Biology and Institute of Molecular and Cellular Biology, University of Leeds, LS2 9JT, UK

Extremophiles (organisms which survive and thrive in the most extreme chemical and physical conditions on Earth) exhibit a range of fascinating cellular- and molecular-level adaptations. The flexibility of extremophilic proteins is one of the key determinants of their ability to function at the extremes of environmental temperatures.

We use single molecule force spectroscopy (SMFS) by atomic force microscopy (AFM) to measure the effect of temperature on the mechanical stability and flexibility of a protein derived from a hyperthermophilic organism.

The study was performed using an AFM SMFS instrument with variable temperature capabilities. We study temperature-dependent changes in the unfolding energy landscape of this protein by measuring changes in the unfolding force with temperature in combination with Monte Carlo simulations. We find that the position of the transition state to unfolding shifts away from the native state with increased temperature, reflecting a reduction in the spring constant of the protein and an increase in structural flexibility [1].

[1] K. M. Tych et al. (2013), Soft Matter (9): 9016-9025

BP 28.3 Wed 15:45 HÜL 386

**Determining the protein folding core: an experimental and computational approach** — •Jack Heal, Claudia Blindauer, Robert Freedman, and Rudolf Römer — University of Warwick, Coventry, England, CV4 7AL

The protein folding problem has been a prevalent concern of structural biology for more than 50 years. We study the folding process by identifying an experimental 'folding core' through hydrogen-deuterium exchange NMR (HDX) as well as a computationally determined folding core based on a combination of coarse-grained simulations using the software FRODA and rigidity analysis using FIRST. We test whether such rapid methods can reliably predict the results of HDX experiments. Our experimental system is Cyclophilin A (CypA), an enzyme that helps proteins to fold. It also binds to and aids the function of the immunosuppressant drug cyclosporin A (CsA) as well as binding to the HIV-1 capsid protein. We characterise the protein and its interaction with CsA using circular dichroism and fluorescence spectroscopy in addition to HDX experiments. From the set of slowly exchanging residues we establish the HDX folding core for both the unbound CypA and the CypA-CsA complex. We are able to improve upon the prediction from the established method of FIRST by using FRODA in combination with normal mode analysis. To accomplish this, we introduce a method of tracking the surface-exposure of backbone N-H atoms through the simulation. In this way, we are in the process of designing computationally undemanding methods that can predict the results of sophisticated experiments characterising ligand binding.

BP 28.4 Wed 16:00 HÜL 386

**Protein dynamical transition * Insights from a combination of neutron scattering and MD simulations** — •Kerstin Kämpf and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt

Evaluating the temperature-dependent mean square displacement (MSD) of proteins with neutron scattering (NS) a non-linear increase due to anharmonic dynamics is found well below room temperature [1]. It is still under debate whether this phenomenon, denoted as protein dynamical transition, occurs in one or two steps and whether these steps result from to a true dynamical onset or from local ($\beta$-) [2] or structural ($\alpha$-) [3] relaxations entering the time window. A promising approach to clarify these issues is to combine NS data with MD simulations [4]. Application of such combination to hydrated elastin shows that NS data obtained from backscattering experiments are highly con-

sistent with MD results. We find that anomalous internal protein dynamics, leading to a subdiffusive time dependence of the MSD and a power-law or logarithmic-like decay of correlation functions [5], dominates the findings in the time window of the experiments. The increase of the MSD is thus a signature of the onset of complex internal protein motion.

[1] Doster et al, Nature, 337, 754, (1989).
[2] Capaccioli et al. J. Phys. Chem. B, 111, 8197, (2007).
[3] Doster et al, J. Non-Cryst. Sol., 357, 622, (2011).
[4] Hong et al, Phys. Rev. Lett., 107, 148102, (2011).
[5] Kämpf et al., J. Chem. Phys., 137, 205105, (2012).

BP 28.5 Wed 16:15 HÜL 386

**Bistable retinal Schiff base photo-dynamics of the histidine kinase rhodopsin HKR1 from the green alga *Chlamydomonas reinhardtii*** — •Alfons Penzkofer[1], Meike Luck[2], Tilo Mathes[2,3], and Peter Hegemann[2] — [1]Fakultät für Physik, Universität Regensburg, Universitätsstrasse 31, D-93053 Regensburg, Germany — [2]Institut für Biologie/Experimentelle Biophysik, Humboldt Universität zu Berlin, Invalidenstrasse 42, D-10115 Berlin, Germany — [3]Department of Exact Sciences / Biophysics, Vrije Universiteit, De Boolelaan 1081A, 1081 HV Amsterdam, The Netherlands

The photo-dynamics of the recombinant rhodopsin fragment of HKR1 [1] was studied. The retinal cofactor of HKR1 exists in two Schiff base forms, RetA (deprotonated 13-*cis* retinal) and RetB (protonated all-*trans* retinal). Blue light exposure converts RetB fully to RetA. UVA light exposure converts RetA to RetB and RetB to RetA giving a mixture of both. The quantum efficiencies of photo-conversion of RetA to RetB and RetB to RetA were determined to be 0.096±0.005 and 0.405±0.01, respectively. In the dark, thermal equilibration occurs between RetA and RetB with a time constant of about 3 days giving mole fractions of 0.8 RetA and 0.2 RetB. Ground state and excited state potential energy curve schemes for the inter-conversion of RetA and RetB were developed. The photo-induced inter-conversions of RetA and RetB are caused by excited-state isomerization on a picosecond timescale, proton transfer, and retinal Schiff base - rhodopsin apoprotein ground-state equilibration on a millisecond timescale.

[1] M. Luck et al., J. Biol. Chem. 287 (2012) 40083.

BP 28.6 Wed 16:30 HÜL 386

**Terahertz spectroscopy on amino acids** — •Sebastian Emmert, Martin Wolf, Peter Lunkenheimer, and Alois Loidl — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

All known proteins are built up from a set of 23 standard amino acids. Their three-dimensionally folded structure is mainly determined by the non-covalent interactions of the amino acid residues, such as hydrogen bonds. Therefore it is crucial to study the binding abilities and vibrational properties of these basic building blocks, to achieve a better understanding of the dynamics of the biological macromolecules.

With the novel technique of terahertz time-domain spectroscopy the interesting, but only rarely explored spectral region between the dielectric and the optical frequency regime can be covered. The amino acids in their crystalline state show numerous characteristic resonant features in the range 0.2 THz to 5 THz. It is shown that only by a thorough investigation of the temperature evolution of these spectral features and by a comparison with additional experimentally and theoretically obtained data, a complete assignment of all resonances is made possible. For this purpose, spectra of various amino acids were measured in the temperature range 4 K to 300 K. Fits were performed to quantify the temperature-induced shifts and intensity variations. In this way, spectral contributions from intra- and intermolecular vibrations could be separated by means of their anharmonicity and the dynamics of specific functional groups could be studied.

BP 28.7 Wed 16:45 HÜL 386

**Genetically Encoded Spin Labelled Artificial Amino Acids** — •Malte Drescher, Moritz Schmidt, and Daniel Summerer — Konstanz Research School Chemical Biology and Department of Chemistry, University of Konstanz, Germany

Recent publications demonstrate the ability of electron paramagnetic resonance spectroscopy (EPR) to provide structural, dynamical and functional data on biomacromolecules in cells. Of particular interest are distance measurements in the nanometer range. The advantages of the method are sensitivity, selectivity, the lack of any limitation imposed by the size of the macromolecule, and the possibility to get information on coexisting conformations via analyzing distance distributions. However, so far, these approaches require microinjection of spin-labelled macromolecules. Moreover, the biomolecules transferred to cells by these means have limited access to natural mechanisms of cellular processing like folding, localization, posttranslational modification and natural decay.

Here, we show for the first time the successfull incorporation of a genetically encoded modified lysine amino acid containing 2, 2, 5, 5, -tetramethyl-pyrrolin-1-oxyl-label into various positions in GFP and TRX mutants in E.coli. First EPR distance measurements on extracted proteins demonstrate the potential of this novel approach.

**15 min. break**

BP 28.8 Wed 17:15 HÜL 386

**Structure and dynamics of interfacial water associated with the climate-active ice nucleating proteins probed by sum frequency generation spectroscopy** — •Ravindra Pandey[1], Janine Fröhlich[2], Ulrich Pöschl[2], Ruth Livingstone[1], Mischa Bonn[1], and Tobias Weidner[1,3] — [1]Max-Planck Institute for Polymer Research, Mainz — [2]Max-Planck Institute for Chemistry, Mainz — [3]Chemical Engineering, University of Washington, USA

Specific Bacteria such as Pseudomonas syringae effectively attack plants by using ice-nucleating proteins (INP) anchored to their outer cell surfaces. INP promotes the growth of ice crystals. To understand the ice formation by INP, it is important to understand the molecular mechanisms by which INP interact with water molecules. In this study, we have investigated the interaction of a monolayer of the INP with water molecules at the air-water interface using static and time resolved sum frequency generation spectroscopy. When cooling the monolayer of the INP with water molecules from room temperature to near-freezing temperature, an increase in the structural order of interfacial water molecules was observed. This effect was not observed for water surface or for proteins lacking ice nucleating activity. By using femtosecond pump probe SFG spectroscopy, we found a decrease of the lifetime of the O-D stretch vibrations as a function of temperature. This may be explained by strongly bound O-D groups, which play a decisive role in the ice nucleating activity. The specific binding at lower temperatures could be due to side chain orientations, which emulate the lattice of ice and hence promote the ice formation.

BP 28.9 Wed 17:30 HÜL 386

**Characterizing Protein Adsorption by *In situ* Atomic Force Microscopy at Single Protein Resolution** — •Christian Kreis, Jonas Heppe, Christian Spengler, Hendrik Hähl, and Karin Jacobs — Department of Experimental Physics, Saarland University, Saarbrücken, 66041, Germany

The adsorption of proteins to surfaces is governed by the mutual interactions of proteins, solution and substrate. To fully characterize the interactions, we have shown before that also the long range van der Waals forces arising from the subsurface of the substrate have to be taken into account [1,2]. However, the uppermost layer defines the surface chemistry and is dominating the strength of the interfacial energy. Studies using e. g. ellipsometry or X-ray reflectometry observe a strong influence of the surface chemistry on protein adsorption. These studies, however, average over hundred thousands of proteins in the measurement and the spatial arrangements of the proteins remain unknown. To resolve the latter, we applied *in situ* AFM measurements in buffer solution and characterized the different protein distributions on hydrophilic and hydrophobic silicon wafers. Additionally, a strong denaturation of the studied proteins can be observed. These results demonstrate the influence of the surface chemistry on protein adsorption and help to elucidate the differences in adsorption kinetics or the final adsorbed layer.

[1] Y. Schmitt et al. *Biomicrofluidics* **4** (2010) 032201
[2] H. Hähl et al. *Langmuir* **28** (2012) 7747–7756

BP 28.10 Wed 17:45 HÜL 386

**Adsorptive Capability and Conformational Efficiency between Lysozyme and Nanosilica/-diamond at pH=7-13** — •Victor Wei-Keh Chao — Department of Chemical and Materials Engineering, National Kaohsiung University of Applied Sciences, 80782 Kaohsiung, Taiwan. — Victor Basic Research Laboratory, e.V. Gadderbaumer-Str. 22, D-33602 Bielefeld, Germany.

Adsorption dynamics of lysozyme and nanosilica(NS)/-diamond(ND) with diameter 100 nm and 0.25 $\mu$g/$\mu$L, lysozyme in 0-1000 nM of 7

mM PPBS at pH=7, 9, 11, and 13 have been investigated by Fluorescence spectroscopy. Chem. instead of phys. adsorption, as well as modification of nanosurface may be necessary for the further investigation of nanocarring of protein or drug through pH-gradients in vivo. Surface of ND was acidified and with approx. 7 % of all covered with COOH groups. Because the acidified surface was only a small part, profile or roughness of the nanosurface is still the decisive factor for the comparison of adsorption strength between NS and ND (adsorption reaction constant NS/ND≈1/4 at four pH values). The highest adsorption capabilities and conformational efficiencies at pH=13 have been obtained. Lysozyme can be prepared, adsorbed and carried with optimal activity and helicity, with 10 and 2 mg/m$^2$ on nanosurface, 150 and 130 mg/g in g of nanoparticle, within the linear coverages at 150-250 nM and four pH values for NS and ND, respectively. They can be prepared in the tightest packed form, with 55 and 20 mg/m$^2$, 580-1100 and 810-1680 mg/g at adsorption thresholds and four pH for NS and ND, respectively. **Ref.** *Chin. J. Chem. Phys.* **26**, 295(2013).

BP 28.11 Wed 18:00 HÜL 386

**Biomolecules at metal interfaces: a novel force field approach including polarization** — •Isidro Lorenzo[1], Hadi Ramezani-Dakhel[2], Hendrik Heinz[2], and Marialore Sulpizi[1] — [1]Johannes Gutenberg University Mainz, Staudinger Weg 7 55099 Mainz — [2]Departament of Polymer Engineering, University of Akron, Ohio 44325

Increasing interest in bio-interfaces for medical and bio-technological applications calls for microscopic understanding and control of protein-surface interactions. In particular here we aim to provide a characterization of peptide / gold interactions at a molecular level in order to explain and interpret recent surface experimental results [1] and to fill the gap between fundamental science and real applications. Atomistic simulations have been performed with the GROMACS package using available force field parameters such as CHARMM27 using 12-6 Lennard-Jones potentials [2] force field. A novel scheme is devised to include the metal polarization (image charge effect) induced by the adsorbed molecules. Extensive tests have been performed for the force field validation and comparisons with quantum mechanics (QM) density functional theory (DFT) are also discussed. Results for the di- and tri-peptide of the insulin-like growth factor on gold are presented.

[1] Anne Vallee, Vincent Humblot, and Claire-Marie Pradier Acc. Chem. Res., 2010, 43 (10), pp 1297*1306

[2] Heinz H, Vaia RA, Farmer BL, Naik RR J. Phys. Chem. C 2008, 112, 17281 17290; Heinz H, Farmer BL, Pandey RB, Slocik JM, Patnaik SS, Pachter R, Naik RR. J. Am. Chem. Soc. 2009, 131, 9704-9714

BP 28.12 Wed 18:15 HÜL 386

**Fibrinogen flexibilty and adsorption properties investigated using atomistic molecular dynamics simulations** — Stephan Köhler[1,2], Friederike Schmid[1], and •Giovanni Settanni[1,3] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [2]Graduate School Materials Science in Mainz — [3]Max Planck Graduate Center mit der Johannes Gutenberg-Universität Mainz

Fibrinogen is a multiprotein complex, fundamental for the coagulation of blood. Adsorption of fibrinogen on material surfaces plays an important role in the viability of those materials for medical implants. Here we use molecular dynamics simulations of fibrinogen in solution and adsorbing on inorganic surfaces to evaluate the behavior of fibrinogen on material surfaces and study the initial adsorption stages. The simulations reveal the extraordinary flexibility of fibrinogen and help to explain how fibrinogen's surface electrostatics influence the adsorption patterns observed experimentally on different inorganic surfaces. This, in turn, may have implications for medical applications such as material design for implants. In addition, the simulation data can ultimately be used to build coarse grained models of fibrinogen to study its aggregation properties[1].

[1] A multiscale model for fibrinogen, S. Köhler, M. McCullagh, F. Schmid, G. Settanni, DPG meeting '14 abstract BP56

## BP 29: Networks – Statistics and Dynamics (joint DY/BP/SOE)

Time: Wednesday 15:00–18:45 Location: ZEU 118

BP 29.1 Wed 15:00 ZEU 118

**Chimera states: spontaneous symmetry-breaking in dynamical networks** — •Eckehard Schöll — Institut für Theoretische Physik, TU Berlin, Hardenbergstr 36, 10623 Berlin, Germany

Systems of nonlocally coupled identical oscillators can exhibit symmetry-breaking in the form of complex spatiotemporal patterns, called chimera states, which consist of coexisting domains of spatially coherent (synchronized) and incoherent (desynchronized) dynamics. We describe the scenario leading from complete coherence to complete incoherence via chimera states [1,2], and present a general analytical calculation of the critical coupling strength at the onset of the chimera states.

[1] I. Omelchenko, Y. Maistrenko, P. Hövel, and E. Schöll: Loss of coherence in dynamical networks: spatial chaos and chimera states, Phys. Rev. Lett. 106, 234102 (2011).

[2] A. Hagerstrom, T.E. Murphy, R. Roy, P. Hövel, I. Omelchenko, and E. Schöll: Experimental observation of chimeras in coupled-map lattices. Nature Physics 8, 658 (2012)

Work in collaboration with A. Hagerstrom, P. Hövel, K. Krischer, Y. Maistrenko, T.E. Murphy, I. Omelchenko, O.E. Omel'chenko, R. Roy, A. Zakharova.

BP 29.2 Wed 15:15 ZEU 118

**Pattern-matching via a network of phase oscillators of different frequency: A novel Architecture** — •Daniel Heger and Katharina Krischer — Technische Universität München, Physikdepartment

Oscillatory networks can in principle be used for pattern recognition. Nevertheless, current architectures either lack scalability towards large numbers of oscillators or need the external input of complex time-dependent coupling functions. In our talk, we will present a novel architecture for pattern matching with oscillatory neural networks. A system of oscillators of different frequencies and coupling functions is used whose dynamics average to the dynamics of an all-to-all coupled oscillator network. In contrast to previous approaches, the necessary coupling functions are automatically generated inside the network and the output pattern can easily be read out binary. By additionally choosing a new type of coupling function, the matching mechanism is stable even for high coupling strengths and the degenerate attractive limit set containing the memorized patterns transforms to a system of seperated attractors for each memorized pattern. Although the system's dynamics do not average to the dynamics of simple coupled Kuramoto oscillators, the appealing mathematical structure permits determination of the stability of all fixed points using nonlinear stability analysis and a dynamic equation solely in pattern space can be derived.

BP 29.3 Wed 15:30 ZEU 118

**Data acquistion by vectorization of high resolution images of vascular networks** — •Jana Lasser — Max-Planck-Institut für Dynamik und Selbstorganisation

Leaf vein networks form highly complex, reticulate, hierarchically organized webs that are believed to be the result of a process of gradual optimization over the course of evolutionary history. These networks form planar graphs dominated by cycles, but to this day the topological properties of such reticulate networks have not been adequately described. We analyze the hierarchical organization of the loops in transport networks from roughly 100 cleared leaf images that are converted into a weighted graph representation using custom tailor-made image analysis tools. We employ tools from statistics and topology, in particular an algorithmic way of assigning a topological tree graph to the leaf's loop graph which represents its hierarchical organization, thus allowing us to make use of specialized tree metrics to unravel the distinguishing characteristics between different network realisations. Our algorithmic tools allow us to quantitatively describe subtle differences between venation phenotypes, and compare reticulate network data with the predictions of optimisation models.

BP 29.4 Wed 15:45 ZEU 118

**Structure and Topology of Optimal Transport Networks in Plant Leaves** — •Henrik Ronellenfitsch and Eleni Katifori —

Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Efficient photosynthesis in plants crucially depends on the ability to transport water from the soil into the leaves, where it can evaporate. To this effect, plants are equipped with a network of pipe-like cells, the xylem, facilitating efficient delivery of water to all parts of the organism. In the leaf, these networks form highly complex, highly reticulate, hierarchically organized webs that are believed to be the result of a process of gradual optimization over the course of evolutionary history. Based on the assumption of functional optimization over the course of evolution, we construct models for optimal transport networks adapted to different kinds of damage (modelling herbivory, diseases, etc...) and fluctuating load (modelling the fact that the stomata, small orifices responsible for the exchange of gasses, open in patches at a time). We numerically solve the resulting optimization problem and analyze the solutions with special regard to structure and hierarchical organization of loops which arise in response to damage and fluctuations.

BP 29.5 Wed 16:00 ZEU 118

**The topology of adaptively controlled networks** — •Judith Lehnert[1], Philipp Hövel[1,2], Alexander Fradkov[3,4], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Bernstein Center for Computational Neuroscience, HU Berlin, Philippstr. 13, 10115 Berlin, Germany — [3]SPb State University, Universitetskii pr.28, St. Petersburg, 198504 Russia — [4]Institute for Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoy Ave, 61, V. O., St. Petersburg, 199178 Russia

Adaptive networks are characterized by a complicated interplay between the dynamics of the nodes and a changing topology: The topology evolves according to the state of the system, while at the same time the dynamics on the network and thus its state is influenced by that topology. Here, we present an algorithm for a changing topology that allows us to control the dynamics on the network. In particular, we control zero-lag and cluster synchronization in delay-coupled networks of Stuart-Landau oscillators.

The emerging topology of the network is modulated by the delay. If the delay time is a multiple of the system's eigenperiod, the coupling within a cluster and to neighboring clusters is on average positive (excitatory), while the coupling to clusters with a phase lag close to $\pi$ is negative (inhibitory). For delay times equal to odd multiples of half of the eigenperiod, we find the opposite: Nodes within one cluster and of neighboring clusters are coupled by inhibitory links, while the coupling to clusters distant in phase state is excitatory.

BP 29.6 Wed 16:15 ZEU 118

**Hierarchical block structures and high-resolution model selection in large networks** — •Tiago P. Peixoto — Universität Bremen, Germany

Many social, technological, and biological networks are composed of modules, which represent groups of nodes which have a similar role in the functioning of the network. The problem of detecting and characterizing these modules is a central one in the broad field of complex systems. However most existing methods used to obtain the modular structure of networks suffer from serious problems, such as the resolution limit on the size of communities. This phenomenon occurs for the very popular approach of modularity optimization, but also for more principled ones based on statistical inference and model selection. Here I construct a nested generative model which, through a complete description of the entire network hierarchy at multiple scales, is capable of avoiding this limitation, and enables the detection of modular structure at levels far beyond those possible by current approaches. Even with this increased resolution, the method is based on the principle of parsimony, and is capable of separating signal from noise. Furthermore, it fully generalizes other approaches in that it is not restricted to purely assortative mixing patterns, directed or undirected graphs, and ad hoc hierarchical structures such as binary trees..

References: [1] Tiago P. Peixoto, Phys. Rev. Lett. 110 14 148701 (2013); [2] Tiago P. Peixoto, arXiv: 1310.4377; [3] Tiago P. Peixoto, arXiv: 1310.4378

BP 29.7 Wed 16:30 ZEU 118

**Temporal networks: Laplacian spectra and synchronization** — •Konstantin Klemm[1,2], Naoki Masuda[3], and Victor M. Eguiluz[4] — [1]Bioinformatics, Institute of Computer Science, Leipzig University, Germany — [2]Bioinformatics and Computational Biology, University of Vienna, Austria — [3]Department of Mathematical Informatics, The University of Tokyo, Japan — [4]Instituto de Fisica Interdisciplinar y Sistemas Complejos, Palma de Mallorca, Spain

Interactions among units in complex systems occur in a specific sequential order thus affecting the flow of information, the propagation of diseases, and general dynamical processes. We investigate the Laplacian spectrum of temporal networks and compare it with that of the corresponding aggregate network. First, we show that the spectrum of the ensemble average of a temporal network has identical eigenmodes but smaller eigenvalues than the aggregate networks. In large networks without edge condensation, the expected temporal dynamics is a time-rescaled version of the aggregate dynamics. Even for single sequential realizations, diffusive dynamics is slower in temporal networks [1]. These discrepancies are due to the noncommutability of interactions. The final part of the presentation uses the calculated spectra to predict the stability of non linear-systems with diffusive temporal couplings.

[1] N. Masuda, K. Klemm, V. M. Eguiluz, Phys. Rev. Lett. 111, 188701 (2013).

**15 min break**

BP 29.8 Wed 17:00 ZEU 118

**Phase Transitions in Cooperative Coinfections: Simulation Results for Networks and Lattices** — •Weiran Cai[1], Li Chen[2,3], Fakhteh Ghanbarnejad[2], and Peter Grassberger[4] — [1]Faculty of Electrical and Computer Engineering, Technische Universität Dresden, Germany — [2]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [3]Robert Koch-Institut P4 - Epidemiologische Modellierung von Infektionskrankheiten, Berlin, Germany — [4]JSC, FZ Jülich, D-52425 Jülich, Germany

In this talk, we study the spreading of a cooperative coinfection on different networks topologies. Previous work has shown that in a mean field approximation, the cooperativity of two diseases in the SIR framework can lead to first-order transitions, where the relative size of the infected cluster changes discontinuously with respect to control parameters. However, due to the mean field approximation, such discontinuous transitions could occur only when the initial density of infected sites is finite. Here we show that the same is true on trees, but not on other networks. On Erdős-Renyi(ER) networks, on networks with long range contacts, and lattices with dimension = 3 we find first order transitions initiated even by a single sick site, while no first order transitions are observed on 2-dimensional lattices, if the contacts are short range. The importance of loops for the presence/absence of discontinuous transitions is discussed.

BP 29.9 Wed 17:15 ZEU 118

**Stability of Boolean and continuous dynamics** — •Fakhteh Ghanbarnejad[1] and Konsatntin Klemm[2,3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Bioinformatics, Institute for Computer Science, University of Leipzig, Germany — [3]Institute for Theoretical Chemistry, University of Vienna, Austria

Regulatory dynamics in biology is often described by continuous rate equations for continuously varying chemical concentrations. Binary discretization of state space and time leads to Boolean dynamics. In the latter, the dynamics has been called unstable if flip perturbations lead to damage spreading. Here, we find that this stability classification strongly differs from the stability properties of the original continuous dynamics under small perturbations of the state vector. In particular, random networks of nodes with large sensitivity yield stable dynamics under small perturbations. (Phys. Rev. Lett. 107, 188701 (2011))

BP 29.10 Wed 17:30 ZEU 118

**Physiological networks studied with time-delay stability analysis** — •Jan W. Kantelhardt[1], Amir Bashan[2], Ronny P. Bartsch[3], Shlomo Havlin[2], and Plamen C. Ivanov[3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Department of Physics, Bar-Ilan University, Israel — [3]Harvard Medical School, Boston, USA

The human organism is an integrated network where complex physiological systems, each with its own regulatory mechanisms, continuously interact, and where failure of one system can trigger a breakdown of the entire network. Identifying and quantifying dynamical networks of diverse systems with different types of interactions is a challenge. We have developed time-delay stability analysis as a framework to probe interactions among diverse systems and identified a physiologi-

cal network from recorded time series data. Each physiological state is characterized by a specific network structure, demonstrating a robust interplay between network topology and function. Across physiological states, the network undergoes topological transitions associated with fast reorganization of physiological interactions on time scales of a few minutes, indicating high network flexibility in response to perturbations.

BP 29.11 Wed 17:45 ZEU 118

**Large networks have small Problems** — •Helge Aufderheide[1] and Thilo Gross[2] — [1]Max-Planck Institut für Physik komlpexer Systeme — [2]University of Bristol, MV School of Engineering Mathematics

On several levels, humans depend on the functioning of complex networks, such as food webs and technical infrastructure networks. However, recent work shows that trying to stabilize a network can lead to large-scale failures. This suggests that it is important to assess not only the risk of a failure, but also its scale. Here we show that instabilities which naturally occur in large networks are typically localized, such that they affect only a relatively small part of the network directly, whereas attempts to stabilize the network can lead to a delocalization, such that instabilities are less likely but will affect a larger number of nodes when they occur. These results may explain how many natural networks can stabilize themselves by sacrificing the parts in which instabilities occur, whereas cases of delocalized systemic failure are known to occur in artificial technical or organizational networks.

BP 29.12 Wed 18:00 ZEU 118

**Outbreaks of coinfections: the critical role of cooperativity** — •Fakhteh Ghanbarnejad[1], Li Chen[1], Weiran Cai[2], and Peter Grassberger[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Faculty of Electrical and Computer Engineering, TU Dresden, Germany — [3]JSC, FZ Jülich, D-52425 Jülich, Germany

Modeling epidemic dynamics plays an important role in studying how diseases spread, predicting their future course, and designing strategies to control them. In this talk, we introduce a model of SIR (susceptible-infected-removed) type which explicitly incorporates the effect of *cooperative coinfection*. More precisely, each individual can get infected by two different diseases, and an individual already infected with one disease has an increased probability to get infected by the other. Depending on the amount of this increase, we prove different threshold scenarios. Apart from the standard continuous phase transition for single disease outbreaks, we observe continuous transitions where both diseases must coexist, but also discontinuous transitions are observed, where a finite fraction of the population is already affected by both diseases at the threshold. All our results are obtained in a mean field model using rate equations, but we argue that they should hold also in more general frameworks. (arXiv:1307.2404)

BP 29.13 Wed 18:15 ZEU 118

**Onset of self-sustained activity in a simple model of excitable dynamics on graphs** — •Christoph Fretter[1,2], Annick Lesne[3], Claus C. Hilgetag[1,4], and Marc-Thorsten Hütt[2] — [1]Department of Computational Neuroscience, Universitätsklinikum Hamburg-Eppendorf, Hamburg, Germany — [2]School of Engineering and Science, Jacobs University Bremen, Germany — [3]LPTMC UMR 7600, Université Pierre et Marie Curie-Paris 6, 4 place Jussieu, F-75252 Paris, France — [4]Department of Health Sciences, Boston Uniersity, Boston, USA

Models of simple excitable dynamics on graphs are an efficient framework for studying the interplay between network topology and dynamics. This subject is a topic of practical relevance to diverse fields, ranging from neuroscience to engineering. Using a discrete excitable node model, we analyse how a single excitation propagates through a random network as a function of the excitation threshold,that is, the percentage of excitations in the neighborhood required for an excitation of a node. Using numerical simulations and analytical considerations, we can understand the onset of sustained activity as an interplay between topological cycle statistics and path statistics. Our findings are interpreted in the context of the theory of network reverberations in neural systems, which is a question of long-standing interest in computational neuroscience.

BP 29.14 Wed 18:30 ZEU 118

**Laplacian Spectrum of 2d Lattice Triangulations** — •Ella Schmidt, Benedikt Krüger, and Klaus Mecke — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Triangulations are an important tool in physics for describing curved geometries. Unimodular triangulations on 2d lattices can also be considered as connected, simple, plane graphs, which allows the appliance of methods from spectral graph theory on triangulations.

We calculate the distribution and averages of eigenvalues of the Laplacian matrix for random and highly ordered unimodular triangulations. Introducing a curvature energy of triangulations we measure microcanonical and canonical averages of the eigenvalues using Monte-Carlo-Simulations. We examine the probability distributions of the spectra of the ensembles of triangulations, the dependence of the eigenvalues on energy and temperature as well as the scaling with the lattice size and compare with random graph models.

In the microcanonical ensemble we find in agreement with our analytical predicitions a linear dependence of the algebraic connectivity and the spectral radius on the energy, in the canonical ensemble we encounter quasi-critical behaviour.

## BP 30: Biomaterials and Biopolymers I (joint CPP/BP)

Time: Wednesday 15:00–18:15 Location: ZEU 222

**Invited Talk** BP 30.1 Wed 15:00 ZEU 222

**Fabrication of 3D Cell Structures Using Self-Folding Polymer Films** — •Leonid Ionov — Leibniz Institute of Polymer Research Dresden

Nature offers an enormous arsenal of ideas for the design of novel materials with superior properties and interesting behaviors. In particular, self-assembly and self-organization, which are fundamental to structure formation in nature, attract significant interest as promising concepts for the design of intelligent materials. Self-folding stimuli-responsive polymer films are exemplary biomimetic materials and can be viewed as model systems for bioinspired actuation. Such films, on one hand, mimic movement mechanisms in certain plant organs and, on the other hand, are able to self-organize and form complex 3D structures. These self-folding films consist of two polymers layers with different properties. For such a bilayer to changes its curvature at least one of these polymers, the active one, must change its volume more than the other one in response to changes in the external environmental such as temperature, pH or light. Because of this non-equal expansion of polymers, these films are able to form tubes, capsules or more 3D complex structures. Self-folding polymeric films provide unique possibilities for the straightforward fabrication of fibers with complex responsive architectures and that cannot be achieved using other currently available technologies. In this presentation, new applications of self-folding films for encapsulation and release of cells, 3D cell patterning as well as design of scaffolds will be demonstrated.

BP 30.2 Wed 15:30 ZEU 222

**Surface-Nanostructure Induced Structural and Dynamical Properties of Adsorbing Protein Layers** — •Thomas F. Keller[1], Robert Schulze[2], Jörg Bossert[2], Mark Kastantin[3], Daniel K. Schwartz[3], and Klaus D. Jandt[3] — [1]Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany — [2]Friedrich Schiller University Jena, Germany — [3]University of Colorado Boulder, USA

Designing implant surface properties on the nanoscale may be one method for tuning the structure and dynamics of adsorbing protein layers. For a set of materials with relevance in the biomedical field, such as ultra high molecular weight polyethylene (UHMWPE), titanium dioxide ($TiO_2$) and polystyrene-b-poly(ethylene oxide) (PS-b-PEO) block copolymers, we show how advanced materials processing permits the creation of surface nanostructures suitable for guiding adsorbing proteins into lateral arrangements that may also affect their dynamic behavior, as determined from mapping using accumulated probe trajectories (MAPT). By atomic force microscopy (AFM), we observed that 1) the surface nanostructure of native UHMWPE may establish a densely packed, ordered arrangement of fibrinogen, which is

one key protein in the implant-induced blood coagulation cascade, 2) adjacent crystalline facets on a nanostructured $TiO_2$ surface create local adsorption sites that guide fibrinogen into different conformational arrangements, and 3) nanoscale phase domains on block copolymer surfaces may serve as nucleation sites for fibrinogen networks. *Ref.:* **ACS Nano 2011**, 5, 3120; **Adv. Funct. Mater. 2012**, 22, 2617; **Acta Biomater. 2013**, 9, 5810; **Macromolecules 2012**, 45, 4740.

BP 30.3 Wed 15:45 ZEU 222

**On the Relationship between Peptide Adsorption Resistance and Surface Contact Angle: A Combined Experimental and Simulation Single-Molecule Study** — •Nadine Schwierz[1], Dominik Horinek[1], Susanne Liese[2], Tobias Pirzer[1], Bizan N. Balzer[1], Thorsten Hugel[1], and Roland R. Netz[2] — [1]Technische Universität München, Germany — [2]Freie Universität Berlin, Germany

Controlling the adsorption of proteins and peptides at synthetic surfaces is the ultimate goal for designing biocompatible implants and fouling resistant surfaces. To gain a microscopic understanding of the transition between peptide adsorption and adsorption resistance, the force-induced desorption of single peptide chains is investigated in closely matched molecular dynamics simulations and atomic force microscopy experiments. In both simulations and experiments, the surfaces become adsorption resistant when their contact angle decreases below $\theta = 50°$-$60°$, thus confirming the so-called Berg limit, established in the context of protein and cell adsorption.

Entropy/enthalpy decomposition of the simulation results reveals that the key discriminator between the adsorption of different residues on a hydrophobic monolayer is of entropic nature and thus is suggested to be linked to the hydrophobic effect. Peptide adsorption resistance is caused by the strongly bound water hydration layer and characterized by the simultaneous gain of both total entropy in the system and total number of hydrogen bonds between water, peptide, and surface. This mechanistic insight into peptide adsorption resistance might help to refine design principles for anti-fouling surfaces.

BP 30.4 Wed 16:00 ZEU 222

**Structural investigation of biomineralization processes in bio(mimetic)-materials by means of solid state NMR** — •Anastasia Vyalikh and Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V.

Solid state NMR is applied to study the structure of biominerals. While the 31P solid state NMR spectra of phosphate containing materials represent a single broad line resulting from the diversity of structural motives, 2D heteronuclear correlation (HETCOR) experiments provide signal separation, and therefore can be used to determine the nature of mineral phases and interfacial organic-inorganic structures. The structure formation of biomimetic apatite-gelatine nanocomposites has been revealed, demonstrating the interaction of mineral domains with the organic matrix in the intergrowth region. HETCOR NMR provides resolution for the identification of different phosphate minerals at very early mineralization stages, which do not yet result in crystallite particles visible in imaging and diffraction techniques. The development of different calcium phosphate species in newly formed tissues has been demonstrated, when dental model implants were inserted in the mandible of minipigs and extracted after various healing time. While in mature bone hydroxyapatite, amorphous calcium phosphate and octacalcium phosphate are observed, the earlier stages include in addition ß-tricalcium phosphate and brushite-like structures. We propose a method, which offers identification of biomineral components as well as the information on crystallite dimensionality based on strength of hydrogen bonds in water related structures.

BP 30.5 Wed 16:15 ZEU 222

**Elucidating insulin structure at hydrophobic interfaces** — •Sergio Mauri[1,2], Tobias Weidner[2], and Heike Arnlods[1] — [1]Surface Science Research Centre, Department of Chemistry, University of Liverpool, UK — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Insulin unfolding and aggregation represents a hot topic for improving the delivery and storage of insulin based drugs.

Human insulin is a small peptide (51 amino acids) that regulates glycemia in the human body. It can be found in the form of hexamers, dimers and monomers: only the latter undergo unfolding and aggregation, forming fibril-like structures (amyloids).

It is generally known that interfaces trigger protein denaturation and eventually aggregation: in particular hydrophobic interfaces (such as the air/water interface) are known to disrupt insulin secondary structure, but the mechanism has not been explained in detail yet, since conventional spectroscopic methods do not have sufficient sensitivity to detect the interfacial protein layer.

Here we address this problem by applying a nonlinear optical technique, infrared-visible sum frequency generation, which is interface sensitive by virtue of optical selection rules and compare it to attenuated total internal reflection IR data at hydrophobic interfaces.

**15 min. break**

BP 30.6 Wed 16:45 ZEU 222

**A theoretical study of intermolecular interactions in crystalline cellulose** — •Johannes Hoja and Alexander F. Sax — Department of Chemistry, University of Graz, Graz, Austria

It is often claimed that cellulose I consists of sheets held together by van der Waals interactions and that each sheet consists of chains held together by hydrogen bonds. Since all weak intermolecular interactions consist of electrostatic, exchange, induction, and dispersion contributions we analyze in this study all intermolecular interactions in cellulose in terms of these four interaction contributions. It was shown that dispersion is crucial for the stabilization of alcohol dimers.[1] This justifies the use of a dispersionless density functional and an additional function that describes the dispersion contribution to the interaction energy for the investigation of the interactions in cellulose I$\alpha$, I$\beta$, and II. For a better understanding of the nature of hydrogen bonds between cellulose chains we investigate model systems of alcohol dimers containing a different number of hydrogen bonds. Especially we study how the dimer stability depends on the intermonomer distance and the topology of the hydrogen bonding networks. For these investigations we use symmetry-adapted perturbation theory based on DFT description of monomers [SAPT(DFT)]. We find that dispersion is not only responsible for the intersheet stabilization but also contributes significantly to the intrasheet interactions. This is in opposition to the general view that only electrostatic interactions are important for hydrogen bonding.

[1] Hoja et al., Chem. Eur. J., DOI: 10.1002/chem.201303528, in press.

BP 30.7 Wed 17:00 ZEU 222

**Biomodified, stimuli responsive surface coatings based on polymer brushes** — •Evmorfia Psarra[1,2], Ulla König[1], Klaus-Jochen Eichhorn[1], Manfred Stamm[1,2], and Petra Uhlmann[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Technische Universität Dresden, Physical Chemistry of Polymer Materials, Dresden, Germany

The main focus of this work is the surface biofunctionalization of ultrathin, stimuli responsive polymer brushes grafted to model surfaces. Different polymer brushes either composed out of a pH responsive component, the Poly(acrylic) acid (PAA), and/or a temperature responsive material, the Poly(N-isopropyl acrylamide) (PNIPAAm) are used to investigate the Arg-Gly-Asp (RGD) peptide binding to the brush surface. Using PNIPAAm mixed with PAA polymer material in order to generate binary brushes will help to create smart surface coatings which are hiding or exposing their functionalities by changing the temperature from physiological (37°C) to room temperature. Binary brushes functionalized with cell-signaling molecules, can lead to intelligent stimuli-responsive bio-nanosurfaces, able to regulate cell adhesion and function. Here we are presenting detailed surface analysis results for the PNIPAA-PAA RGD modified system.

BP 30.8 Wed 17:15 ZEU 222

**Microtopographic substrates for controlling cell adhesion at the nanoscale** — •Laith Kadem, Julia Purtov, Constanze Lamprecht, and Christine Selhuber-Unkel — Biocompatible Nanomaterials, Institute for Materials Science, University of Kiel

Diblock-copolymer micelle nanolithography has in recent years proven to be a valuable tool for controlling the adhesion of cells at the nanoscale by offering a control over spacing variation in binding sites of single-cell adhesion receptors. Here we present a novel method to additionally control binding sites spacing on regular micropatterns. We use a micro-structured topography on Si substrates that can be easily produced with photolithography followed by wet etching. Performing a diblock-copolymer micelle nanolithography procedure on such substrates introduces nanoparticle arrays of different densities and spacings in the pattern provided by the microtopography in a single-step. With this technique, we can achieve spacing variations

in the micropattern of up to 25 nm. The microstructured domains patterned with nanoparticle arrays were biofunctionlized with RGD ligands in order to make them attractive for integrin binding in order to further study the effect of ligand spacing on cell adhesion. Thus, our micro-patterned nanostructured surfaces now provide a versatile platform for studying cellular adhesion processes that are influenced by micro-nanostructured ligand spacing and density.

BP 30.9 Wed 17:30 ZEU 222

**Thermal Melting of Protein Beta Sheet Crystals** — Andreas Wurm[1], Evgeny Zhuravlev[1], Xiao Hu[2], David Kaplan[2], Peggy Cebe[2], and •Christoph Schick[1] — [1]University of Rostock, Institute of Physics, Germany — [2]Tufts University, Medford MA, USA

The remarkable stability that makes silk useful in garments and surgical sutures has impeded efforts by scientists to study its thermophysical properties. Here, we use fast scanning chip calorimetry and report the first reversible thermal melting of protein beta-pleated-sheet crystals, exemplified by silk fibroin. Heating nanogram-sized samples at 2000K/s, allowed us to avoid thermal decomposition, and demonstrate that beta-pleated-sheet crystals melt to become random coils, helices and turns. We establish that following melting silk can be recrystallized into beta-pleated-sheets, and remelted. The similarity between thermal melting behavior of beta-pleated-sheet crystals and crystals of synthetic polymers is confirmed. Significance for controlling beta-pleated-sheet content during thermal processing of biomaterials is envisioned based on these findings. Demonstration of reversible thermal transitions in silk, the most beta-pleated-sheet-enriched and stable protein, suggests important new insights can also be gained with the broader range of proteins where beta-pleated-sheets serve as critical control points in structural transitions.

**Invited Talk** BP 30.10 Wed 17:45 ZEU 222

**Biopolymer Network Mechanics: Nonlinearity and Hierarchy.** — •Cornelis Storm — Department of Applied Physics and Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands.

Biological materials possess some remarkable mechanical properties. Cells and tissues can adjust, remodel, stiffen, soften, in some cases even pack up and leave when circumstances require action. Surprisingly, most systems that exhibit this stunningly complex response, such as the cytoskeleton inside cells and the extracellular matrix, share a common design: under a microscope, they are crosslinked, hierarchical networks of biological polymers. Even more surprisingly, many of the in vivo behaviors can be reproduced in vitro in reconstituted proteinaceous polymer gels. Many of these systems, most notably collagen, play a purely structural role in living organisms. In other words, their function *is* their mechanical response. Biopolymer networks are therefore particularly suited to begin to understand the complex relationship between structural design and functionality in living systems.

In this seminar, I will discuss our efforts to bridge the gap from microscopic structure to macroscopic mechanical response of such nonlinear systems using collagen as an example. Towards the end, I will discuss our first steps towards controlling the nonlinear mechanical properties of biomimetic synthetics.

## BP 31: Cell adhesion, mechanics and migration II

Time: Wednesday 17:00–18:30 Location: ZEU 250

**Topical Talk** BP 31.1 Wed 17:00 ZEU 250

**Active torque generation by the actomyosin cortex** — •Stephan Grill — BIOTEC, TU Dresden, Germany — MPI-PKS Dresden, Germany — MPI-CBG Dresden, Germany

Many developmental processes break left/right symmetry with a consistent handedness, which requires cellular processes that are chirally asymmetric. Here we describe a novel process of active torque-generation in the actomyosin cortex. We present evidence that active torques drive chiral counter-rotating cortical flow in the polarizing Caenorhabditis elegans zygote, depend on myosin activity, and can be specifically altered through changes in cortical structure and dynamics. Notably, genes that affect the establishment of the C. elegans left/right body axis also control active torques. Our work suggests that actomyosin-based cell chirality provides a fundamental mechanism for chiral morphogenesis in development.

BP 31.2 Wed 17:30 ZEU 250

**Keratocyte-like movement of the slime mold *Physarum polycephalum*** — •Christina Oettmeier, Jonghyun Lee, Erik Bernitt, and Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen, 28359 Bremen

We report on a particular motility pattern in *P. polycephalum*, which closely resembles the forward movement of fish keratocytes. When microplasmodia are plated upon an agar surface, they will fuse and form a network in a percolation transition [1]. However, under certain environmental conditions, the microplasmodia fuse into wedge-shaped structures ("satellites") and start to move outwards for several hours. The satellites are laterally elongated, with one large, curved growth front along the front arc. They move unidirectionally for several cm and maintain a half-moon shape. This behaviour has not been described in *P. polycephalum* locomotion before, but is characteristic for, e.g., fish keratocytes. One mutant *Dictyostelium* cell line, however, was shown to exhibit this movement as well [2]. We characterize the morphology and different phases of development of the satellites, using light microscopy, fluorescence imaging and electron microscopy. The fact that both *Dictyostelium* amoebae and vertebrate cells are relatively small whereas *P. polycephalum* is huge and multinucleate, makes the discovery of a seemingly common movement pattern significant for further investigation of universal modes of motility. [1] Fessel, Oettmeier, Bernitt, Gauthier, Döbereiner, *PRL* **109** (2012) [2] Asano, Mizuno, Kon, Nagasaki, Sutoh, Uyeda, *Cell Motility and the Cytoskeleton* **59** (2004)

BP 31.3 Wed 17:45 ZEU 250

**Actin-MT interactions result in mutual sensing and remodeling** — •Florian Huber[1], Magdalena Preciado López[1], Michel O. Steinmetz[2], Anna Akhmanova[3], Gijsje Koenderink[1], and Marileen Dogterom[1] — [1]FOM Institute AMOLF, Amsterdam, The Netherlands — [2]Laboratory of Biomolecular Research, Paul Scherrer Institut, Switzerland — [3]Division of Cell Biology, Utrecht University, The Netherlands

The cooperative functioning of actin and microtubules (MTs) is increasingly regarded as a central element for many cellular key processes including cell division, cell migration, and adhesion. Several specific actin-MT linker molecules have been discovered, but a detailed understanding of their effects on actin-MT co-organization remains elusive. For a more profound and quantitative understanding of actin-MT crosstalk we developed a simple yet realistic reconstituted model system. To account for the diversity of cytoskeleton architectures we confront dynamic MTs with loose actin networks or rigid bundles. Coupling between the two cytoskeleton components is introduced in form of transient binding of growing MT plus ends to actin filaments using a physiologically relevant actin-MT linker (MACF). We find that MACF allows growing microtubules to steer actin bundle formation and to transport actin filaments. In return, existing actin bundles can reliably capture and guide growing microtubules. Facing a wide spectrum of different geometrical and mechanical settings, the same dynamic actin-MT cross-linker can hence lead to a rich repertoire of co-organizational effects, independent of biochemical regulation.

BP 31.4 Wed 18:00 ZEU 250

**Speed and nuclear deformations during cancer cell migration through narrow pores** — •Christoph Kämmerer[1], Lena Lautscham[1], Sebastian Lachner[1], Amy Rowat[2], Carolin Gluth[1], and Ben Fabry[1] — [1]Department of Physics, Biophysics Group, University of Erlangen-Nuremberg, Germany — [2]Department of Integrative Biology and Physiology, UCLA, USA

To metastasize, cancer cells migrate through the narrow pores of the extracellular matrix. To study cell migration and nuclear deformations in narrow pores, we use soft lithography to fabricate a series of channel segments ($18\mu m$ length, $3.7\mu m$ height, decreasing width from $10.5 - 1.7\mu m$), each separated by a $20x20\mu m$ chamber so that cells can spread and relax between channel crossings. We compare highly invasive HT1080 fibrosarcoma cells with less invasive MDA-MB-231 breast carcinoma cells. Cells are stained with Hoechst 33342 dye to

track the speed and shape of the nucleus. For channels $> 7\mu m$, cell migration is largely unimpeded. When encountering smaller channels, the cell nucleus stalls while the cell body migrates through the channel. Eventually, the nucleus elongates and enters the channel. Once fully elongated, the nucleus glides through and exits the channel with higher speed. Highly invasive HT1080 cells migrate faster through narrow channels compared to MDA-MB-231 cells. These data show that the nucleus is the principal source of resistance against migration through narrow channels. The stalling of the nucleus when entering a channel, and the speed-up of the nucleus when exiting a channel indicate that cells need to build up traction forces to pull the nucleus along.

BP 31.5 Wed 18:15 ZEU 250

**Real-time and high-throughput mechanical phenotyping of suspended cells** — •Oliver Otto[1], Philipp Rosendahl[1], Stefan Golfier[1], Alexander Mietke[1], Salvatore Girardo[1], Stefano Pagliara[2], Ulrich Felix Keyser[2], and Jochen Guck[1,2] — [1]Biotechnology Center, TU Dresden, Tatzberg 47/49, 01307 Dresden, Germany — [2]Cavendish Laboratory, University of Cambridge, JJ Thomson Avenue, Cambridge, CB3 0HE, UK

The mechanical properties of cells have been emerging as label-free, inherent marker of biological function and disease. Concerted utilization has so far been hampered by the availability of a convenient and robust measurement technique. We report the development and characterization of a microfluidic system for mechanical single cell classification in real-time with analysis rates of several hundred cells per second.

A cell suspension is driven through the constriction zone of a microfluidic chip resulting in cell deformation due to hydrodynamic interactions only. Our custom-built image processing software is capable of performing image acquisition, image analysis and data storage on the fly allowing for mechanical phenotyping of several hundred cells per second in real-time.

The ensuing deformations can be described by an analytical hydrodynamic model. Initial experiments based on our novel technology with different cell types are in agreement with results obtained with atomic force microscopy and optical stretcher. Our method allows continuous mechanical phenotyping of large cell populations with a throughput previously only known from flow cytometry.

## BP 32: BP Mitgliederversammlung

Time: Wednesday 19:00–20:00 Location: HÜL 386

**Discussion**

## BP 33: Active cell and tissue mechanics (focus session) I

Time: Thursday 9:30–12:30 Location: HÜL 386

**Invited Talk** BP 33.1 Thu 9:30 HÜL 386

**Self-Focusing of the Ran Gradient in Mitosis: Signaling, Mechanics, and Spindle Size** — •Daniel Needleman and Doogie Oh — Harvard University, Cambridge, MA 02138, USA

During spindle assembly, microtubules are highly enriched near chromatin by a process which, in many systems, is driven by the GTPase Ran. The Ran pathway has been proposed to establish a reaction-diffusion network that generates gradients in the behaviors of soluble proteins around chromatin, but the manner in which this happens is poorly understood. To better characterize the behavior of the Ran pathway, we developed a novel form of fluorescence fluctuation spectroscopy capable of quantitatively measuring the concentration, diffusion, and interactions of soluble proteins simultaneously at hundreds of locations throughout cells. We use this technique to study the behaviors of soluble Ran, importin-alpha, importin-beta, RanBP1, RanGAP, and a variety of downstream cargo proteins throughout mitotic human tissue culture cells, and we investigate how the spatial organization of this network changes in response to perturbations. Our results suggest that a self-focusing of the Ran pathway is produced by an interplay between soluble gradients of upstream signaling molecules and the mechanics of the microtubule network they generate. This feedback has interesting implications for models of spindle assembly and the maintenance of spindle size.

BP 33.2 Thu 10:00 HÜL 386

**Surface tension governs the shape of confined mitotic HeLa cells** — •Elisabeth Fischer-Friedrich[1,2], Anthony A. Hyman[2], Frank Jülicher[1], Daniel J. Müller[3], and Jonne Helenius[3] — [1]MPI PKS, Dresden, Germany — [2]MPI CBG, Dresden, Germany — [3]D-BSSE, ETHZ, Basel, Switzerland

During mitosis, adherent cells round up, by increasing the tension of the contractile actomyosin cortex while increasing the internal hydrostatic pressure. In the simple scenario of a liquid cell interior, the surface tension is related to the local curvature and the hydrostatic pressure by Laplace's law. However, verification of this scenario for cells requires accurate measurements of cell shape. Here, we use wedged micro-cantilevers to uniaxially confine single cells and determine confinement forces while concurrently determining cell shape using confocal microscopy. We fit experimentally measured confined cell shapes to shapes obeying Laplace's law with uniform surface tension and find quantitative agreement. Geometrical parameters derived from fitting the cell shape, and the measured force were used to calculate hydrostatic pressure and surface tension of cells. We find that HeLa cells increase their internal hydrostatic pressure and surface tension from $\approx 40\,\mathrm{Pa}$ and $0.2\,\mathrm{mNm}^{-1}$ during interphase to $\approx 400\,\mathrm{Pa}$ and $1.6\,\mathrm{mNm}^{-1}$ during metaphase. The method introduced provides a means to determine pressure and surface tension of rounded cells accurately and with minimal cellular perturbation, and should be applicable to characterize the mechanical properties of various cellular systems.

BP 33.3 Thu 10:15 HÜL 386

**Active pulsatory patterns** — •Vijay Krishnamurthy[1,2], Justin Bois[3], Frank Jülicher[1], and Stephan Grill[1,2,4] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]BIOTEC, Technische Universität Dresden, Tatzberg 47/49, 01307 Dresden, Germany — [3]UCLA Department of Chemistry and Biochemistry, 611 Charles E Young Drive East, Los Angeles, CA 90095, USA — [4]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauer Straße 108, 01307 Dresden, Germany

We study pulsatory patterns in a system of two chemical species suspended in a thin film active fluid. Active stress in the fluid is regulated by the concentrations of the two species, which diffuse and are also advected by the flows generated by active stress gradients. We demonstrate that this system exhibits spontaneous pulsatory patterns when the following conditions are met: (i) the fast-diffusing species up-regulates the active stress and the slow-diffusing species down-regulates the active stress, or (ii) the active-stress up-regulator turns-over faster compared to the active-stress down-regulator. Our study motivated by the actomyosin cortex of cells provides a simple generic mechanism for oscillatory patterns in active fluids.

BP 33.4 Thu 10:30 HÜL 386

**Characterizing the functionality of engineered cardiac tissue using computational motion tracking: A noninvasive alternative to electrophysiological methods** — •Peter Loskill[1], Nathanial Huebsch[2], Natalie C. Marks[1], Anurag Mathur[1], Zhen Ma[1], C. Ian Spencer[2], Bruce R. Conklin[2], and Kevin E. Healy[1] — [1]Department of Bioengineering, UC Berkeley, Berkeley, United States — [2]Gladstone Institute of Cardiovascular Disease, San Francisco, United States

Drug discovery and development to date has relied on animal models, which are useful, but fail to mimic human physiology. The discovery of iPS cells has led to the emergence of a new paradigm of drug screening using human organ-like cultures in a dish. A crucial requirement for

the application of *in vitro* organ models is the ability to characterize *in situ* their functionality. In the case of cardiac tissue, electrophysiological methods are commonly applied. These are, however, limited in terms of choice of substrate and versatility. To overcome these limitations, we have developed a user-friendly motion capturing software that quantifies the mechanical movement of engineered cardiac tissue. The software is based on a block matching algorithm and optimized to capture beating motions of cardiomyocytes and cardiac microtissue. Without the necessity for staining or tracers, multiple parameters such as beat rate, beat duration, and contractility can be obtained using phase contrast microscopy. The software was validated by comparing the obtained result to electrophysiological methods and was applied to study the drug response of various 3D cardiac tissue constructs.

BP 33.5 Thu 10:45 HÜL 386

**Tissue packing dynamics during morphogenesis of the early Drosophila m. embryo, in toto.** — •Stefan Günther[1], Sebastian Streichan[2], Uros Krzic[3], Marvin Albert[1], Timothy Saunders[4], and Lars Hufnagel[1] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Kavli Institute For Theoretical Physics, USA — [3]Carl Zeiss Microscopy, TASC, Munich, Germany — [4]Mechanobiology Institute and Department of Biological Sciences, Singapore

The organization of tissues is challenged by the propagation dynamics of the cells which constitute the tissue. How the dynamic motion shape tissues in vivo during early development is poorly understood due to a lack of quantifiable data. We use a selective plane illumination microscope (MuVi-SPIM) and automated image analysis to quantify the dynamics of the nuclei packing in 3D. High temporal and spatial resolution allows us to analyze the relationship between the packing of nuclei in the entire embryo and the orientation of the division axis of nuclei. Lineages of all nuclei through several rounds of division are used to explore the role of a nucleus' spatio-temporal history for its local packing. We further use computational models in order to propose the necessary interactions that can lead to the orderliness and the dynamics of the observed nuclei packing and test the predictions using laser ablations to locally perturb the developing embryo.

**30 min. break**

BP 33.6 Thu 11:30 HÜL 386

**Living cells: Active at long times but passive at short times** — Wylie Ahmed, Matthias Bussonnier, and •Timo Betz — Physical-Chemistry-Curie, Institut Curie, Paris, France

Living cells are per definition out of thermodynamic equilibrium as they consume energy to maintain their organization. This has an important impact on their mechanical properties and on the measurement of these properties. Up to now, the correct description of cell mechanics by using passive techniques such as particle tracking based microrheology inside living cells remains a challenge, since these measurements suffer from incomplete knowledge about the active contribution of cellular dynamics. Active microrheology, where the probe particles are moved by a controlled force, provides a solution to this problem since it offers independent access to the mechanical properties. We combine active and passive microrheology to directly determine the active contribution of intracellular dynamics. These experiments suggest that at short timescales equilibrium thermodynamics hold, while it is violated in long timescales. Using phagocytosed beads and cell organelles we can determine the timescale of this difference which is found to be dependent of the cell type and varies between $\approx 5 - 100$ms. Using this information we exploit the high frequency regime to calibrate the optical forces on cell organelles which gives direct and simple access to the mechanical properties important for organelle transport. This method can be also used in 3D cultures to directly measure the differences in intracellular mechanics for 2D versus 3D cultures. Hence, we can show that at short timescales even a living cell behaves like dead material.

BP 33.7 Thu 11:45 HÜL 386

**The role of mechanics in leaf primary vein morphogenesis** — •Jonathan Edward Dawson[1], Irina Kneuper[2], William Teale[2], Klause Palme[2], Franck Ditengou[2], and Eleni Katifori[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Albert-Ludwigs-Universität Freiburg, Institute of Biology, Freiburg, Germany

The veins of plant leaves exhibit a large variety of morphological patterns. Growth and development of leaf veins is a highly regulated process. Mechanisms that regulate the formation of veins and vascular architecture are largely unknown. In addition to genetic regulation, cell mechanics must also play an important role in these processes. However, to what extent cell mechanics and the interplay between mechanics and biochemistry plays a role in vascular patterning is not well understood. Using a cell based model in which cells are polygons, here we describe the vascular development in early stages of growing leaf primordia. Here we investigate the formation of leaf primary vein. We simulate tissue growth driven by inter-cellular diffusion of the plant hormone auxin, from auxin synthesizing cells. We show that dynamic modulation of the cell mechanical properties based on cell auxin concentration can reproduce realistic mid vein as observed in growing leaf primordia. We further tested our model by comparing with perturbation experiments, in which the inter-cellular auxin transport as well as auxin biosynthesis in leaf primordia is affected.

BP 33.8 Thu 12:00 HÜL 386

**PAR dependent regulation of mechanical activity of the actomyosin cortex in C. elegans zygotes** — •Peter Gross[1,2], Vijay Krishnamurthy[2,3], Nathan Goehring[4], Justin Bois[5], and Stephan Grill[1,2,3] — [1]MPI-CBG, Dresden, Germany — [2]BIOTEC, TU Dresden — [3]MPI-PKS, Dresden, Germany — [4]London Research Institute, UK — [5]UCLA, Los Angeles, CA

The interplay between biochemistry and cell mechanics is critical for a broad range of morphogenetic changes. A prominent example hereof is the emergence of cell polarity during the early embryogenesis of C. elegans, resulting in a patterned state of the membrane-associated PAR polarity proteins. Crucial for the robust emergence of the patterned state are large-scale flows in the membrane-associated actomyosin cortex, which are observed concomitantly with the emergence of PAR polarization. The coupling of biochemistry and large-scale transport via cortical flows, driving this mechanochemical patterning processes, remain poorly understood. We demonstrate a regulatory role of the PAR polarity domains on actomyosin cortex contractility, which can generate cortical flows at the onset of polarization. We quantify the spatial regulation of non-muscle myosin II (nmy-2) turnover in the cortex by a combination of Fluorescence Recovery After Photobleaching (FRAP) and RNA interference (RNAi). Furthermore we present a theoretical description of this process in the framework of active fluids combined with PAR biochemistry in a coupled reaction-diffusion-contraction-advection approach, and show that this model captures all aspects of the dynamics of the PAR polarization process quantitatively.

BP 33.9 Thu 12:15 HÜL 386

**Pattern formation in nematic active fluids** — •Fabio Staniscia[1], Anne-Cécile Reymann[2], Ralph Bohme[2], Justin Bois[3], Frank Jülicher[1], Stephan Grill[1,2], and Guillaume Salbreux[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]UCLA Department of Chemistry and Biochemistry, Los Angeles, USA

We study the patterns formed in a nematic active fluid submitted to active stress generated by myosin activity. The fluid is described by a hydrodynamic theory including the fields of myosin concentration, actin velocity and nematic order parameter describing the local alignment of actin filaments. The pattern-forming region in the parameters space is found through a linear stability analysis, and the effects of the nonlinearities is studied both analytically and numerically. The structure and dynamics of these patterns are reminiscent of the process of formation of myosin foci connected by actin cables in the C. Elegans embryo cortex. Using measurements of the velocity and alignment profiles in the polarization flow of the C. Elegans embryo, we can show that there is indeed a relation between these two quantities which can be explained by our model.

# BP 34: Imaging

Time: Thursday 9:30–11:45 Location: ZEU 250

BP 34.1 Thu 9:30 ZEU 250

**Fast Frame-Rate FLIM for Applications in Molecular Biology and Photosynthesis Research** — •Franz-Josef Schmitt[1], Danilo Bronzi[2], Marco Vitali[1], Cornelia Junghans[1], Franco Zappa[2], and Thomas Friedrich[1] — [1]Institute of Chemistry, Biophysical Chemistry, TU Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany — [2]Dipartimento di Elettronica Informatica e Bioingegneria, Politecnico di Milano, Piazza Leonardo Da Vinci 25, I-20133 Milano, Italy

A monolithic 64x32 CMOS image sensor for fluorescence detection is presented. Each pixel consists of three 9-bit gated counters and a single-photon avalanche diode (SPAD). Thanks to their inherent digital nature, SPADs have a sensitivity limited only by photon shot noise and therefore single-photon imaging at very high-frame rate is enabled. Moreover, we used a sliding-time window scheme to achieve time-resolved photon detection for measuring the fluorescence lifetime with a temporal resolution down to 200 ps. The described sensor has been used for simultaneous imaging of the fluorescence amplitude and lifetime of a pH-sensitive dual-emission GFP fusion protein (deGFPpHSens) expressed in chinese hamster ovary cells (CHO). This allows to monitor over time the pH distribution within individual compartments and organelles of living cells. Additionally, we present fluorescence induction images at the frame-rate of 1 kfps of dark adapted living cells of the blue alga Synechocystis sp. PCC 6803.

BP 34.2 Thu 9:45 ZEU 250

**3D-Density Measurements of the Bacterium Deinococcus Radiodurans by Tomo-Ptychographic X-ray Imaging** — •Robin N. Wilke[1], Marius Priebe[1], Matthias Bartels[1], Klaus Giewekemeyer[2], Ana Diaz[3], Malte Vassholz[1], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Universität Göttingen, Germany — [2]European XFEL, Hamurg, Germany — [3]Paul Scherrer Institut, Villigen, Switzerland

D.radiodurans[1,2] is famous for its extraordinary resistance to high doses of ionizing radiation, which has been tentatively linked to the structural organization of DNA in the nucleoid[3,4]. Determination of the mesoscopic density in the nucleoid would help to test these ideas and eventually to discriminate different models of DNA packing.

Ptychographic phasing[5-9] is one promising (coherent) X-ray imaging technique for this particular problem and other biological applications. We present results of quantitative 3D resolved mass density maps of D.radiodurans by a combination of ptychography and tomography of unstained, unsliced and freeze-dried bacterial cells[8]. In addition, we show how ptychographic results can be enhanced by increasing the dynamic range of pixel detectors by introducing a Semi-Transparent Central Stop[9].

[1]Levin-Zaidman et al.,Science299,2003
[2]Eltsov&Dubochet,J.Bacteriol.187,2005
[3]Eltsov&Dubochet,J.Bacteriol.188,2006
[4]Minsky et al.,J.Bacteriol.188, 2006
[5]Rodenburg et al.,PRL98,2007.
[6]Thibault et al.,Science321,2008
[7]Giewekemeyer et al.,PNAS107,2010
[8]Wilke et al.,Opt.Expr.20,2012
[9]Wilke et. al.,ActaCryst.A69,2013

BP 34.3 Thu 10:00 ZEU 250

**Imaging of biological cells with helium-ion microscopy** — •André Beyer[1], Natalie Frese[1], Henning Vieker[1], Matthias Schürmann[2], Barbara Kaltschmidt[2], Christian Kaltschmidt[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany — [2]Cell Biology, University of Bielefeld, 33615 Bielefeld, Germany

Helium-ion microscopy (HIM) images are generated by scanning a beam of helium ions while recording the emitted secondary electrons. Advantages of HIM include the high resolution, high surface sensitivity as well as an efficient charge compensation mechanism, which allows imaging of insulating samples without the need for a conductive coating.

In this contribution, a HIM imaging study of biological cells is presented. This study focuses on neuronal differentiated inferior turbinate stem cells as well as mouse neurons which were prepared in different ways for imaging under the required vacuum conditions. Charging of specimens without conductive coating was effectively compensated by an electron flood gun. Therewith, extremely small features at cell surfaces were imaged with an estimated edge resolution of 1.5 nm. Indications of lipid rafts at the surface of all investigated cells will be discussed.

BP 34.4 Thu 10:15 ZEU 250

**Suitability of the echo-time-shift method as laboratory standard for thermal ultrasound dosimetry** — •Tina Fuhrmann[1], Olga Georg[2], Julian Haller[2], and Klaus-Vitold Jenderka[1] — [1]University of Applied Sciences, Merseburg, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany

Ultrasound therapy is a promising, non-invasive medical application. It is used e.g. for physiotherapy and lithotripsy for the destruction of kidney stones and has high potential for surgical and therapeutic applications like treatment of cancer, bone repair and treatment of stroke with high intensity focused ultrasound (HIFU). To further develop this technique, to ensure a save clinical application and repeatability of the treatment, laboratory dosimetry standards and quality control mechanisms for therapeutic devices are necessary.

Our approach is to measure temperature with a diagnostic ultrasound device by tracing the time-shift in the backscattered signal. This shift is mainly due to the temperature dependence of speed of sound. We evaluated the suitability of this echo-time shift method for laboratory dosimentry and quality control, especially its general suitability, uncertainties and limitations.

**15 min. break**

BP 34.5 Thu 10:45 ZEU 250

**Optical tweezers based coherent sub-diffraction 3D imaging of helical bacteria and sensing of deformation forces** — •Matthias Koch, Julian Roth und Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Simple living cells such as bacteria are often regarded as model systems in order to analyse basic cellular reactions. The size of a bacterial cell or of small protrusions is often in the range of only a few tens to hundreds of nanometres and their shape may change rapidly. Therefore, advanced photonic measurement techniques are needed which are also capable of extracting forces and energetics on a broad temporal bandwidth. We show how an optical tweezers setup can be used to generate high contrast, 3D super-resolution movies of an only 200nm thin helical bacterium at rates up to 1kHz without any object staining [1]. Images are generated by analysing the interference pattern of the incident and the coherently scattered laser light in the back focal plane of a detection lens. Our system allows the simultaneous measurement and manipulation of fast shape changes and deformation forces generated by the cell. The bacterium itself uses a unique linear motor composed of cytoskeletal protein ribbons for propulsion/swimming. The subunits of these ribbons undergo subsequent conformational changes associated with force generation of the cell body. We show how this technique can be used to analyse the force an torque generation of the motor under different environmental situations.

[1] Koch, M. & A. Rohrbach (2012). Nature Photonics 6(10): 680-686

BP 34.6 Thu 11:00 ZEU 250

**Scanning probe magnetic spin imaging of the protein complex ferritin** — •Dominik Schmid-Lorch, Thomas Häberle, Andrea Zappe, Friedemann Reinhard, and Jörg Wrachtrup — 3. Physikalisches Institut und Forschungszentrum SCoPE, Universität Stuttgart, Germany

We present a novel technique to image nanoscale magnetic fields. It is based on the nitrogen-vacancy (NV) center, a color center in diamond, which can be used as a novel magnetic field sensor by monitoring the Zeeman-shift of its spin sublevels [1]. Mounted to the tip of an atomic-force microscope (AFM), this atomic-sized color center promises to map magnetic fields with a resolution in the atomic range [2-3]. Being sensitive enough to detect single electron and nuclear spins in its close environment, it could enable imaging and structure determination of

single biomolecules.

We will demonstrate imaging of magnetic resonance contrast agents with a resolution in the 10 nm range using this technique. Specifically, we have been able to image small ensembles of Ferritin, an iron storage protein complex [4], by detecting its spin noise with a scanning NV center probe. Beyond these results, we will present our progress towards imaging of single Ferritin complexes.

[1] G. Balasubramanian et al., Nature, Vol 455, 648-651 (2008)
[2] L. Rondin et al., Appl. Phys. Lett., Vol 100, 153118 (2012)
[3] P. Maletinsky et al., Nat. Nanotech., Vol 7, 320-4 (2012)
[4] M. Uchida et al., Magn. Reson. Med., Vol 60, 1073-1081 (2008)

BP 34.7 Thu 11:15 ZEU 250

**The nitrogen vacancy in nanodiamonds as a bio-marker for resolving dynamics of bio molecules** — •Torsten Rendler, Seoyoung Paik, Sany-Yun Lee, and Jörg Wrachtrup — 3. Physikalisches Institut, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Fluorescent probes are essential for bio imaging application. Therefore several different types of fluorescent markers like dye molecules, quantum dots and fluorescent nanodiamonds (fND) have been developed and studied for their purpose as bio-markers. Besides the superior long time stability of the fluorescent emissions, fNDs decorated with the nitrogen-vacancy (NV) color center exhibit another interesting property based on its electron spin system: The NV can probe both the orientation and strength of magnetic field in its environment [1]. This allows not only to locate the fND but also to detect its relative orientation to an external magnetic field in real time on a ms-timescale [2]. It also has been suggested that the rotational diffusion rate of nanodiamonds even in faster time scales are accessible [3]. These works motivate the development of experimental techniques to resolve the rotational diffusion of fNDs, which will also open the door for molecular motion tracing, like monitoring fast conformational changes of working bio molecules. As a preliminary test, we investigate the spin dynamics of NVs in freely rotating fNDs.

[1] Balasubramanian, G. et al., Nature 455, 648-651 (2008). [2] McGuinness, L. P. et al., Nat. Nanotech. 6, 358-363 (2011). [3] Maclaurin,D. et al.,PRL 108 240403(2012).

BP 34.8 Thu 11:30 ZEU 250

**Detection of vancomycin resistances in enterococci using a combined dielectrophoresis-Raman setup and a three-level chemometric model** — •Ulrich Schröder[1,2], Cora Assmann[2], Claudia Beleites[1], Uwe Glaser[1,2], Uwe Hübner[1], Wolfgang Pfister[4], Wolfgang Fritzsche[1], Jürgen Popp[1,2,3], and Ute Neugebauer[1,2] — [1]Institute of Photonic Technology, Jena, Germany — [2]Center for Sepsis Control and Care, Jena University Hospital, Germany — [3]Institute of Physical Chemistry and Abbe Center of Photonics, University Jena, Germany — [4]Institute of Medical Microbiology, Jena University Hospital, Germany

The rising resistances of pathogens towards antibiotics represent a significant problem in human health-care. In this context, enterococci have become one of the most challenging nosocomial problems. It is of utmost interest to detect these resistances early in time to initiate appropriate tailored antibiotic therapies. We present a combined DEP-Raman setup which traps bacteria directly from dilute suspension within micro sized regions so as to perform highly specific Raman spectroscopic analysis. The setup is used to analyze the response of sensitive and resistant enterococci with respect to the antibiotic vancomycin. In combination with a three-level chemometric model based on PLS and LDA we are able to detect the induced drug resistance within less than three hours. Compared to standard microbiological methods which take 24 hours and more our method holds the potential to reduce diagnosis time by orders of magnitude. Acknowledgement: Financial support of BMBF (FKZ 01EO1002) is highly acknowledged.

## BP 35: The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (Symposium SYCP, joint CPP/BP/DY)

Time: Thursday 9:30–12:15 Location: HSZ 02

**Invited Talk** BP 35.1 Thu 9:30 HSZ 02

**Why do polymer collapse and polymer topology frustrate each other** — •Alexander Y. Grosberg — Department of Physics and Center for Soft Matter Research, New York University, NY, USA

Polymer topology is most commonly studied in the context of a melt or concentrated solution. Here, the role of topological constraints is discussed in the context of a single chain swelling or collapse behavior, both in kinetics and in equilibrium (the latter in case topology is quenched, one way or another). Biological aspects are discussed in the context of both chromatin and proteins.

**Invited Talk** BP 35.2 Thu 10:00 HSZ 02

**Nanoscopy of nuclear Genome Structure** — •Christoph Cremer — Institute of Molecular Biology (IMB), D-55128 Mainz — Kirchhoff-Institute of Physics (KIP) University Heidelberg, D-69120 Heidelberg — Institute of Pharmacy and Molecular Biotechnology (IPMB) University Heidelberg, D-69120 Heidelberg

Numerical models as well biochemical data indicate a decisive functional role of genome nanostructure; but due to the conventional resolution limits of far-field light microscopy, direct light microscopic tests of such models were believed to be impossible. However, novel developments in optical technology and photophysics succeeded to radically overcome these conventional limits. With such"superresolution" techniques, it has become possible to analyze nuclear genome structure with a greatly enhanced light optical resolution down to a few tens of nanometer. Application examples will be presented on the use of such "nanoscopy" procedures to measure in cell nuclei the size of individual small chromatin domains, of replication and transcription complexes, as well as the spatial distribution of individual nuclear proteins and of short specifically labelled DNA sequences. It is anticipated that the wealth of nanoscale information on nuclear genome nanostructure accessible by the novel superresolution approaches will substantially contribute to the theoretical understanding of the folding in space and time of the huge polymers called chromosomes, and its functional consequences.

**Invited Talk** BP 35.3 Thu 10:30 HSZ 02

**Blood Clotting Inspired Polymer Physics** — •Alfredo Alexander-Katz — Massachusetts Institute of Technology

Nature has devised creative and efficient ways of solving complex problems, and one of these problems is that of blood clotting in flowing conditions. In fact, nature has used a novel combination of polymer physics and chemistry that enhances the self-healing propensity of a vessel when strong flows are present while avoiding coagulation when the flow is diminished, a rather counter-intuitive phenomenon. Underlying this process is a globular biopolymer, the so-called von Willebrand Factor, whose function is strongly regulated by flow. In this talk I will present our work on this macromolecule starting from the single molecule approach and building up to the multi component system that more closely resembles blood. I will emphasize how new concepts have emerged from trying to understand such a complex system, in particular I will show how these polymers can display giant non-monotonic response to shear, as well as a very large propensity to form polymer-colloid composites in flow while being a stable dispersed suspension in quiescent conditions. In fact, the aggregation behavior is universal and can be explained with simple scaling arguments. These novel concepts and results are in principle not unique to blood clotting and can have important ramifications in other areas.

**15 min. break**

**Invited Talk** BP 35.4 Thu 11:15 HSZ 02

**Modeling dynamic spatial genome organization in yeast** — •Christophe Zimmer — Institut Pasteur, 25 rue du Docteur Roux, 75015 Paris

The spatial organization and dynamics of chromosomes plays important roles for gene expression, DNA repair and replication, but its underlying principles remain poorly known. We will present quantitative experimental data and simulation results showing that the territorial organization the interphase yeast nucleus and the dynamics of chromosomes can be largely predicted by a model based on generic polymer

physics with a minimal set of DNA sequence-specific constraints and assumptions. We will also discuss extensions of our budding yeast model to other organisms and address implications of this model for a quantitative understanding of DNA repair.

**Invited Talk** BP 35.5 Thu 11:45 HSZ 02

**Ring polymers in the melt state: the physics of crumpling** — •Ralf Everaers[1] and Angelo Rosa[2] — [1]Laboratoire de Physique et Centre Blaise Pascal, ENS Lyon, CNRS UMR5672, 46 allée d'Italie, 69364 Lyon, France — [2]SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste (Italy)

The conformational statistics of ring polymers in melts or dense solutions is strongly affected by their quenched microscopic topological state. The effect is particularly strong for non-concatenated unknotted rings, which are known to crumple and segregate and which have been implicated as models for the generic behavior of interphase chromosomes. Here we use a computationally efficient multi-scale approach to identify the subtle physics underlying their behavior, where we combine massive Molecular Dynamics simulations on the fiber level with Monte Carlo simulations of a wide range of lattice models for the large scale structure. We show that (i) topological constraints may be neglected on scales below the standard entanglement length, $L_e$, (ii) that rings with a size $1 \leq L_r/L_e \leq 30$ exhibit nearly ideal lattice animal behavior characterized by primitive paths which are randomly branched on the entanglement scale, (iii) that larger rings are weakly swollen relative to ideal lattice animals with gyration radii $\langle R_g^2(L_r)\rangle \propto L_r^{2\nu}$ and $\nu \approx 1/d > 1/4$, and (iv) that ring melts can be *quantitatively* mapped to coarse-grained melts of *interacting* randomly branched primitive paths.

## BP 36: Evolutionary Game Theory and Economic Models (joint SOE/BP/DY)

Time: Thursday 11:00–12:15 Location: GÖR 226

BP 36.1 Thu 11:00 GÖR 226

**Learning dynamics explains human behavior in Prisoner's Dilemma on networks** — •Giulio Cimini[1] and Angel Sanchez[1,2] — [1]Grupo Interdisciplinar de Sistemas Complejos (GISC), Universidad Carlos III de Madrid, 28911 Leganés, Madrid, Spain — [2]Instituto de Biocomputación y Física de Sistemas Complejos (BIFI), Universidad de Zaragoza, 50018 Zaragoza, Spain

Cooperative behavior lies at the very basis of human societies, yet its evolutionary origin remains a key unsolved puzzle. Whereas reciprocity or conditional cooperation is one of the most prominent mechanisms proposed to explain the emergence of cooperation in social dilemmas, recent experimental findings on networked Prisoner's Dilemma games suggest that conditional cooperation also depends on the previous action of the player—namely on the 'mood' in which the player currently is. Roughly, a majority of people behave as conditional cooperators if they cooperated in the past, while they ignore the context and free-ride with high probability if they did not. However, the ultimate origin of this behavior represents a conundrum itself. Here we aim specifically at providing an evolutionary explanation of moody conditional cooperation. To this end, we perform an extensive analysis of different evolutionary dynamics for players' behavioral traits—ranging from standard processes used in game theory based on payoff comparison to others that include non-economic or social factors. Our results show that only a dynamic built upon reinforcement learning is able to give rise to evolutionarily stable moody conditional cooperation, and at the end to reproduce the human behaviors observed in the experiments.

BP 36.2 Thu 11:15 GÖR 226

**Human coordination in the presence of local and global information: A laboratory experiment** — •Alberto Antonioni[1,2], Marco Tomassini[1], and Angel Sánchez[2] — [1]University of Lausanne, Switzerland — [2]Universidad Carlos III de Madrid, Spain

Pure coordination games arise in many situations that affect the functioning of society. In fact, many frequent social and economic activities require individuals to coordinate their actions on a common goal since in many cases the best course of action is to conform to the standard behavior. In particular, social coordination can be studied through coordination games between individuals located in space. Here we study the behavior of humans in the laboratory when they play a pure coordination game in a setting in which subjects are situated in a virtual two-dimensional grid space and can move around. We compare a local information setting situation to one in which global information is available. In the local information treatment subjects can see only the eight cells that are their spatial neighbors in the grid and they can decide if they want to move and/or pay a cost to switch to the other strategy type. In the global treatment subjects are in the same condition as before but they possess also the global information about the current fraction of strategies in the population. We observe that in the local information treatment people tend to converge to two separated monomorphic clusters each playing a different strategy. In contrast, in the global setting this can lead to full predominance of one strategy when strategy fluctuations reach a threshold such that imitation of the majority sets in.

BP 36.3 Thu 11:30 GÖR 226

**Differential value of information in non-cooperative games** — Nils Bertschinger[1], David H. Wolpert[2], •Eckehard Olbrich[1], and Jürgen Jost[1,2] — [1]Max Planck Institut für Mathematik in den Naturwissenschaften, Leipzig — [2]Santa Fe Institute, NM, USA

We study how players value changes in the information structure of non-cooperative games with imperfect information.

We use the functionals central to Shannon's information theory to quantify amounts of information study how changes in the values of those functionals are related to changes in the expected utility of the players. Our approach is based on the Multi-Agent Influence Diagram representation of games, and is based on a generalization of the concept of marginal utility in decision scenarios to apply to infinitesimal changes of the channel parameters in non-cooperative games. Using that framework we derive general conditions for the possibility of a negative value of information, and show that generically, these conditions hold in all games unless one imposes a priori constraints on the allowed changes to information channels. In other words, in any game in which a player values some aspect of the game's specification beyond the information provided in that game, there will be an infinitesimal change to the parameter vector specifying the game that increases the information but hurts the player.

We demonstrate these results numerically for a leader-follower game and discuss their general implications.

BP 36.4 Thu 11:45 GÖR 226

**Stability of Zero-Sum Games in Evolutionary Game Theory** — •Johannes Knebel, Torben Krüger, Markus F. Weber, and Erwin Frey — Ludwigs-Maximilians-Universität, München, Deutschland

Evolutionary game theory has evolved into a successful theoretical concept to study mechanisms that govern the evolution of ecological communities. On a mathematical level, this theory was formalized in the framework of the celebrated replicator equations (REs) and its stochastic generalizations.

In our work, we analyze the long-time behavior of the REs for zero-sum games with arbitrarily many strategies, which are generalized versions of the children's game Rock-Paper-Scissors (1). We demonstrate how to determine the strategies that survive and those that become extinct in the long run. Our results show that extinction of strategies is exponentially fast in generic setups, and that conditions for the survival can be formulated in terms of the Pfaffian of the REs' antisymmetric payoff matrix. Consequences for the stochastic dynamics, which arise in finite populations, are reflected by a generalized scaling law for the extinction time in the vicinity of critical reaction rates.

Our findings underline the relevance of zero-sum games as a reference for the analysis of other models in evolutionary game theory.

(1) J. Knebel, T. Krüger, M.F. Weber, E. Frey, Phys. Rev. Lett. 110, 168106 (2013)

BP 36.5 Thu 12:00 GÖR 226

**Opportunistic strategies and the emergence of responsible punishment** — •Arne Traulsen — Max-Planck-Institute for Evolutionary Biology, Evolutionary Theory Group, Plön, Germany

One way to promote cooperation among selfish actors is to allow for

the opportunity to punish those peers who do not cooperate. However, the vast majority of models and behavioral experiments considers situations in which actors cannot assess whether it is likely that they will be punished. If this information is available, opportunistic strategies that act according to this information become possible and lead to the emergence of responsible punishment targeted at non-cooperators only, without the problems of antisocial punishment, second order free-riding or spite. Also for institutional, so called pool punishment, such opportunistic strategies are successful, which implies that the presence of punishment institutions should be made public.

## BP 37: Networks, From Topology to Dynamics II (joint SOE/DY/BP)

Time: Thursday 12:15–13:00 Location: GÖR 226

BP 37.1 Thu 12:15 GÖR 226

**Synchronization in two-layer multiplex networks of conformist and contrarian interactions** — •Maximilian Sadilek[1] and Stefan Thurner[1,2,3] — [1]Section for Science of Complex Systems, Medical University of Vienna, Spitalgasse 23, A-1090, Austria — [2]Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA — [3]International Institute for Applied Systems Analysis, Schlossplatz 1, A-2361 Laxenburg, Austria

Several mathematical models have been proposed to describe synchronization in social, biological and physical systems, the most known being the Kuramoto model (KM).

We present a Kuramoto-type model on two layers which is designed to capture the interplay of synchronization-enhancing (conformist) and -reducing (contrarian) links in a multiplex network. The model is a combination of a KM on the first layer and a phase shifted KM on the second layer. The topology of the layers varies from random networks to small world networks.

We find indications of a phase transition from the synchronized to the unsynchronized phase in terms of the phase shift parameter of the model. Further, we observe an upward shift of the dominant frequencies in the power spectra with increasing values of the phase shift parameter.

These results may elucidate the understanding of synchronization modes in the human brain and their consequences.

BP 37.2 Thu 12:30 GÖR 226

**Controllability of Temporal Networks** — •Márton Pósfai[1,2] and Philipp Hövel[2,3] — [1]Department of Physics of Complex Systems, Eötvös University, Budapest, Hungary — [2]Institut für Theoretische Physik, TU Berlin, Berlin, Germany — [3]Bernstein Center for Computational Neuroscience, HU Berlin, Berlin, Germany

The control of complex systems is an ongoing challenge of complexity research. Resent advances making use of structural control made it possible to deduce a wide range of control related properties from the network representation of complex systems. Here we examine the controllability of complex systems for which the timescale of the dynamics we control and the timescale of changes in the network topology are comparable. We provide analytical and computational tools to study the controllability of such systems based on temporal network characteristics of the system. We apply these results to investigate the controllable subnetwork using a single input. We present analytical results for a simple class of temporal network models, and we preform measurements using data collected from real systems. Depending on the density of the interactions compared to the timescale of the dynamics, we witness a phase transition describing the sudden emergence of a giant controllable subspace spanning a finite fraction of the network. We also study the role of temporal patterns in real data making use of various randomization processes, with special focus on the role of the hubs.

BP 37.3 Thu 12:45 GÖR 226

**Analysis of local network structure by node-specific triadic Z-score profiles** — •Marco Winkler and Jörg Reichardt — Institute for Theoretical Physics, University of Würzburg, Germany

Over the last decade so called network motifs have attracted high attention. A motif is a subgraph pattern that appears significantly more often than in a random network with the same degree distribution as the original one. Triadic Z-score profiles, $\vec{Z}$, assign every possible triadic subgraph pattern $i$ a score $Z_i$, corresponding to the magnitude of over-/underrepresentation of the pattern compared to the random null model. These Z-score profiles are a common tool to analyze complex networks.

However, triad patterns are not necessarily homogeneously distributed over the network. Therefore, we introduce the concept of *node-specific Z-scores*. For the node-specific Z-score profile, $\vec{Z}^{\alpha}$, of a node $\alpha$, only the triads it participates in are taken into account. The node-specific Z-score profiles can then be used for classification of a network's vertices into different structural groups. We present results for various real-world data sets including neural networks and transcription networks.

## BP 38: Active cell and tissue mechanics (focus session) II

Time: Thursday 15:00–17:30 Location: HÜL 386

**Topical Talk** BP 38.1 Thu 15:00 HÜL 386

**Analyzing integrin's force transduction using novel biosensors** — •Carsten Grashoff — Max-Planck-Institute of Biochemistry, Group of Molecular Mechanotransduction, Am Klopferpsitz 18, 82152 Planegg, Germany

Cell adhesion to the extracellular matrix is mediated by integrin receptors which connect to the cytoskeleton in complex structures called focal adhesions (FAs). The ability of these adhesions to bear and transduce mechanical forces is central to many developmental or homeostatic processes and plays an important role in a range of pathological situations; yet our understanding of how integrin forces are propagated in FAs remains fragmentary.

One reason for our limited understanding has been the lack of suitable methods to study force propagation on the sub-cellular level in the living cell. Therefore, we have previously developed a FRET-based method to visualize and quantify mechanical forces within cells.

Here, I will introduce a novel, calibrated biosensor and describe its application to the integrin activator talin-1.

BP 38.2 Thu 15:30 HÜL 386

**Transduction channel's gating controls friction on vibrating hair-cell bundles in the ear** — •Volker Bormuth[1], Jérémie Barral[1], Jean-François Joanny[1], Frank Jülicher[2], and Pascal Martin[1] — [1]Laboratoire Physico-Chimie Curie, CNRS, Institut Curie, UPMC; 75005 Paris, France — [2]2Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Hearing starts when sound-evoked mechanical vibrations of the hair-cell bundle activate mechanosensitive ion channels, giving birth to an electrical signal. As for any mechanical machine, friction impedes movements of the hair bundle and thus constrains the sensitivity and frequency selectivity of auditory transduction. Using dynamic force measurements on single hair-cell bundles, we demonstrate here that the opening and closing of the transduction channels produce internal friction forces that can dominate viscous drag on the micrometric hair-bundle structure. A theoretical analysis reveals that channel friction arises from coupling the dynamics of the conformational change associated with channel gating to tip-link tension. We propose that this intrinsic source of friction contributes to the process that sets the hair cell's characteristic frequency of responsiveness.

BP 38.3 Thu 15:45 HÜL 386

**Mechanical properties of syncytial Drosophila embryos by high-speed video microrheology** — •Alok D. Wessel and Christoph F. Schmidt — Drittes Physikalisches Institut, Georg-

August-Universität Göttingen, Germany

In the early syncytial stage Drosophila melanogaster embryos nuclei are duplicating, but are not yet separated by membranes. They are interconnected by cytoskeletal polymer networks consisting of actin and microtubules. Between division stages 9 and 13, nuclei and the cytoskeletal networks form a well-ordered 2D cortical layer. To understand the underlying mechanical properties and dynamics of this self-organizing "pre-tissue", we have measured shear elastic moduli of the interior of the embryo and its cortical layer by high-speed video microrheology. We have recorded position fluctuations of injected micron-sized fluorescent beads with a high-speed camera at kHz sampling frequencies. In that manner we can analyze the local mechanics of the embryo in time and space. The interior of syncytial embryos shows a homogeneous, viscously dominated character with a viscosity approximately 300 times higher than water. In the actin-rich outer layers, near the nuclei, we measured a viscoelastic response. Furthermore we were able to resolve temporal variations of the shear modulus inside the layer.

BP 38.4 Thu 16:00 HÜL 386

**Active mechanics and dynamics of epithelia during morphogenesis** — •Amitabha Nandi[1], Marko Popovic[1], Matthias Merkel[1], Raphaël Etournay[2], Suzanne Eaton[2], Guillaume Salbreux[1], and Frank Jülicher[1] — [1]Max-Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Max-Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstrasse 108, 01307 Dresden, Germany

During development of an organism, epithelial tissues are dynamically remodeled due to forces generated in the cells, cellular rearrangements, and cell division and apoptosis. Such remodeling occurring over long time-scales leads to reorganization of the tissue allowing to establish the shape of the organism. In this work, we introduce a physical description of the slow timescale behavior of an epithelium. We obtain the hydrodynamic constitutive equations describing the continuum mechanics of an epithelium in two dimensions on spatial scales larger than a cell. Within this framework, topological rearrangements relax elastic stresses in the tissue and can be actively triggered by internal cell processes. We study simple limit cases of the flows and deformation predicted by the continuum theory. Using segmentation of the wing disc cell packing at pupal stage of the fly, we analyze experimental coarse-grained patterns of flow field and tissue shear. We show that our continuum theory can account for the key features of the cell flow and deformation fields. We find that a gradient of active contractile stress acting together with active cell rearrangement that are polarized in the tissue plane can explain the flow patterns observed in experiments.

**15 min. break**

BP 38.5 Thu 16:30 HÜL 386

**Impact of heating on passive and active biomechanics of suspended cells** — •Chii Jou Chan[1,2], Graeme Whyte[1,3], Lars Boyde[1], Guillaume Salbreux[4], and Jochen Guck[1,2] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, UK — [2]Biotechnology Center, TU Dresden, Dresden, Germany — [3]Department of Physics and Institute of Medical Biotechnology, University of Erlangen-Nuremberg, Germany — [4]MPI PKS, Dresden, Germany

Heating can have a dramatic effect on cell mechanical properties, similar to its impact on the dynamics of artificial polymer networks. We investigated such mechanical changes by the use of an optical stretcher which allowed us to probe single-cell mechanics at different heating conditions and time-scales. We find that HL60/S4 myeloid precursor cells become mechanically more compliant and fluid-like when subjected to either a sudden temperature increase or a prolonged exposure to higher ambient temperature. Above a critical temperature of 52°C, we observed active cell contraction which was strongly correlated with calcium influx through temperature-sensitive TRPV2 ion channels. The change from passive to active cellular response can be effectively described by a mechanical model incorporating cell viscoelastic components and an additional time-dependent active component. Our work highlights the role of TRPV2 in regulating the thermo-mechanical response of cells, and offers insights on how cortical tension and osmotic pressure can actively regulate cell shape changes in response to heat and mechanical stress.

BP 38.6 Thu 16:45 HÜL 386

**The mechanics of cultured cell monolayers** — •Guillaume Charras — University College London, London, UK

One-cell thick monolayers are the simplest tissues in multi-cellular organisms, yet they fulfil critical roles in development and normal physiology. In early development, embryonic morphogenesis results largely from monolayer rearrangement and deformation due to internally generated forces. Later, monolayers act as physical barriers separating the internal environment from the exterior and must withstand externally applied forces. Though resisting and generating mechanical forces is an essential part of monolayer function, simple experimental methods to characterise monolayer mechanical properties are lacking. Using a novel tensile testing system that enables examination of monolayer mechanics at subcellular, cellular and tissue-scales, we provide measurements of monolayer elasticity and show that this is two orders of magnitude larger than the elasticity of their isolated cellular components. Monolayers could withstand more than a doubling in length before failing through rupture of intercellular junctions. Measurement of stress at fracture enabled a first estimation of the average force needed to separate cells within truly mature monolayers, ˜9-fold larger than measured in pairs of isolated cells. As in single cells, monolayer mechanical properties were strongly dependent on the integrity of the actin cytoskeleton, myosin, and intercellular adhesions interfacing adjacent cells. This multiscale study of monolayer response to deformation enabled by our novel device provides the first quantitative investigation of the link between monolayer biology and mechanics.

BP 38.7 Thu 17:00 HÜL 386

**Individual cell phenotype determines growth modes of cell colonies** — •Ben Fabry[1], Janina Lange[1], Pamela Strissel[2], Julian Steinwachs[1], and Claus Metzner[1] — [1]Department of Physics, University of Erlangen-Nuremberg, Erlangen, Germany — [2]Women's Hospital, University Clinics, Erlangen, Germany

Many tumor cells proliferate without anchorage to the matrix and often lack the cell-contact inhibition that normally prevents cells from proliferating beyond confluency. It is unclear, however, how individual cells contribute to the collective behavior and growth in a colony. Here we study colonies of different tumor and non-tumor cells lines on planar substrates. Despite the stochastic behavior of individual cells, deterministic features emerge at the colony level that are qualitatively independent of cell type, such as the linear increase of colony radius with time, a global radial streaming motion of cells away from the colony center, and a strong increase of streaming velocity and persistence at the colony border. Quantitatively, however, we find systematic differences between 6 differently adhesive and cohesive cell lines. All measured collective and single cell parameters showed a strong covariance, and no single parameter emerged as a principle component. Rather, all parameters correlated or anticorrelated strongly with the ranking order of these cell lines from a mesenchymal to an epithelial cell phenotype, suggesting that collective behavior is tightly linked with individual cell mechanical behavior.

BP 38.8 Thu 17:15 HÜL 386

**Furrow constriction in animal cell cytokinesis** — •Hervé Turlier[1,2], Basile Audoly[3], Jean-François Joanny[1,4], and Jacques Prost[1,4] — [1]Physico-chimie Curie, Institut Curie, Paris, France — [2]EMBL, Heidelberg, Germany — [3]Institut Jean-le-Rond d'Alembert, UPMC, Paris, France — [4]ESPCI, Paris, France

Cytokinesis is the process of physical cleavage at the end of cell division; it proceeds by ingression of an actomyosin furrow at the equator of the cell. Its failure leads to multinucleated cells and is a possible cause of tumorigenesis. We calculate the full dynamics of furrow ingression and predict cytokinesis completion above a well-defined threshold of equatorial contractility. The cortical acto-myosin is identified as the main source of mechanical dissipation and active forces. Thereupon, we propose a viscous active nonlinear membrane theory of the cortex that explicitly includes actin turnover and where the active RhoA signal leads to an equatorial band of myosin overactivity. The resulting cortex deformation is calculated numerically, and reproduces well the features of cytokinesis such as cell shape and cortical flows toward the equator. Our theory gives a physical explanation of the independence of cytokinesis duration on cell size in embryos. It also predicts a critical role of turnover on the rate and success of furrow constriction. Scaling arguments allow for a simple interpretation of the numerical results and unveil the key mechanism that generates the threshold for cytokinesis completion: cytoplasmic incompressibility results in a competition between the furrow line tension and the cell poles* surface tension.

# BP 39: The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (accompanying session, joint CPP/BP/DY)

Time: Thursday 15:00–17:30 Location: ZEU 250

BP 39.1 Thu 15:00 ZEU 250

**Collapse and self-organization of polymer structures in poor solvent - A Monte Carlo Study** — •Marco Werner[1,2], Christoph Jentzsch[1,2], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

We investigate poor solvent effects in polymer structures such as single polymer globules [1], collapsed polymer brushes as well as self-assembled lipid bilayer membranes [2] by using the bond-fluctuation model with explicit solvent. Focussing on the coil-to-globule transition of single polymer chains we show that even in the case of very poor solvent our coarse grained lattice model avoids freezing effects and preserves dynamic fluctuations at the polymer-solvent interface in contrast to corresponding implicit solvent models. We demonstrate that fluctuations will be necessary for a complete description of the force-extension curve during the unravelling process of a single polymer globule. In particular in the region of coexistence of collapsed and stretched part we observe a fluctuating ensemble of globules along the chain, which smooths the force-extension curve.

[1] C. Jentzsch, M. Werner, und J.-U. Sommer, J. Chem. Phys. 138 (9), 094902 (2013).

[2] J.-U. Sommer, M. Werner, und V. A. Baulin, Europhys. Lett. 98, 18003 (2012).

BP 39.2 Thu 15:15 ZEU 250

**Melts of unconcatenated and unknotted polymer rings revisited** — •Joachim Wittmer, Hendrik Meyer, and Albert Johner — Institut Charles Sadron & CNRS, 23 Rue du Loess, 67034 Strasbourg CEDEX 2, France

A paradigmatic example for soft matter systems ruled by topological interactions is provided by melts of unconcatenated polymer rings. Recent computational studies suggest that sufficiently long rings become compact which begs the question of whether the irregular surfaces of these compact objects may be characterized by a finite fractal surface dimension $d_s < 3$. We revisit the scaling analysis of the intramolecular structure factor by Halverson et al. [J. Chem. Phys. 134, 204904 (2011)] claiming $d_s \approx 2.8$. Our analysis suggests that this conclusion might be due to an inappropriate application of the Generalized Porod Law. We present then in the second part of our talk a "decorated Gaussian loop model" which does not require a finite fractal surface dimension $d_s < 3$. In this approach the topological interactions between different rings are taken into account by a self-similar and space-filling random tree of polydisperse Gaussian loops ranging from the entanglement length to a skeleton ring of length $N^{2/3}$. Individual rings are predicted to be marginally compact with an average chain size $R^2 \sim N^{2/3}(1 - 1/N^{1/3})$ where all prefactors have been omitted for clarity. Sluggish $1/N^{1/3}$-corrections to the leading power-law behavior are also shown to arise for other experimentally relevant properties.

BP 39.3 Thu 15:30 ZEU 250

**Fractal globule as an artificial molecular machine** — •Nechaev Sergei — LPTMS (Orsay, France)

The relaxation of an elastic network, constructed by a contact map of a fractal (crumpled) polymer globule is investigated. We found that: i) the slowest mode of the network is separated from the rest of the spectrum by a wide gap, and ii) the network quickly relaxes to a low-dimensional (one-dimensional, in our demonstration) manifold spanned by slowest degrees of freedom with a large basin of attraction, and then slowly approaches the equilibrium not escaping this manifold. By these dynamic properties, the fractal globule elastic network is similar to real biological molecular machines, like myosin. We have demonstrated that unfolding of a fractal globule can be described as a cascade of equilibrium phase transitions in a hierarchical system. Unfolding manifests itself in a sequential loss of stability of hierarchical levels with the temperature change.

BP 39.4 Thu 15:45 ZEU 250

**Conformation and Structural Changes of Diblock Copolymers with Octopus-Like Micelle Formation under the Influence of Water Vapor** — •Kirsten Dammertz[1], Masoud Amirkhani[1], Christoph Jentzsch[2], Jens-Uwe Sommer[2,3], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm Univeristy — [2]Leibniz-Institute of Polymer Research Dresden — [3]Institute of Theoretical Physics, TU-Dresden

External stimuli like vapors, pressure or electric fields can be used to manipulate the polymer configurations of diblock-copolymers. Due to the conformational flexibility of such polymers, AB-diblock copolymers constitute a valuable tool to develop functional nanomaterials and devices.

We study the conformation and structural response of PS-b-PMMA, PS and PMMA adsorbed on mica under water vapor, respectively. At polymer concentrations below the minimum needed for the development of thin films, octopus-like surface micelles are formed. By applying water vapor to a system containing polar PMMA chains, additional mobility can be provided to the polymers. In contrast, PS is less affected since it does not contain a permanent dipole moment. Furthermore, collapse and decollapse effects were observed.

In addition to AFM measurements, we performed BFM Monte Carlo simulations to analyze the formation process of the micellular structures as well as their response to water vapor.

**Invited Talk** BP 39.5 Thu 16:00 ZEU 250

**Universal aspects of chromosome folding** — •Angelo Rosa — Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste (Italy)

The dynamics of the mm-long chromatin (*i.e*, DNA+histones) fibers in the cell nucleus is subject to strong topological constraints [Sikorav & Jannink (1994)]. In particular, their incomplete equilibration during interphase [Rosa & Everaers (2008)] results in territorial, crumpled globule-like chromosome conformations [Grosberg *et al.* (1993)].

It has been suggested [Rosa & Everaers, *ibid.*; Vettorel *et al.* (2009)], that this incomplete relaxation might underlie a subtle analogy between interphase chromosomes and corresponding solutions of non-concatenated ring polymers. Here, we start from our recent multi-scale computational approach for explicit construction of equilibrated solutions of giant ring polymers [Rosa & Everaers (2013); see talk by R. Everaers] to further explore the physical and biological consequences of this analogy.

We show that not only the territorial confinement [Cremer & Cremer (2001)] but also other characteristic features of chromosome folding such as their conformational statistics [Sachs *et al.* (1995); Lieberman-Aiden *et al.* (2009)] and the loop-on-loop structure of internal contacts [Cook (2010)] arise as a generic consequence of the polymeric nature of chromosomes. Integrated with biological information on intra- and inter-chromosomal interactions, our results pave the way for the systematic modeling of the nuclear structure and dynamics.

**15 min break**

BP 39.6 Thu 16:45 ZEU 250

**Effects of nucleosome positioning on condenstation of short and long chromatin fibers** — Robert Schöpflin[1], Oliver Müller[1], Christin Weinberg[1], Vladimir B. Teif[2], Karsten Rippe[2], and •Gero Wedemann[1] — [1]CC Bioinformatics, University of Applied Sciences Stralsund, Stralsund, Germany — [2]Deutsches Krebsforschungszentrum & BioQuant, Heidelberg, Germany

In eukaryotes DNA is associated with proteins in a complex structure termed chromatin. The basic packaging unit of chromatin is the nucleosome in which DNA is wrapped around a histone octamer. Experiments indicate that chromatin has different packaging conditions connected to distinct activation states. Experimental evidence showed that packaging and activation states are closely linked to positions of nucleosomes on the DNA which are actively regulated. To improve the understanding of the interplay between nucleosome positions and chromatin structure we applied computer simulations of a coarse-grained chromatin model including fundamental physical properties such as elasticity, electrostatics and nucleosome interactions using a feedback-optimized replica exchange protocol. We calculated the effect of nucleosome positioning on the structure of polynucleosomes of different length scales, up to the size of a gene locus. We compared chromatin models based on synthetic positions with models based on experimen-

tally derived nucleosome positions from cells at different stages of cell differentiation. Simulation results revealed a significant influence of nucleosome positions on the three dimensional structure of chromatin.

BP 39.7 Thu 17:00 ZEU 250

**Loop models in Magnetic Spin Ice crystals** — •Ludovic Jaubert[1], Masud Haque[2], and Roderich Moessner[2] — [1]OIST, Okinawa, Japan — [2]MPI-PkS, Dresden

Loops are ubiquitous in physics, either as tangible entities such as polymers, or as emergent phenomena, especially where we do not expect them. In this talk, we shall focus on the latter case, where loops appear as extended degrees of freedom in spin ice crystals.

Spin ice has become a canonical member of the large and growing family of frustrated magnets, where excitations take the form of magnetic monopoles. The ground state of this system is highly degenerate and can be mapped exactly onto a fully packed loop model. We studied the statistics of this model both in 2 and 3 dimensions [1], making contact with Stochastic-Loewner Evolution processes (SLE), percolation and polymer physics, before illustrating implications of these results in related problems (Heisenberg magnets, itinerant electrons [2]).

[1] Jaubert, Haque, Moessner, PRL, 107, 177202 (2011)
[2] Jaubert, Pitaecki, Haque & Moessner, PRB, 85, 054425 (2012)

BP 39.8 Thu 17:15 ZEU 250

**Membrane-driven collapse of DNA macromolecules and semiflexible filamentous virus particles** — Anastasiia B. Artemieva[1], Christoph Herold[2], Andrey G. Cherstvy[3], Petra Schwille[1], and •Eugene P. Petrov[1] — [1]Max Planck Institute of Biochemistry, 82152 Martinsried, Germany — [2]BIOTEC, Technische Universität Dresden, 01307 Dresden, Germany — [3]University of Potsdam, 14476 Potsdam-Golm, Germany

Interaction of (bio)macromolecules and colloidal particles with lipid membranes is one of the important problems of the modern bio-inspired soft matter physics. Earlier, we have found [1] that interaction of DNA molecules with strongly charged freestanding cationic lipid bilayers [2] leads membrane-mediated coil-globule transition of membrane-absorbed DNA macromolecules. Our recent experimental observations show that membrane-driven interactions at higher membrane charge densities are strong enough to induce the membrane-mediated collapse of much stiffer *fd* virus particles ($l_p \sim 2.2$ $\mu$m). We discuss these experimental findings in the framework of our new theoretical treatment [3] which takes into account membrane-polyelectrolyte electrostatic interactions, local membrane deformations, and polyelectrolyte bending rigidity.

[1] C. Herold, P. Schwille, and E. P. Petrov, *Phys. Rev. Lett.* **104** (2010) 148102.
[2] C. Herold, G. Chwastek, P. Schwille, and E. P. Petrov, *Langmuir* **28** (2012) 5518.
[3] A. G. Cherstvy and E. P. Petrov, *PCCP* (2014) in press.

## BP 40: Stochastic Dynamics of Growth Processes in Biological and Social Systems (Symposium SYGP, joint DY/BP/SOE)

Time: Thursday 15:00–17:45 Location: HSZ 02

**Invited Talk** BP 40.1 Thu 15:00 HSZ 02

**Noisy invasions: large fluctuations in stochastic invasion models** — •Baruch Meerson — Racah Institute of Physics, Hebrew University of Jerusalem, Jerusalem 91904 Israel

Invasion fronts have been recognized as important, and often fateful, phenomena in ecology, epidemiology and biological evolution. The position of an invasion front fluctuates because of the shot noise of individual reactions. What is the probability to observe, at a given time, a front displacement that is considerably smaller or larger than that predicted from deterministic theory? The answer strongly depends on whether the front propagates into a metastable or unstable state, and I will review recent theoretical progress in both cases. The progress is mostly based on a dissipative version of WKB theory which assumes many individuals in the front region. In this theory the most likely history of the system, for a given front displacement, is encoded in a special trajectory of the underlying effective Hamilton mechanics, a classical field theory. This special trajectory is described by a traveling front solution. For fronts, propagating into unstable states, very large front displacements are much more likely than very small ones. The leading contribution to the probability density of a large displacement comes from a few fastest particles running ahead of the front. For such fronts the WKB theory breaks down, and new methods are needed.

**Invited Talk** BP 40.2 Thu 15:30 HSZ 02

**Fractal clustering of inertial particles in random velocity fields** — •Bernhard Mehlig and Kristian Gustavsson — Department of Physics, University of Gothenburg, 41296 Gothenburg, Sweden

Independent particles suspended in incompressible turbulent or randomly mixing flows may cluster together even though incompressible flows exhibit no sinks. This is an inertial effect: inertia allows the particles to detach from the flow. Distinct mechanisms have been invoked to explain clustering in incompressible flows. The two most common ones are "preferential concentration" and "multiplicative amplification". Preferential concentration refers to the tendency of heavy particles to avoid vortical regions of the flow. Multiplicative amplification, by contrast, explains clustering in terms of the logarithmic amplification of the sequence of many small kicks that the suspended particles experience.

In order to quantify the relative importance of the two mechanisms it is necessary to compute the fluctuations of the flow-velocity gradients that the particles experience as they move through the flow. We show how this can be achieved systematically by means of perturbation expansions that recursively take into account how the flow affects the actual particle trajectory. We analyse the statistics of particle- and flow-velocity gradients as seen by the particles. Based on these results we show that in random velocity fields multiplicative amplification has a much stronger effect than preferential concentration, except at very small Stokes numbers. We discuss the implications of these findings for particles suspended in turbulent flows.

**Invited Talk** BP 40.3 Thu 16:00 HSZ 02

**Stochastic population dynamics on rugged fitness landscapes** — •Joachim Krug — Institut für Theoretische Physik, Universität zu Köln

Biological evolution is inherently noisy because of random mutations and stochasticity induced by sampling in finite populations. Since the sampling noise is inversely proportional to population size, one expects deterministic dynamics to emerge in large populations, but in practice this regime is hardly every attainable and fluctuations dominate the behavior even in the largest microbial populations. In this talk I will show how the interplay of the stochastic population dynamics with the structure of the underlying fitness landscape can lead to counter-intuitive phenomena such as an adaptive advantage of small populations and a non-monotonic dependence of evolutionary predictability on population size. If time permits, the adaptive benefits of recombination in rugged fitness landscapes will be briefly addressed as well. The talk is based on joint work with Kavita Jain, Johannes Neidhart, Stefan Nowak, Su-Chan Park, Ivan Szendro and Arjan de Visser.

**15 min break**

**Invited Talk** BP 40.4 Thu 16:45 HSZ 02

**Modeling cancer as a stochastic process** — •Tibor Antal — School of Mathematics at Edinburgh University, Edinburgh, UK

Stochasticity is essential when modeling initiation of tumors, progression of tumors from benign to malignant states, or metastasis formation. Many aspects of these phenomena can be modeled by simple multi-type branching processes, and the results compare fairly well with experimental and clinical data. These models then can be used to optimize drug treatments. Spatial heterogeneity of tumors are also important for treatment, and their exploration has recently begun by modeling the interplay between tumor shapes and genetic mutations.

**Invited Talk** BP 40.5 Thu 17:15 HSZ 02

**Von Neumann's growth model: from statistical mechanics to cell metabolism** — •Andrea De Martino — Sapienza Universita'

di Roma & CNR, Roma, Italy

This talk reviews the basic properties of Von Neumann's model of growth in production economies, mainly from a statistical mechanics perspective. In addition, I will discuss its recent applications in quantitative biology, for the profiling of a cell's metabolic activity and of its thermodynamics. Finally, a class of Boolean constraint-satisfaction problems based on Von Neumann's idea will be presented, whose solutions allow to shed new light on the modular organization of metabolic networks.

## BP 41: Biomaterials and Biopolymers II (joint CPP/BP)

Time: Thursday 15:00–18:45 Location: ZEU 222

BP 41.1 Thu 15:00 ZEU 222

**Observing the onset of amyloid fibril formation at interfaces with Reflection Anisotropy Spectroscopy** — •Heike Arnolds, Sergio Mauri, Caroline Smith, and Peter Weightman — Surface Science Research Centre, University of Liverpool, Oxford Road, Liverpool L69 3BX, UK

The interaction of proteins with surfaces facilitates misfolding and leads to the formation of amyloid fibrils. This has a major impact on human health, because fibril formation during drug storage and injection decreases drug activity, for example in human insulin, and fibril formation at cell membranes is associated with diseases such as Alzheimer's. The key event is the formation of $\beta$-sheet structures which further self-assemble into amyloid fibrils, but there is little mechanistic understanding to date due to a dearth of experimental techniques which are sensitive and informative enough. Reflection anisotropy spectroscopy (RAS) provides structural information of adsorbates from the azimuthal angular variation of the optical spectrum about the direction of the incident light. It has been used for example to monitor the conformational change in cytochrome P450 in real time [1]. Here we apply the technique to the adsorption of human insulin on model methyl and amine terminated stepped Si(111) surfaces. By comparison to attenuated total reflection infrared spectra of the amide I band, we show that RAS can detect a helical $\beta$-sheet structure, which likely represents the onset of fibril formation.

[1]P. Weightman et al, Phys Rev E 88, 032715 (2013)

BP 41.2 Thu 15:15 ZEU 222

**UV treatment of stretchable polymer foils for bio-applications** — •Ruxandra-A. Barb[1], Birte Magnus[2], Theresia Greunz[4], David Stifter[4], Rainer Marksteiner[2], Siegfried Innerbichler[3], and Johannes Heitz[1] — [1]Institute of Applied Physics, Johannes Kepler University Linz, Austria — [2]Innovacell Biotechnologie AG, Innsbruck, Austria — [3]Innerbichler GmbH, Breitenbach am Inn, Austria — [4]CDL-MS-MACH, Johannes Kepler University Linz, Austria

Polymers are often used as substrates for cell cultivation. Stretchable polymer foils are required in a cell stretcher, which allows to investigate the behavior of cells during uni-axial mechanical strain or compression [1]. However, many stretchable polymers have weak cyto-compatibilty. We demonstrate here that the cyto-compatibility of fluorinated ethylene propylene (FEP) or polyurethane (PU) can be significantly enhanced by UV photo-modification in a reactive atmosphere by means of a Xe2* excimer lamp emitting at 172 nm. Cells seeded on the treated polymer foils show enhanced cell adhesion and proliferation. Water contact angle and XPS measurements indicate that this is a result of improved wettability and a significant change in surface chemistry. However, tensile tests show that UV induced chain scissions can also lead to a degradation of the mechanical stability. But with suitable irradiation dose and foil thickness, repeatedly stretchable polymer foils with sufficient cell adhesion can be prepared.

[1] A. Gerstmair, G. Fois, S. Innerbichler, P. Dietl, E. Felder, J. Appl. Physiol. 107, 613-620 (2009).

BP 41.3 Thu 15:30 ZEU 222

**Mechanics of engineered spider silk microparticles** — •Martin Peter Neubauer[1], Claudia Bluem[2], Thomas Scheibel[2], and Andreas Fery[1] — [1]Department of Physical Chemistry II, University of Bayreuth, Germany — [2]Department of Biomaterials, University of Bayreuth, Germany

Spider silk fibers are well known for their high tensile strength and elasticity. Further, spider silk is biocompatible and -degradable. Thus, application perspectives can be envisaged for pharmaceutics or cosmetics. Employing recombinant synthesis spider silk proteins are readily available and can be processed into different morphologies such as particles, capsules or films.[1]

We focus on mechanical properties of spider silk microparticles.[2] These could serve as fillers in composite materials or for drug delivery [3]. In this context, the understanding and controlling of mechanics is essential. From AFM force spectroscopy experiments we could show the drastic influence of hydration on the particles' elastic modulus which drops by orders of magnitude. Other investigated parameters include crosslinking and molecular weight. These mechanical studies are accompanied by the examination of structure, swelling and thermal behavior.

[1] Humenik, M., Smith, A. M., Scheibel, S., Polymers 2011, 3: 640-661

[2] Neubauer, M. P., Bluem, C., Agostini, E., Engert, J., Scheibel, S., Fery, A., Biomater. Sci. 2013, 1: 1160-1165

[3] Bluem, C., Scheibel, T., BioNanoSci. 2012, 2: 67-74

BP 41.4 Thu 15:45 ZEU 222

**Multivalent Ligand Design** — •Susanne Liese — FU Berlin, Berlin

The binding strength of multivalent ligands of different geometry and rigidity is studied, using an analytic statistical mechanics model. By varying the spacer length between the ligand units, the binding strength is optimized. It is found that for low association constants of the monovalent ligand, even an optimized multivalent structure, does not bind better than the monovalent correspondent. The critical association constant above which a multivalent ligand enhances binding, depends cubically on the distance between the receptor binding sites. In all systems we find that a multivalent ligand binds best, if the average spacer length is in the range of the receptor binding site distance and if the spacer is as stiff as possible.

BP 41.5 Thu 16:00 ZEU 222

**Structure/Property-Correlation of Alinate-Surfactant Mixtures at the Water Surface** — •Patrick Degen[1], Victoria Jakobi[2], Michael Paulus[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, Germany — [2]Analytical Chemistry - Biointerfaces, Ruhr-Universität Bochum, Germany

Usually soft colloids, such as emulsion droplets or foam bubbles are stabilized by adsorbed layers of surfactants, polymers and mixtures of both. In recent years industrial researchers focus on polymers that are biocompatible such as gum acacia, chitosan or alginate. Such mixtures are found in pharma-ceutical and food applications, in cosmetic products, detergents, and so forth. Nevertheless, the knowledge of basic properties of oil-water interfaces stabilized by surfactant-polymer mixtures is challenged by the complexities of the interactions involved. We present complementary investigations of surface tension and surface rheology properties on the alginate/surfactant system. In combination with dynamic light scattering and fluorescence spectroscopy this work provides new insights into the interactions between alginate and different surfactants in bulk and at the interface. Additionally, X-ray reflectivity measurements give information about the microscopic structure of such interfacial films. We demonstrate that some of the characteristic rheological features related to polymer - surfactant associations correlate with the X-ray reflectivity results, where the formation of large-scale complexes, depending on the surfactant concentration was observed.

BP 41.6 Thu 16:15 ZEU 222

**Determining the Specificity of Monoclonal Antibody HPT-101 to Tau-Peptides with Optical Tweezers** — •Tim Stangner[1], Carolin Wagner[1], David Singer[2], Stefano Angioletti-Uberti[3], Christof Gutsche[1], Joachim Dzubiella[3], Ralf Hoffmann[2], and Friedrich Kremer[1] — [1]University of Leipzig, Department of Experimental Physics I, D-04103 Leipzig, Germany — [2]University of Leipzig, BBZ, D-04103 Leipzig, Germany — [3]Humboldt University Berlin, De-

partment of Physics, Berlin 12489, Germany

Optical tweezers-assisted dynamic force spectroscopy (DFS) is employed to investigate specific receptor/ligand bindings on the level of single binding events. Here, the binding of the phosphorylation-specific antibody HPT-101 to tau-peptides (pThr231/pSer235) with two potential phosphorylation sites is analyzed. According to ELISA-measurements, the antibody binds only specificity to the double-phosphorylated tau-peptide. It is shown by DFS that HPT-101 binds also to each sort of the mono-phosphorylated peptides. By analyzing the measured rupture-force distributions characteristic parameters are determined for all interactions. Using the extracted bond parameters, we build a simple theoretical model to predict features of the unbinding process for the double-phosphorylated peptide purely based on data on the monophosphorylated ones. Furthermore we introduce a method to estimate the relative affinity of the bonds. The values obtained for this quantity are in accordance with ELISA, showing how DFS can offer important insights about the dynamic binding process that are not accessible with this common and widespread assay.

**15 min. break**

**Invited Talk** BP 41.7 Thu 16:45 ZEU 222

**Threading DNA through nanopores for biosensing applications** — •Maria Fyta — Insitute for Computational Physics, University of Stuttgart

The use of nanopores to read-out in an ultra-fast and cheap way the information inherent in DNA is being intensively investigated the last two decades. A biomolecule, like DNA, in a salt solution is electrophoretically threaded through a nanometer sized pore altering the ionic current that flows through the pore. Simultaneously, measuring the transverse tunneling currents across the nanopore can possibly lead to distinguishable electronic signatures for each DNA unit. Here, we will review some of our work related with the statistical and dynamical characteristics of the translocation process and the ionic current through the pore as obtained through multiscale simulations. Using more accurate simulations we will then report on our attempts to optimize the nanopore. Our efforts are focused on proper functionalization of the nanopore in order to enhance the transverse ionic current for reading-out the genetic information in DNA.

BP 41.8 Thu 17:15 ZEU 222

**DNA Interactions in Crowded Nanopores** — Nadanai Laohakunakorn[1], Sandip Ghosal[2], Oliver Otto[1], Karolis Misiunas[1], and •Ulrich F. Keyser[1] — [1]Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, CB3 0HE Cambridge, UK — [2]Northwestern University, Evanston, IL 60208-3109, USA

The motion of DNA in crowded environments is a common theme in physics and biology. Examples include gel electrophoresis and the self-interaction of DNA within cells and viral capsids. Here we study the interaction of multiple DNA molecules within a nanopore by tethering the DNA to a bead held in a laser optical trap to produce a *molecular tug-of-war*. We measure this tether force as a function of the number of DNA molecules in the pore and show that the force per molecule decreases with the number of molecules [1]. A simple scaling argument based on a mean field theory of the hydrodynamic interactions between multiple DNA strands explains our observations. At high salt concentrations, when the Debye length approaches the size of the counterions, the force per molecule becomes essentially independent of the number of molecules. We attribute this to a sharp decrease in electroosmotic flow which makes the hydrodynamic interactions ineffective.

[1] N. Laohakunakorn, S. Ghosal, O. Otto, K. Misiunas, and U. F. Keyser. DNA Interactions in Crowded Nanopores. Nano Letters, 13(6):2798-2802, (2013).

BP 41.9 Thu 17:30 ZEU 222

**Diffusion regulation in the basal lamina** — •Fabienna Arends[1,2] and Oliver Lieleg[1,2] — [1]Zentralinstitut für Medizintechnik, Technische Universität München, Boltzmannstr.11, 85748 Garching — [2]Fakultät für Maschinenwesen,Technische Universität München, Boltzmannstr.15, 85748 Garching

The permeability of the basal lamina, a biological hydrogel found at the basolateral side of the epithelium, is an important property for the design of both new drug delivery systems and biomimetic hydrogels. Moreover, it is highly desirable to understand the diffusion of colloidal particles and macromolecules such as drug delivery vehicles, nutrients, growth factors, and proteins across the basal lamina. The mobility of those objects in this highly complex gel is regulated by a broad range of factors including geometric constraints and different types of physical interactions between the particles/molecules and the hydrogel constituents.

Here, we quantify the diffusion of colloids and molecules within an extracellular matrix gel (ECM) purified from the Engelbreth-Holm-Swarm sarcoma, which is a model system for the basal lamina. For this quantification we use single particle tracking techniques and measure the formation of a concentration gradient of solutes across the ECM. From our data we aim at deciphering the underlying mechanisms responsible for the permeability properties of the hydrogel.

BP 41.10 Thu 17:45 ZEU 222

**Induction phase of entropic DNA segregation in bacteria** — •Elena Minina and Axel Arnold — Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569, Stuttgart, Germany

Cell division is a complex mechanism which consists of two main processes – DNA replication and segregation. In primitive bacteria such as Escherichia coli, which has a rod-like shape and a single chromosome, the dsDNA molecule of the mother cell is split into two daughter strands which are complemented again. During the replication these daughter strands segregate, i.e. move towards opposite sides of the cell to create two new cells. It was previously shown that the segregation of confined linear polymers (DNA) is entropically driven and does not need to involve any active mechanisms [A. Arnold and S. Jun, Phys. Rev. E 76 (2007)]. However, the initial configuration of fully overlapping polymers is perfectly symmetrical. Initiation of segregation requires to break this symmetry. This period of time is called induction and has a rather broad distribution, which significantly reduces the efficiency of entropic segregation. In the present study we investigate the induction more closely and determine the mechanism that breaks the symmetry of the system. Combination of MD simulations with theory based on free energy calculation shows that the induction is not diffusive as it was predicted, but is a process related to the ordering of the polymer ends during breaking the system symmetry, when the tail of one strand tries to pass the tail of the other strand. Our findings might explain the segregation delay observed in experiments on E.coli.

BP 41.11 Thu 18:00 ZEU 222

**The influence of topology and thermal backbone fluctuations on sacrificial bonds** — •Soran Nabavi[1], Matthew J. Harrington[2], Oskar Paris[1], Peter Fratzl[2], and Markus A. Hartmann[1] — [1]Institute of Physics, Montanuniversität Leoben, Leoben, Austria — [2]Max-Planck-Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

One strategy to improve the mechanical performance of natural materials is sacrificial bonding that can be found in bone, wood, and in some softer biological materials like silk, mussel byssus threads. Sacrificial bonds (SBs) are reversible bonds which are weaker than the covalent bonds that hold the structure together. Thus, upon loading SBs break before the covalent bonds rupture. The rupture of SBs reveals hidden length providing a very efficient energy dissipation mechanism. Furthermore, SBs can reform after their rupture providing molecular repair and self-healing. We use Monte Caro simulations to examine the influence of topology and SBs density on mechanical properties of single polymeric chains. The influence of SB density, topology and thermal backbone fluctuations on mechanical behavior are investigated by computationally mimicking tensile and cyclic loading test. Increasing the SBs density increases the work to fracture and also the energy dissipation in cyclic loading whereas the topology (determines the position and spacing of peak force) and thermal fluctuations (determine height of SB force) changes the mechanical properties. The results bear important implications for the understanding of natural systems and for the generation of strong and ductile biomimetic polymers.

BP 41.12 Thu 18:15 ZEU 222

**Dynamic glass transition in room temperature ionic liquids with calorimetric methods.** — •Evgeni Shoifet[1,2], Heiko Huth[1], Sergey Verevkin[2,3], and Christoph Schick[1,2] — [1]Institute of Physics, Rostock University, Rostock, 18051, Germany — [2]Interdisciplinary Faculty, Rostock University, Rostock, 18051, Germany — [3]Institute of Chemistry, Rostock University, Rostock, 18051, Germany

Many ionic liquids are good glass formers. Nevertheless, only a few studies of the glass transition in ionic liquids are available so far. Par-

ticularly the frequency dependence of the dynamic glass transition ($\alpha$-relaxation) is not known for most ionic liquids. The standard technique for such studies - dielectric spectroscopy - is not easily applicable to ionic liquids because of the high electrical conductivity. We try to use calorimetric techniques to obtain complex heat capacity and to investigate the dynamic glass transition of room temperature ionic liquids (RTILs) in a wide frequency range. This can give an insight in cooperative motions of ions and ion clusters in RTILs.

BP 41.13 Thu 18:30 ZEU 222

**Unusual behavior of vapor deposited glasses of 1-pentene and ethylcyclohexane investigated by fast-scanning and AC chip nanocalorimetry** — •Yeong Zen Chua[1], Mathias Ahrenberg[1], Christoph Schick[1], Katherine Whitaker[2], Michael Tylinski[2], and Mark Ediger[2] — [1]Institute of Physics, University of Rostock, Rostock 18051, Germany — [2]Department of Chemistry, University of Wisconsin, Madison, Wisconsin 53706, United States

Glasses produced by physical vapor deposition exhibit different densities and relaxation behaviors, depending upon the deposition conditions. Glasses deposited at temperatures of about 0.85 of glass transition temperature $T_g$, called stable glass, have low enthalpy, low heat capacity, high kinetic stability and high density, while glasses deposited at much lower temperatures than $T_g$ have opposite properties. We have investigated the glasses of 1-pentene and ethylcyclohexane created from PVD in a wide range of deposition temperatures between 10 K and 120 K by fast-scanning and AC chip nanocalorimetry. Fast-scanning calorimetry provides information about the enthalpy of the deposited samples, while AC chip nanocalorimetry allows for a highly sensitive heat capacity measurement on the same samples.

## BP 42: Biotechnology and bioengineering

Time: Friday 9:30–12:00 Location: HÜL 386

BP 42.1 Fri 9:30 HÜL 386

**Massively parallel computation with self-propelled biological agents in nanofabricated networks** — •Till Korten[1], Dan V. Nicolau Jr.[2], Mercy Lard[3], Falco van Delft[4], Malin Persson[5], Elina Bengtsson[5], Alf Månsson[5], Stefan Diez[1], Heiner Linke[2], and Dan V. Nicolau[6] — [1]B CUBE - Center for Molecular Bioengineering, TU Dresden, Dresden, Germany — [2]University of California, Berkeley, USA — [3]Lund University, Lund, Sweden — [4]Philips Research, Eindhoven, The Netherlands — [5]Linnaeus University, Kalmar, Sweden — [6]McGill University, Montreal, Canada

Combinatorial optimization problems are important for network routing, protein folding, and decrypting encoded messages. Solving such a problem often requires computation of all possible combinations of the elements in a problem set. However, the number of combinations - and thus the number of calculation operations - grows exponentially with the number of elements. Because they work sequentially, conventional computers are quickly overwhelmed with solving even relatively small problem sets of this type. We demonstrate a new parallel and scalable computation approach by encoding the NP-complete subset-sum problem in a physical network of lithographically defined nanochannels. The network, and thereby solution space, is explored in a massively parallel fashion by a large population of cytoskeletal filaments powered by molecular motors. All possible subset sums are recovered from the final positions of the filaments. The method is scalable, energy efficient, and may be used to augment conventional computing devices for solving combinatorial optimization problems.

BP 42.2 Fri 9:45 HÜL 386

**A droplet based microfluidic device for single paramecia cell trapping and viability measurements** — •Rico Illing[1], Daniel Pfitzner[2], Corinna Burkart[2], Dirk Jungmann[2], Larysa Baraban[1], and Gianaurelio Cuniberti[1,3] — [1]Institute for Materials Science, Max Bergmann Center of Biomaterials Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, (Germany) — [2]Technische Universitaet Dresden Faculty of Environmental Sciences Institute of Hydrobiology — [3]Center for Advancing Electronics Dresden, 01062 Dresden, (Germany)

Digital microfluidics, enabling entrapping of living cells inside of the emulsion droplets, is an attractive platform for rapid single-cell analysis. Here we present a simple way for encapsulating and observing the viability and growth kinetics of single paramecia cells in droplets (approx. 200 nL). The aim of the work is to measure the viability of single cells within hundreds of microreactors, exposed to different silver nitrate concentrations. Hundreds of droplets were created which were containing paramecia cells, culture media, viability indicator resazurin and silver nitrate. Detection of the cells activity was done by measuring the fluorescence intensity of the viability indicator, added to each droplet. To be flexible with different viability indicators, the spectrum of every single droplet was measured in less than one minute. With the help of the spectra counting and labelling of the droplet was also achieved. Finally, our detection platform enabled precise determination of a number of encapsulated cells per droplet relying only on metabolic activity of the paramecia cell.

BP 42.3 Fri 10:00 HÜL 386

**Aerographite for biomedical applications** — •Constanze Lamprecht[1], Carsten Grabosch[1], Arnim Schuchardt[1], Ingo Paulowicz[1], Matthias Mecklenburg[2], Karl Schulte[2], Rainer Adelung[1], and Christine Selhuber-Unkel[1] — [1]Institute for Materials Science, University of Kiel, Kiel, Germany — [2]Istitute of Polymers and Composites, Hamburg University of Technology, Hamburg, Germany

Aerographite is a novel carbon based material that exists as a seamless 3D network of interconnected nano- and microtubes. The material exhibits outstanding physical properties such as ultra-lightweight, excellent electrical conductivity, and mechanical robustness, which are shared by the related material of carbon nanotubes (CNTs). CNTs have found a multitude of possible applications in a variety of disciplines including biomedical and tissue engineering. Notably CNT substrates have been shown to promote cell attachment, growth, and differentiation. However, the natural scaffold of tissues, the extracellular matrix, is a 3D structure with nano- and microscale features such as interconnecting pores, ridges, and fibers. While these requirements pose a difficult challenge for CNT composites, Aerographite (AG) might present new bioengineering possibilities, as it naturally provides a stable porous 3D scaffold that offers accessibility and penetrability of surfaces. AG can be synthesized as a macroscopic self supportive 3D scaffold in a variety of micro- and nano-architectures tailored by the growth conditions. This structural flexibility may prove as competitive advantage of AG for biomedical applications.

BP 42.4 Fri 10:15 HÜL 386

**Two-photon composition and modification of a PEG-based hydrogel** — •Christiane Jungnickel[1], Mikhail Tsurkan[2], Carsten Werner[2], and Michael Schlierf[1] — [1]B CUBE - Center for Molecular Bioengineering, Dresden, Germany — [2]IPF - Leibniz-Institut für Polymerforschung Dresden e.V, Dresden, Germany

Hydrogels are used on an everyday basis in a lot of different fields like contact lenses [1], biomimetic scaffolding [2] and drug delivery [3]. Hydrogels are becoming increasingly popular in biological and medical sciences because of their broad application possibilities for tissue engineering.

Here, we present a novel approach to build up a hydrogel with nanometer precision in 3D around a living cell via two-photon reaction [4]. In comparison to previous approaches, the polymer based hydrogel does not require photoinitiators for its reaction. The two-photon process allows a high spatial and temporal control and enables furthmore a precise surface or volume structuring with a broad selection of functionalized biomolecules. Therefore it is now possible to trap cells in a hydrogel cage, manipulate and release them afterwards.

[1] O. Wichterle et al., Nature 185, 117 (1960)
[2] P.B. Welzel et al., Polymers 3, 602 (2011)
[3] T. Nermonden et al., Chem. Rev. 112, 2853 (2012)
[4] M.Pawlicki et al., Angew. Chem. Int. Ed. 48, 3244 (2009)

BP 42.5 Fri 10:30 HÜL 386

**A versatile 3D tubular platform for single cell analysis and study** — •Wang Xi[1,2], Samuel Sanchez[1,2], Christine K. Schmidt[3], David H. Gracias[4], Richard Butler[3], Rafael E. Carazo-Salas[3], Stephen P. Jackson[3,5], and Oliver G. Schmidt[1,6,7] — [1]Institute

for Integrative Nanosciences, IFW Dresden, Dresden, Germany — [2]Max Planck Institute for Intelligent Systems, Stuttgart, Germany — [3]The Gurdon Institute, Cambridge, UK — [4]Johns Hopkins University, Baltimore, US — [5]The Wellcome Trust Sanger Institute, Cambridge, UK — [6]Material Systems for Nanoelectronics, Chemnitz University of Technology, Chemnitz, Germany — [7]Center for Advancing Electronics Dresden, Dresden University of Technology, Dresden, Germany

We use micropatterning and strain engineering to encapsulate single live mammalian cells into 3D rolled-up transparent nanomembrane architectures suitable for the scrutiny of cellular dynamics within confined 3D-microenvironments with high- and super-resolution microscopy. We show that during cell division in non-transformed RPE1 cells and transformed HeLa cancer cells the extent of spatial confinement correlates strikingly with chromosome missegregation, delayed mitotic progression, cortex bipolarisation and membrane blebbing, highlighting both conserved and novel phenomena compared to the effects previously reported in 2D cultured mammalian cells. Collectively, this novel approach represents a multifunctional device which enables the detection and scrutinization of single cell inside the 3D space of cavity of microtubes which would capture more of the complexity present in tissue scaffold.

**15 min. break**

BP 42.6 Fri 11:00 HÜL 386

**Heart-on-a-chip - Design, Fabrication, and Characterization of a Microphysiological Platform for Drug Screening in Cardiac Tissue** — •Peter Loskill[1], Anurag Mathur[1], Zhen Ma[1], Micaela Finnegan[1], Natalie C. Marks[1], SoonGweon Hong[1], Bruce R. Conklin[2], Luke P. Lee[1], and Kevin E. Healy[1] — [1]Department of Bioengineering, UC Berkeley, Berkeley, United States — [2]Gladstone Institute of Cardiovascular Disease, San Francisco, United States

Drug discovery and development to date has relied on animal models, which are useful, but fail to resemble human physiology. The discovery of human induced pluripotent stem (iPS) cells has led to the emergence of a new paradigm of drug screening using human disease-specific organ-like cultures in a dish. One promising approach to produce these organ-like structures is the use of microfluidic devices, which can simulate 3D tissue structure and function with microphysiological features. Using microfabrication techniques we have developed a 3D microphysiological platform that mimics human cardiac tissue and is amenable to drug screening. The microfluidic 3D culture platform consists of three functional components: endothelial like barriers that are 2 $\mu$m wide; 30 $\mu$m wide capillary like media channels; and 100-200 $\mu$m wide cell culture channels. The platform is able to create a functional cardiac microtissue with physiological beat rates (60-80 beats/min) and with viability for multiple weeks. Assessing the physiological response to various cardiac drugs validated function of the cardiac microtissue. The microphysiological platform is extremely versatile and can be used for drug toxicity screening and therapeutic applications.

BP 42.7 Fri 11:15 HÜL 386

**Biocompatibility of $Fe_{70}Pd_{30}$ ferromagnetic shape memory films for cell sensing** — •Mareike Zink[1], Uta Allenstein[1], Yanhong Ma[2], Florian Szillat[2], and Stefan G. Mayr[2,3] — [1]Division of Soft Matter Physics, Institute for Experimental Physics I, Universität Leipzig, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung (IOM) e.V., Leipzig — [3]Translationszentrum für Regenerative Medizin and Fakultät für Physik und Geowissenschaften, Universität Leipzig, Germany

Ferromagnetic shape memory alloys (FSMAs) have received great attention recently as an exciting class of smart functional materials. In comparison to conventional shape memory alloys, FSMA bear the significant potential for miniaturized devices for single cell actuation which is capable of yielding magnetically controllable shear strains and/or volume dilations of several percent. However, biocompatibility of this material remains to be confirmed. Our in vitro assessments show that various cell types adhere and proliferate well on Fe-Pd. Since adhesion and spreading is mediated by the interaction of the amino acid sequence RGD which binds to integrin receptors on the cell surface, we further compared the interaction of RGD molecules with Fe-Pd by ab initio simulation, delamination and cell tests. We could demonstrate that the adhesion force of RGD with Fe-Pd is larger compared to the binding strength of RGD with integrin receptors - a prerequisite for good bioactivity of the surface.

BP 42.8 Fri 11:30 HÜL 386

**Label free biomolecular interaction studies with imaging ellipsometry * an Overview.** — •Peter H. Thiesen — Accurion GmbH, Göttingen, Germany

Interactions between biomolecules play a central roles in every life process. Surface plasmon resonance (SPR) in Kretschmann configuration is state of the art in bio molecular interaction analysis, but a number of papers in literature show that the high lateral resolution, the capability of mapping and ellipsometric contrast micrographs performed by Imaging SPR in the ellipsometric mode or imaging surface plasmon resonance enhanced ellipsometry (i-SPREE) is promising for the development of new options in detection and screening of biomolecular interaction. Valiokas et al. [1] characterized differential protein assemblies on micro patterned surfaces with nitriletriacetic acid based surface functionalization. Klenkar et al. [2] used the technique to follow the addressable adsorption of lipid vesicles and subsequent protein interaction studies and to detect Narcotics trace detection [3]. Schuy et al. report a mimetic approach to the active drug target for fusion inhibitors of HIV (human immunodeficiency virus) and SIV (simian immunodeficiency virus) [4]. Beside reviewing, new applications in the field of protein adsorption, protein/protein and single strain DNA interaction, the capability of imaging ellipsometry in QC of arrays and also basic surface coating will be addressed. [1] Valiokas et al., ChemBioChem 7, 1325 (2006) [2] Klenkar et al., Biointerphases 3, 29(2008) [3] Klenkar et al., Anal Bioanal Chem 391, 1679(2008) [4] Schuy et al., Journal of Structural Biology 168, 125 (2009)

BP 42.9 Fri 11:45 HÜL 386

**Tiny nanodiamonds as potential DNA detectors** — •Ganesh Sivaraman and Maria Fyta — Institute for Computational Physics. University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Diamondoids are tiny hydrogen-terminated diamond clusters with a variety of doping and functionalization possibilities. These nanostructures can show strong quantum confinement effects and are potential candidates as nanoscale biosensors. Along these lines, we investigate the possibility of chemically modified diamondoids to detect biomolecules, such as DNA. Quantum mechanical calculations are performed to study the specific interactions of diamondoids with DNA units and reveal the bonding characteristics and distinguishable electronic properties of diamondoid-DNA complexes. At a second step, we perform electronic transport measurements along a DNA placed between two diamondoid-functionalized surfaces in order to reveal whether the diamondoid can enhance the electronic signal differences arising from different DNA units. In the end, we discuss the relevance of our results in view of biosensing applications and specifically nanopore sequencing of DNA.

# BP 43: Neurosciences

Time: Friday 9:30–11:45 Location: ZEU 250

**Topical Talk** BP 43.1 Fri 9:30 ZEU 250

**The Dynamics of Neuronal Circuits** — •Fred Wolf — Max Planck Institute for Dynamics and Self-Organization — Bernstein Center for Computational Neuroscience, Göttingen University — Faculty of Physics, Göttingen University

Current advances in photonic live imaging, the ability to *instrument* living cells with genetically encoded sensors and effectors, and emerging techniques for the large-scale mapping of neuronal micro-circuits are currently driving a revolutionary change in the science of biological nervous systems. These advances are opening up exciting avenues for studying the collective dynamics and cooperative phenomena underlying the function of neuronal systems. This talk will first provide a condensed survey of emerging experimental techniques for observing and perturbing neuronal circuits. I will then present examples from our own theoretical and experimental work[1-8] on the dynamics of neocortical circuits that exemplify challenging dynamical systems and statistical physics problems that need to be solved to understand biological neuronal circuits.

[1]M. Kaschube et al., Science 330, 1113 (2010). [2]T. Tchumatchenko et al., Phys Rev Lett 104, 58102 (2010). [3]W. Wei and F. Wolf, Phys Rev Lett 106, 88102 (2011). [4]T. Tchumatchenko et al. J Neurosci 31, 12171 (2011). [5]M. Monteforte and F. Wolf, Phys Rev Lett 105, 1 (2010). [6]M. Monteforte and F. Wolf, Phys. Rev. X 2, 041007 (2012). [7]V. Ilin et al., Neurosci 33, 2281 (2013). [8]W. Keil et al., Science 336, 413 (2012).

BP 43.2 Fri 10:00 ZEU 250

**The neuronal action potential as a nonequilibrium first order phase transition** — •Benjamin Schäfer[1,3], Bernhard Altaner[2], Federico Faraci[1], and Marc Timme[1,4] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Ogranization, 37077 Göttingen, Germany — [2]Dynamics of Complex Fluids, Max Planck Institute for Dynamics and Self-Ogranization, 37077 Göttingen, Germany — [3]Otto-von-Guericke University Magdeburg, 39106 Magdeburg, Germany — [4]Bernstein Center for Computational Neuroscience (BCCN) Göttingen

Neuroscience has become one of the fastest growing topics in science, with aims ranging from understanding brain function to medical applications. Foundational assumptions underlying theoretical and modeling approaches are rarely questioned, in particular if they are already "long-estabilished". For example the excitation of a single nerve was explained in 1952 with a mathematical model by Hodgkin and Huxley and this model was since then modified and supplemented with overwhelming success in characterizing experimental data.
Is this the only way to explain neuronal excitation? This talk addresses the question whether models based on a complementary perspective of phase transitions can consistently explain nerve excitation. We start with a short review on the Hodgkin-Huxley model and several experiments performed on nerves. The idea of the neuronal action potential modeled as a phase transition is presented and the relation to existing models is shown. The talk ends by giving an exemplary biological mechanism that could realize the phase transition in biological nerve cells.

BP 43.3 Fri 10:15 ZEU 250

**Asymmetric two-trace model for STDP** — •Rodrigo Echeveste and Claudius Gros — Institut für Theoretische Physik, Johann Wolfgang Goethe Universität, Max-von-Laue-Str. 1, Frankfurt am Main, Germany

In the present work we propose a simple model formulating synaptic potentiation and depression in terms of two interacting traces, representing the fraction of open NMDA receptors and the $Ca^{2+}$ concentration in the post-synaptic neuron, respectively. These two traces then determine the evolution of the synaptic weight. We first test that the standard STDP curve for low frequency trains of pairs of pre- and post-synaptic spikes is obtained and we then evaluate high frequency effects. Secondly, we study triplets. In this case, we are interested in non-linear effects and, in particular, in possible asymmetric response to pre-post inversion.

Having a low number of parameters and composed of only polynomial differential equations, the model is able nonetheless to reproduce key features of LTP and LTD. Moreover, since the parameters of the model are easily related to the dynamical properties of the synapse, it permits to make a connection between the observed synaptic weight change and the behaviour of the underlying traces.

BP 43.4 Fri 10:30 ZEU 250

**Including intrinsic thalamic currents in a population model of the thalamo-cortical system during deep sleep** — Michael Schellenberger Costa[1], Arne Weigenand[1], Thomas Martinetz[1], and •Jens Christian Claussen[2,1] — [1]INB, Universität zu Lübeck, Germany — [2]Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

Sleep has been shown to be beneficial for the consolidation of memories [1, 2]. As the thalamocortical interaction is important for both the processing of sensory stimuli and the generation of slow waves a detailed understanding of its dynamical properties is needed, to reveal the influence of one on the other. Population models have been used to investigate the behaviour of awake brain networks [3,4,5]. These models lack the hallmarks of a sleeping thalamus e.g. rebound bursts and waxing/waning of spindles [6]. Therefore we adapt a cortical population model proposed [7] and extend it with the respective intrinsic properties specific in the RE and TC neurons.
[1] L. Marshall et al, Nature, 444, 610 (2006) [2] H V V Ngo et al, J Sleep Res (2013), Neuron (2013). [3] M. Ursino et al, NeuroImage, 52, (2010). [4] R. C. Sotero et al, Neur Comp 19, 478 (2007) [5] B S Bhattacharya et al, Neural Networks 24, 631 (2011). [6] A Destexhe, T J Sejnowski, Physiol Rev 83, 1401 2003) [7] D. Steyn-Ross et al, J Biol Phys 31, 547 (2005)

BP 43.5 Fri 10:45 ZEU 250

**Statistics of neural spiking under non-Poissonian stimulation** — •Tilo Schwalger[1] and Benjamin Lindner[2,3] — [1]EPFL, Lausanne, Switzerland — [2]Humboldt-Universität zu Berlin, Berlin, Germany — [3]Bernstein-Center for Computational Neuroscience, Berlin, Germany

Nerve cells in the brain generate sequences of spikes with a complex statistics. To understand this statistics, the synaptic input received from other neurons is often modeled by temporally uncorrelated input (Poissonian shot noise), which possesses a flat (white) power spectrum. However, realistic input is temporally correlated because presynaptic neurons exhibit refractoriness, bursting or adaptation, carry a time-dependent signal in their spikes and are subject to short-term synaptic plasticity. The effect of such "colored noise" input is poorly understood theoretically because the the associated first-passage-time problem with colored noise is generally a hard problem. Based on a weak-noise expansion of a multi-dimensional Fokker-Planck equation, we derive simple analytical formulas for essential spike train statistics for a tonically firing neuron driven by arbitrarily correlated synaptic input. We show that synaptic input with power-law correlations also leads to power laws in the interspike interval correlations and the Fano factor. Furthermore, input spikes that are more regular than Poisson, as well as neurons with short-term synaptic depression, cause negative interval correlations similar to neurons with adaptation. Our results provide a framework for the interpretation of spiking statistics measured in vivo.

BP 43.6 Fri 11:00 ZEU 250

**Asymmetric neural coding in the honeybee brain** — Elisa Rigosi[1,2], Gianfranco Anfora[3], Renzo Antolini[4], Paul Szyszka[5], Giorgio Vallortigara[2], and •Albrecht Haase[2,4] — [1]BIOtech center, Dep. of Industrial Engineering, University of Trento, Mesiano (TN), Italy — [2]Center for Mind/Brain Sciences, University of Trento, Mattarello (TN), Italy — [3]Research and Innovation Center, Fondazione Edmund Mach, San Michele a/A (TN), Italy — [4]Department of Physics, University of Trento, Povo (TN), Italy — [5]Department of Biology, Neurobiology, University of Konstanz, Konstanz, Germany

Left-right asymmetric processing of symmetric stimuli is a common property of sensory systems, yet little is known about asymmetric neuronal coding. We studied this aspect in the honeybee using various methods to trace asymmetries along the olfactory pathway. Electron microscopy was used to image the odour receptor sensilla and electroantennography for the olfactory receptor neurons to characterize the input to the primary processing centers, the antennal lobes (ALs). Two photon microscopy visualizes the AL morphology and in vivo

functional imaging of the projection neurons describes the output of the ALs. We identified for the first time a left-right asymmetry in the neural coding during odour processing. Neurophysiological distances between odours in the right antennal lobes are higher than in the left ones. Moreover, mixture processing differs between sides. Behavioural experiments support the brain imaging results. The implementation of different neuronal coding strategies in the left and right brain side may serve to increase coding capacity by parallel processing.

BP 43.7 Fri 11:15 ZEU 250

**Computer simulation of the distribution of histone deacetylases 1 and 3 in the brain** — •Davoud Pouladsaz — Department of Biological Physics, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Since their abnormal activities have been implicated in various neurological disorders, including oncogenesis, neurodegenerative and psychiatric disorders, histone decaetylases (HDACs), a class of enzymes that alter the chromosome structure and affect the gene expression, are potential targets for therapeutic development. Therefore, understanding the distribution of HDACs in the brain can serve as a valuable tool in this regard. We perfom Monte Carlo simulations in order to calculate the distribution of HDAC1 and HDAC3 in the brain based on previous experimental results of patterns of histone acetylation in the brain in response to MS-275, a benzamide derivative with in vivo antitumor activity and selectivity against HDAC1 and HDAC3. The results show significant correlation to experimental measurements.

BP 43.8 Fri 11:30 ZEU 250

**The fly on a swing- Generation of complex locomotor pattern through nonlinear coupling to a prototypical dynamic environment** — •Jan Bartussek[1,2,3], Hannah Haberkern[3], and Martin Zapotocky[2] — [1]Department of Animal Physiology,University of Rostock, Albert-Einstein-Str. 3, 18059 Rostock, Germany — [2]Institute of Physiology, Academy of Sciences of the Czech Republic, Videnska 1083, 14220 Praha 4, Czech Republic — [3]Institute of Neuroinformatics, ETH/Uni Zurich, Winterthurerstr. 190, 8057 Zurich, Switzerland

We investigated the mutual, dynamic coupling of flying flies with their environment. By gluing single fruit flies to a steel tether with defined mechanical properties, we replaced the dynamics of the natural world by a prototypical environment, which can be modelled as a simple harmonic oscillator. We used an interferometer to measure the vibrations of the tether induced by the flying fly. Depending on the tether resonance frequency, the forces from the fly were inducing a large cumulative motion of the tether and activation of the fly's mechanosensors. The fly therefore received delayed feedback dependent on its previous activity. This lead to a variety of observed dynamical locomotor patterns, including locking of the wingbeat to the tether resonance frequency. We were able to reproduce most of the observed dynamical features in a simple nonlinear model of two mutually coupled oscillators. Aerodynamic calculations indicate that even in natural free flight, the wingbeat might be continuously locked to mechanosensory feedback due to body oscillations. We argue how this locking can improve flight control on fast time scales.

## BP 44: Stochastic Dynamics of Growth Processes in Biological and Social Systems (accompanying session, joint DY/BP/SOE)

Time: Friday 10:00–12:45 Location: GÖR 226

BP 44.1 Fri 10:00 GÖR 226

**Evolution of increasingly complex linear molecules** — •Philipp Zimmer[1], Emanuel Gregor Worst[2], Eva Wollrab[2], Albrecht Ott[2], and Karsten Kruse[1] — [1]Universität des Saarlandes, Theoretische Biologische Physik, Postfach 151150, 66041 Saarbrücken — [2]Universität des Saarlandes, Biologische Experimentalphysik, Postfach 151150, 66041 Saarbrücken

Darwinian evolution is based on variation and selection acting on mutations, reproduction, or the metabolism of a species. These processes can only take place when the underlying system is out of thermodynamical equilibrium. For natural evolution the species as well as their relation network has continuously been gaining complexity. The conditions necessary for a steady increase in complexity are not well understood. Performing stochastic simulations as well as experiments with DNA, we analyze a chemical system consisting of autocatalytically concatenating chains. We find that, despite its inherent stochastical nature, the system evolves along a reproducible path towards states of increasing complexity if the autocatalytic activity exceeds a critical value.

BP 44.2 Fri 10:15 GÖR 226

**Autocatalysis in a primordial broth** — •Sabrina Scherer, Eva Wollrab, and Albrecht Ott — Biologische Experimentalphysik, Universität des Saarlandes

In many energetically driven systems non-linearities lead to pattern formation. Here we study the dynamics of a driven primordial broth, synthesized from a gas mixture of methane, ammonia and steam that is triggered by eletric discharge and heat. Using real-time mass spectrometry, we observe the generation of many hundreds of different molecules in a mass range from 50 to 1000 Dalton. The temporal course of the primordial broth reveals the spontaneous emergence and disappearance of several oligomeric groups that consist primarily of polyethylene glycol (PEG) surfactants. These oligomers appear in aperiodic oscillations. This requires stronger non-linearities than a simple autocatalytic reaction. PEG and -surfactants are well known phase-transfer catalysts, able to favour biochemical reactions by inhibiting hydrolysis. We suggest that autocatalytic phase-transfer leads to self-organizing processes in a primordial broth and enables the production of relevant biomolecules.

BP 44.3 Fri 10:30 GÖR 226

**Cooperation in suddenly changing environments** — •Karl Wienand[1], Jonas Cremer[2], Anna Melbinger[2], and Erwin Frey[1] — [1]Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Theresienstrasse 37, 80333 München, Germany — [2]UC San Diego, 9500 Gilman Dr., La Jolla, CA 92093, U.S.A.

The interdependence of evolutionary and growth dynamics shapes the evolutionary fate of populations. This is especially the case in microbial populations, where volatile population sizes and capricious environments are the rule rather than the exception. A suddenly changing carrying capacity, which periodically oscillates between abundance and scarcity of resources, represents such changing environment and causes the population size to grow and shrink. The variation in size, in turn, affects the evolutionary dynamics. Studying this complex interplay, we find most oscillating environments enhance demographic fluctuations and cooperative behavior.

BP 44.4 Fri 10:45 GÖR 226

**Selection and drift in expanding bacterial colonies** — •Fred Farrell[1], Bartlomiej Waclaw[1], Davide Marenduzzo[1], and Oskar Hallatschek[2] — [1]School of Physics, University of Edinburgh, Edinburgh, UK — [2]Department of Physics, University of California, Berkeley, California, USA

In an expanding population, such as a bacterial colony growing on a surface in the laboratory or in nature, evolution proceeds very differently to in a well-mixed population with a static population size. This is mostly due to the so-called founder effect, where individuals close to the expanding front of the population have a much better chance of passing their genes on to future generations than those deep within the population. Since there are relatively few of these founders, rates of genetic drift are much higher, and the probability that a beneficial mutation will fixate in the population much lower. This is important as it will impact the speed with which such a population adapts to its environment, for example developing antibiotic resistance.

I will present my work using a fairly detailed agent-based biophysical simulation model of an expanding microbial colony to estimate probabilities of fixation of beneficial mutations, and how these depend on the fitness advantage and the properties of the cells, and compare these results to analytical theories of selection in expanding populations.

BP 44.5 Fri 11:00 GÖR 226

**Bacterial population genetics in antibiotic concentration gradients: Accelerated evolution of antibiotic resistance** — •Philip Greulich[1,2], Bartlomiej Waclaw[2], and Rosalind Allen[2] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]School of Physics and Astronomy, University of Edinburgh, Edinburgh, UK

The increased emergence of antibiotic resistance poses a major threat to human health nowadays. Evolution of antibiotic resistance occurs by a sequence of mutations (mutational pathway) when bacteria are exposed to the selection pressure of an applied antibiotic. Recent experiments indicate that the spatial distribution of an antibiotic plays an important role for the evolution of antibiotic-resistant bacterial strains. I will present a stochastic model for the population genetics of bacteria growing in different spatial distributions of an antibiotic. This model reveals an intriguing interplay between the mutational pathway and the spatial structure of the drug distribution. It shows that spatial gradients in antibiotic concentrations can strongly accelerate the emergence of resistance when the mutational pathway involves a long sequence of mutants. However, gradients may slow down evolution if the pathway is short or crosses a fitness valley.

BP 44.6 Fri 11:15 GÖR 226

**Evolution of the size distribution of colloidal particles: focussing, breakdown of scaling, and asymptotic distributions** — •Martin Rohloff[1,2] and Jürgen Vollmer[1,2] — [1]Max Planck Institute for Dynamics and Self-Organisation (MPIDS), 37077 Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, 37077 Göttingen, Germany

Mechanisms underlying the synthesis of mono-disperse colloids and nanocrystals are under vivid discussion. A common feature of the recipies is the growth of an assembly of particles subjected to a flux of material, provided e.g. by a chemical reaction like the decomposition of precurser.

We present analytical and numerical studies on diffusion dominated growth of particles with a constant overall volumetric growth rate. The resulting particle growth is qualitatively different from Ostwald ripening, and it leads to narrow and non-universal asymptotic size distributions.

BP 44.7 Fri 11:30 GÖR 226

**Multi-Species Range Expansions: Frequency-Dependent Selection at Rough Fronts** — •Jan-Timm Kuhr and Holger Stark — Institut für Theoretische Physik, Technische Universtität Berlin

Growing microbial colonies have recently been used as model systems for macroscopic colonization events, known as range expansions, since growth in the Petri dish is comparably fast and controllable.

Employing the statistical Eden model, already single-strain colonies feature remarkable properties like self-affine fronts, which have also been found in experiments. Multi-species settings promise a plethora of possible phenomena, e.g. irreversible mutations resulting in a non-equilibrium phase transition to an absorbing state [1].

Whereas a simple selective advantage entails quasi-deterministic fixation of the faster growing strain, local frequency-dependent selection gives rise to non-trivial outcomes. We focus on representations of social dilemmas, where local group selection brings about extremely rough fronts, the effects of which are neglected in other approaches.

[1] J.-T. Kuhr, M. Leisner, and E. Frey, *Range expansion with mutation and selection: dynamical phase transition in a two-species Eden model*, New J. Phys. **13**, 113013 (2011).

BP 44.8 Fri 11:45 GÖR 226

**Clonal interference and Muller's ratchet in spatial habitats** — Jakub Otwinowski[1] and •Joachim Krug[2] — [1]Biology Department, University of Pennsylvania, Philadelphia, USA — [2]Institute for Theoretical Physics, University of Cologne, Cologne, Germany

Competition between independently arising beneficial mutations is enhanced in spatial populations due to the linear rather than exponential growth of the clones. The resulting fitness dynamics is analogous to a surface growth process, where new layers nucleate and spread stochastically, leading to the build up of scale-invariant roughness. This scenario differs qualitatively from the standard view of adaptation in that the speed of adaptation becomes independent of population size while the fitness variance does not, in apparent violation of Fisher's fundamental theorem. Here we exploit recent progress in the understanding of surface growth processes to obtain precise results for the universal, non-Gaussian shape of the fitness distribution for one-dimensional habitats. We then consider a version of the model where all mutations are deleterious, that is, a spatial version of Muller's ratchet. Based on an analogy to models of nonequilibrium wetting, we show that the system displays a phase transition related to directed percolation. The transition is governed by the ratio $U/s^2$, where $U$ denotes the deleterious mutation rate and $s$ the selection coefficient of mutations. For $U/s^2 > 1$ the speed of the ratchet remains finite in the limit of infinite habitat size.

BP 44.9 Fri 12:00 GÖR 226

**A Non-Equilibrium Phase Transition in a Biofilm Growth Model in a Fluctuating Environment** — •Florentine Mayer and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNs), Department of Physics, Ludwig-Maximilians-Universität München, Germany

Bacterial communities represent complex and dynamic ecological systems. They appear in the form of free-floating bacteria and biofilms in nearly all parts of our environment. They are highly relevant for human health and disease. Spatial patterns arise from heterogeneities of the underlying landscape or are self-organized by the bacterial interactions, and play an important role in maintaining species diversity. Bacteria must rapidly adapt to fluctuating environments in order to survive. In biofilms this is often achieved by phenotypic diversity, where bacteria can switch between different phenotypic states. Survival of the population can increase if each of these phenotypes is adapted to different environmental conditions.To analyze biofilm growth we set up a two-species automaton model in which growth, death and switching rates depend on the environmental conditions. These fluctuate, resulting in periodically interchanged reaction rates. Depending on the rates we find either fast extinction or thriving biofilms with intriguing spatio-temporal patterns. Close to the region of extinction patterns become self-affine, which is typical for a phase transition to an absorbing state. Employing extensive stochastic simulations we measure critical exponents of our non-equilibrium phase transition and find universal scaling behaviour characterising the universality class of our model.

BP 44.10 Fri 12:15 GÖR 226

**Discrete scale invariance in growing networks** — Wei Chen[1,2,3], •Malte Schröder[4], Raissa M. D'Souza[3], Didier Sornette[5], and Jan Nagler[5,4] — [1]Chinese Academy of Sciences, Beijing — [2]Peking University, Beijing — [3]University of California, Davis — [4]MPI DS Göttingen — [5]ETH Zürich

Discrete scale invariance (DSI) arises in systems where the usual (continuous) scale invariance (for example at phase transitions) is partially broken, leading to a remarkable discrete hierarchy of resonances in the system order parameter. DSI has broad technical, physical and biological relevance, penetrating statistical physics (Potts model, Singularities), hydrodynamics, turbulence, astronomy, evolution, fracture and economics. (D. Sornette, Phys. Rep. 297, 239 (1998)).

A hierarchy of discrete micro-transitions leading up to the transition to global connectivity in models of continuous and discontinuous percolation is observed. These transitions can in some cases be observed in the relative variance of the size of the largest cluster even in the thermodynamic limit.

Depending on the model these cascades exhibit either genuine discrete scale-invariance or a generalized (novel) form. In contrast to average values, the size of the largest cluster before the phase transition is limited to integer values. This leads to a family of scaling relations that describe the behavior of the micro-transition cascade (Chen, Schröder, D'Souza, Sornette, Nagler (under review)). Our findings open up the possibility for the prediction of tipping in complex systems that are dominated by large-scale disorder.

BP 44.11 Fri 12:30 GÖR 226

**Firm growth and inter-organizational flows in the Stockholm region, 1990-2003** — •Hernan Mondani[1], Petter Holme[2,3,1,4], and Fredrik Liljeros[1,4] — [1]Department of Sociology, Stockholm University, Sweden — [2]Department of Energy Science, Sungkyunkwan University, Korea — [3]IceLab, Department of Physics, Umeå University, Sweden — [4]Institute for Futures Studies, Stockholm, Sweden

Explaining the emergence of fat-tailed growth-rate distributions in terms of the action of individual agents remains an important open question in the study of socio-economic systems. Studies of organizational growth statistics are limited by the quantity and level of detail of the available information. Large databases have little or no information about the composition of each workplace, and the time-dependent

variables are often reported at the level of the organization.

In this empiric study, we use Swedish register data, a quite unique individual-level longitudinal database that provides data on organizational membership of all workers in the Stockholm region, for a period of 14 years (1990-2003). With this dataset, we can analyze how individual attributes are aggregated at the organizational level, and track individual movements on a yearly basis.

We compute statistics for organizational size and growth, and look at their time evolution in the period of analysis. We further study the distribution of individual-level properties across organizations, especially the in- and out-flow of people moving between organizations.