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Fachverband Biologische Physik (BP)

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Overview of Invited Talks and Sessions

(Lecture Rooms H43, H44, and H46; Poster B2 and C)

Plenary Talks related to BP

PV I	Mon	8:30– 9:15	H1	**Optical Dressing of Molecules and Materials** — •Thomas W. Ebbesen
PV VII	Tue	14:00–14:45	H15	**Self-assembly, Self-organization and Control of Colloidal Suspensions** — •Sabine H. L. Klapp
PV IX	Wed	8:30– 9:15	H1	**Mechanics and dynamics of rapid cell movement** — •Julie Theriot
PV XVII	Thu	14:00–14:45	H15	**Observing the Interactions of Ions with Solid-Liquid Interfaces using X-rays** — •Paul Fenter

Invited Talks of BP sessions

BP 1.1	Mon	9:30–10:00	H43	**Motor-clutch model for substrate stiffness sensing by living cells** — •David Odde, Benjamin Bangasser, Steven Rosenfeld
BP 2.1	Mon	9:30–10:00	H44	**Energy conversion mechanisms of heat shock proteins** — •Thorsten Hugel
BP 5.1	Mon	15:00–15:30	H43	**Cytoskeletal pattern formation: Self organization of driven filaments** — •Andreas Bausch
BP 12.1	Tue	9:30–10:00	H43	**Motor and Track Systems for Navigating the Cytoskeleton** — Joanna Kalita, •Ronald Rock
BP 12.7	Tue	11:15–11:45	H43	**Molecular Motors from DNA** — •Andrew Turberfield
BP 13.1	Tue	9:30–10:00	H44	**Ultrasensitive detection, microscopy, tracking, and manipulation of nano-objects** — •Vahid Sandoghdar
BP 15.1	Tue	12:00–12:30	H43	**Protein diffusion on DNA** — •Ralf Seidel
BP 17.1	Wed	9:30–10:00	H43	**Processing of recombinant proteins for biomaterials applications: about spider silk and more** — •Thomas Scheibel
BP 18.1	Wed	9:30–10:00	H44	**Out-of-equilibrium membrane physics and cellular organelles.** — •Pierre Sens
BP 20.1	Wed	15:00–15:30	H43	**Challenges of Neurophysics** — •Theo Geisel
BP 21.1	Wed	15:00–15:30	H46	**Mimicking cellular membranes: lessons from reconstitution** — •Eva Schmid
BP 27.1	Thu	9:30–10:00	H43	**DNA Origami: Applications in Physics and Biotechnology** — •Tim Liedl
BP 28.1	Thu	9:30–10:00	H44	**Advanced Fluorescence Methods for Investigating the Lifecycle of Viruses** — •Don C. Lamb
BP 28.7	Thu	11:30–12:00	H44	**Looking at proteins inside live cells with atomic resolution: Science fiction or science reality?** — •Phil Selenko
BP 30.1	Thu	15:00–15:30	H43	**Inversion and perversion in biomechanics: from microscopic anisotropy to macroscopic chirality.** — •Alain Goriely
BP 30.5	Thu	16:15–16:45	H43	**A noisy path to order: refinement of a developing tissue** — •Buzz Baum

Invited Talks of the Joint Symposium Charge Transfer Effects in Molecular Materials

Organizers Wolfgang Brütting and Frank Schreiber. For more details see SYCT.

SYCT 1.1	Mon	9:30–10:00	H1	**A coarse grained QM/MM approach for the description of charge transfer in complex systems** — •Marcus Elstner
SYCT 1.2	Mon	10:00–10:30	H1	**Identifying and resolving charge separation in organic solar cells** — •Eberhard Riedle
SYCT 1.3	Mon	10:30–11:00	H1	**Quantifying the energy of charge transfer states: From molecular crystals to donor-acceptor blends** — •Reinhard Scholz
SYCT 1.4	Mon	11:00–11:30	H1	**Efficient Exciton Generation and Collection in Organic Solar Cells** — •Mark Thompson, Cong Trinh, Steve Forrest, Jeramy Zimmerman
SYCT 1.5	Mon	11:30–12:00	H1	**Electron transport in organic single-crystal transistors and Schottky-gated heterostructures** — •Alberto Morpurgo

Invited Talks of the Joint Symposium Magnetic Nanoparticles in Biomedical Diagnostics and Therapy

Organizers Gernot Güntherodt and Eckart Rühl. For more details see SYBD.

SYBD 1.1	Mon	15:00–15:30	H1	**Functionalization and Pharmaceutical Aspects of Magnetic Nanoparticles (Magnetic Carriers)** — •Urs O. Häfeli
SYBD 1.2	Mon	15:30–16:00	H1	**Fluid mechanical aspects of therapeutic application of suspensions of magnetic nanoparticles** — •Stefan Odenbach
SYBD 1.3	Mon	16:00–16:30	H1	**Magnetic Particle Imaging: A new Medical Imaging Modality** — •Thorsten Buzug
SYBD 1.4	Mon	16:30–17:00	H1	**Superparamagnetic iron oxide nanoparticles for MR-visible mesh implants and novel drug targeting models** — •Ioana Slabu, Anjali Roeth, Christiane Kuhl, Thomas Schmitz-Rode, Martin Baumann
SYBD 1.5	Mon	17:00–17:30	H1	**Magnetic measurement techniques assisting biomedical applications of magnetic nanoparticles** — •Lutz Trahms

Invited Talks of the Joint Symposium Computational Challenges in Scale-Bridging Modeling of Materials

Organizers Gianaurelio Cuniberti and Frauke Gräter. For more details see SYMM.

SYMM 1.1	Thu	9:30–10:00	H1	**Challenges for first-principles based computation of properties of oxide materials** — •Karsten Albe
SYMM 1.2	Thu	10:00–10:30	H1	**Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales** — •Peter Gumbsch, Matous Mrovec, Kinshuk Srivastava, Daniel Weygand
SYMM 1.3	Thu	10:30–11:00	H1	**Crucial Issues and Future Directions of Through-Process Modeling** — •Guenter Gottstein
SYMM 1.4	Thu	11:00–11:30	H1	**Adaptive Resolution Simulations for Soft Matter: Applications and New Developments** — •Kurt Kremer
SYMM 1.5	Thu	11:30–12:00	H1	**Materials by design** — •Markus Buehler

Invited Talks of the Joint Focus Session Publishing in the Age of the Internet (with jDPG)

Organizers Stephan Köhler (jDPG) and Ulrich Schwarz (BP).

BP 6.1	Mon	15:30–16:00	H44	**Publishing in Physical Review Letters** — •Karsten Kruse
BP 6.2	Mon	16:00–16:30	H44	**The Opportunities of Open Access Publishing** — •Eberhard Bodenschatz

Invited Talks of the Joint Focus Session Dynamics of Adaptive Networks (with SOE and DY)

Organizers Eckehard Schöll and Jens Christian Claussen.

SOE 15.1	Wed	9:30–10:00	H37	**Adaptive Networks: Of social interactions and mathematical tools** — •Anne-Ly Do

SOE 15.8	Wed	11:30–12:00	H37	**Bio-molecular Networks: Structure, Function, Evolution** — •Michael Lässig
SOE 15.9	Wed	12:00–12:30	H37	**Adaptive networks and critical dynamics** — •Stefan Bornholdt

Invited Talks of the Joint Focus Session Biomechanics (with jDPG)

Organizers Jochen Schneider (jDPG) and Ulrich Schwarz (BP).

AGjDPG 3.1	Wed	15:00–15:30	H6	**Active Mechanical Processes in Cells and Tissues** — •Frank Jülicher
AGjDPG 3.2	Wed	15:30–16:00	H6	**Cell mechanics: An experimental biophysicist's perspective** — •Jochen Guck

Sessions

BP 1.1–1.12	Mon	9:30–13:00	H43	**Cell migration**
BP 2.1–2.11	Mon	9:30–12:45	H44	**Proteins**
BP 3.1–3.8	Mon	9:30–11:30	H47	**Statistical Physics in Biological Systems I (joint with DY)**
BP 4.1–4.5	Mon	9:30–12:00	H1	**Symposium Charge Transfer Effects in Molecular Materials (SYCT, joint with CPP, HL and DS)**
BP 5.1–5.7	Mon	15:00–17:00	H43	**Cytoskeleton**
BP 6.1–6.2	Mon	15:30–17:30	H44	**Publishing in the Age of the Internet (joint with jDPG)**
BP 7.1–7.5	Mon	15:00–17:30	H1	**Symposium Magnetic Nanoparticles in Biomedical Diagnostics and Therapy (SYBD, joint with MA, CPP and ST)**
BP 8.1–8.30	Mon	17:30–19:30	Poster B2	**Posters: Proteins**
BP 9.1–9.10	Mon	17:30–19:30	Poster B2	**Posters: Membranes**
BP 10.1–10.17	Mon	17:30–19:30	Poster B2	**Posters: Imaging**
BP 11.1–11.24	Mon	17:30–19:30	Poster B2	**Posters: Statistical Physics in Biological Systems (joint with DY)**
BP 12.1–12.7	Tue	9:30–11:45	H43	**Molecular Motors**
BP 13.1–13.9	Tue	9:30–12:00	H44	**Imaging**
BP 14.1–14.12	Tue	9:30–13:00	H34	**Biomaterials and Biopolymers I (joint with CPP)**
BP 15.1–15.7	Tue	12:00–14:00	H43	**DNA/RNA and related enzymes**
BP 16.1–16.4	Tue	15:00–16:00	H37	**Evolutionary Game Theory (joint with SOE and DY)**
BP 17.1–17.11	Wed	9:30–12:45	H43	**Biomaterials and Biopolymers II (joint with CPP)**
BP 18.1–18.9	Wed	9:30–12:15	H44	**Membranes and Vesicles I**
BP 19.1–19.9	Wed	9:30–12:30	H37	**Focus Session: Dynamics of Adaptive Networks (joint with SOE and DY)**
BP 20.1–20.9	Wed	15:00–17:30	H43	**Statistical Physics in Biological Systems II (joint with DY)**
BP 21.1–21.5	Wed	15:00–16:30	H46	**Membranes and Vesicles II**
BP 22.1–22.5	Wed	15:00–16:45	H6	**Biomechanics (joint focus session with jDPG)**
BP 23.1–23.5	Wed	15:45–17:00	H37	**Networks, From Topology to Dynamics (joint with SOE and DY)**
BP 24.1–24.34	Wed	17:30–19:30	Poster C	**Posters: Physics of Cells**
BP 25.1–25.21	Wed	17:30–19:30	Poster C	**Posters: Cytoskeleton**
BP 26.1–26.12	Wed	17:30–19:30	Poster C	**Posters: Biomaterials and Biopolymers (joint with CPP)**
BP 27.1–27.8	Thu	9:30–12:00	H43	**Biotechnology and Bioengineering**
BP 28.1–28.11	Thu	9:30–13:00	H44	**Focus session: Intracellular Spectroscopy**
BP 29.1–29.5	Thu	9:30–12:00	H1	**Symposium Computational Challenges in Scale-Bridging Modeling of Materials (SYMM, joint with CPP, DY and MM)**
BP 30.1–30.8	Thu	15:00–17:30	H43	**Tissue**
BP 31.1–31.10	Thu	15:00–17:30	H46	**Statistical Physics in Biological Systems III (joint with DY)**
BP 32.1–32.13	Fri	9:30–13:00	H43	**Cell Adhesion and Mechanics**
BP 33.1–33.12	Fri	9:30–12:45	H44	**Statistical Physics in Biological Systems IV (joint with DY)**

Annual General Meeting of the Biological Physics Division

Wednesday 19:00–20:00 H43

- Award of the EPL poster prizes for biological physics
- Report of the current speakers
- Election of the new speakers
- Lessons learned and spring meeting Dresden 2014
- Miscellaneous

BP 1: Cell migration

Time: Monday 9:30–13:00 Location: H43

Invited Talk BP 1.1 Mon 9:30 H43

Motor-clutch model for substrate stiffness sensing by living cells — •David Odde[1], Benjamin Bangasser[1], and Steven Rosenfeld[2] — [1]Department of Biomedical Engineering, University of Minnesota, Minneapolis, MN, USA — [2]Brain Tumor and Neuro-Oncology Center, Cleveland Clinic, Cleveland, OH, USA

Cells sense the mechanical stiffness of their environment to control cell shape, differentiation, survival, proliferation, and migration. How cells sense the Young's modulus of an elastic environment to make these vital decisions is not clear. We recently showed that a simple 'motor-clutch' model exhibits stiffness sensitivity (Chan and Odde, Science, 2008). In particular, the F-actin retrograde flow rate and traction force exhibit a biphasic response to substrate Young's modulus, an effect that we confirmed using embryonic chick forebrain neurons. We now further explore the behavior of the motor-clutch model, and assess which model parameters control the stiffness at which sensing is optimal. Our exploration of parameter space reveals that no single parameter in the motor-clutch model can strongly control the set-point for optimal stiffness sensing. Rather, parameters need to be changed coordinately to effectively change the set-point. In particular, coordinate increases of both motor and clutch numbers effectively increases the set-point stiffness. Our recent experimental studies with glioma cells are consistent with predictions of the motor-clutch model. We speculate that the motor-clutch model may be useful for in silico identification of combination drug targets for brain cancers.

BP 1.2 Mon 10:00 H43

Mechanics of Collagen Gels - What Cells Feel — •Julian Steinwachs, Claus Metzner, Stefan Münster, Nadine Lang, and Ben Fabry — University of Erlangen-Nürnberg, Germany

Collagen gels are frequently used to study cell migration in a three-dimensional environment. Their mechanical properties are governed by non-affine deformation of the collagen fibrils, such as buckling and tautening, resulting at the macroscopic scale in pronounced strain stiffening under shear and strong lateral contraction under stretch. It is currently unknown how these properties play out at the microscopic scale of a migrating cell. To explore this question, we develop a nonlinear elastic material model for collagen gels based on observations from confocal microscopy that fibrils evade mechanical stress by deforming in a non-affine manner, resulting in a nonlinear force-length relationship. Our model replicates the macroscopic strain stiffening and lateral contraction of collagen and predicts that tautening of fibrils results in a strong stiffening against expanding forces that can arise, for example, when the diameter of a migrating cell is larger than the network pore diameter. Using the model, we compute cell induced stresses and local material properties during cell migration from collagen fiber displacements measured with confocal reflection microscopy. We find that mesenchymally migrating cells exert highly localized forces onto the matrix with an average magnitude of 65nN. As a result, the collagen matrix stiffens locally by approximately two-fold.

BP 1.3 Mon 10:15 H43

Effects of adhesion dynamics and substrate compliance on shape and motility of crawling cells — •Falko Ziebert[1,2] and Igor Aranson[3,4] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Institut Charles Sadron, 67034 Strasbourg, France — [3]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA — [4]Engineering Sciences and Applied Mathematics, Northwestern University, Evanston, IL 60202, USA

Understanding physical mechanisms of cell motility and its relation to substrate properties is essential e.g. for morphogenesis or wound healing or for the development bio-active surfaces. We present an effective computational model, based on the cell's shape deformation mediated by the actin cytoskeleton, coupled to the dynamics of adhesion site formation and the elastic response of the substrate. We reproduce and analyze key experimental observations, like transitions from steady cell motion to stick-slip motion with concomitant shape oscillations. We present 'phase' diagrams for the different types of motion as a function of the determining parameters like actin protrusion rate, substrate stiffness, and the rates of adhesion site formation. The model also has been investigated for substrates with stripe-patterned adhesiveness: on hard adhesive substrates, cells move along the stripes, while for softer and/or less adhesive substrates motion perpendicular to the stripes occurs, a prediction that might be relevant for the design of selective bio-active substrates for e.g. cell sorting.

BP 1.4 Mon 10:30 H43

Cytoskeletal polarization during amoeboid motion in narrow microfluidic channels — •Oliver Nagel[1], Matthias Theves[1], Meghan Driscoll[2], Can Guven[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 study the quasi one-dimensional motion of *Dictyostelium discoideum* amoebae inside narrow microfluidic channels with a cross section of 10 x 20 micrometer. While many cells perform a quasi one-dimensional random walk with frequent switches in the direction of motion, we regularly observe cells that show a markedly different type of motion. They move persistently in one direction along the channel for more than half an hour without reversing their direction of motion. We perform laser scanning confocal imaging with a transfected *Dictyostelium* cell line that expresses myosin II-GFP together with LimE-mRFP, a marker for filamentous actin. Our experiments reveal a polarized structure of the cell cortex that differs from polarized cells in absence of confinement. We characterize this type of polarized cell motion using custom made software tools for cell shape analysis to monitor the dynamics of local protrusions and retractions on the membrane together with the accompanying intracellular distributions of actin and myosin II in the cell cortex.

BP 1.5 Mon 10:45 H43

Spatiotemporal dynamics of self-organized waves in electrofused amoeboid cells. — •Matthias Gerhardt, Michael Walz, and Carsten Beta — Institut für Physik und Astronomie, Karl-Liebknecht-Strasse 24/25, 14476 Potsdam, Germany

We investigated the intracellular dynamics of PIP3 and F-Actin in electro-fused Dictyostelium discoideum cells by confocal laser scanning microscopy, using the markers PHCRAC-GFP and LimE-mRFP, respectively. The obtained fusion products were approximately 10-100 times larger than native Dictyostelium cells. In the substrate-attached cortex, they exhibit self-organized actin waves, similar to non-fused cells. However, due to the increased size of the fused cells, we can now observe the dynamics of the actin waves for the first time in much larger spatial domains. The wave patterns show many characteristic features that are well known from excitable reaction-diffusion systems. The dynamics is characterized by expanding circular and elliptic waves as well as rotating spirals. If such waves collide, they annihilate each other. The distribution of the fluorescent markers indicate that F-actin is concentrated at the leading front of the wave followed by a PIP3 enriched zone containing only little F-actin. Using a custom written software, the recorded wave patterns were fitted either by ellipses or spiral-functions to determine the cell displacement, the wave velocity, and the curvature of individual waves for further analysis. Furthermore, our data suggest an important role of the F-actin waves in cell motility, an observation that can be accounted for in terms of a simple mechanical model.

BP 1.6 Mon 11:00 H43

Mechanics of bleb formation in filamin-negative cancer cells — Julia Peukes and •Timo Betz — Institut Curie, UMR 168, Paris, France

The formation of cellular blebs is a well described dynamical process that can be associated with cell motility, cell division and apoptosis. While recent research has shown a direct relation between cell contractility, cell cortex mechanics and bleb formation, a detailed mechanical model of cell bleb formation containing quantitative values for the mechanical parameters is still under work. Here we show new quantification of the membrane advancement of filamin negative cancer cells during bleb formation as measured by an interferometric technique that gives sub-nm precision at kHz repetition rate. These new experiments allow to determine the fluctuations of the cell bleb membrane during the extension of the bleb, the polymerization of the actin cortex and the myosin driven bleb retraction. Using simple arguments we can

translate the fluctuations into an effective actin-cortex tension that is consistent with previous measurements. More detailed analysis of the fluctuation shows mechanical details of the different bleb phases. Furthermore, we can identify clear separations of the bleb growth rates into distinct extension velocity regimes that we attribute to different levels of the actin polymerization under the cell membrane. These findings give hints towards a more detailed model on the different events involved in cellular blebbing.

15 min break

BP 1.7 Mon 11:30 H43

Sensing the surface: shortcuts for bacteria — •Siddharth Deshpande[1], Isabelle Hug[2], Urs Jenal[2], and Thomas Pfohl[1] — [1]Department of Chemistry, University of Basel, Switzerland — [2]Biozentrum, University of Basel, Switzerland

Caulobacter crescentus is an oligotrophic bacterium which divides asymmetrically to generate a sessile stalked cell and a flagellated swarmer cell. While the stalked cell immediately enters the next cell cycle, the swarmer cell remains in G1 phase for a definite time before differentiating into a stalked cell by losing the flagellum, pilli and producing an adhesive organelle, the holdfast. This cell cycle progression is controlled by cyclic di-GMP signaling and associated phosphorylation networks. We have developed a microfluidic assay to show that swarmer cells can attach immediately after the cell division if they encounter a surface during growth, suggesting that the cell cycle program for motile-sessile transition can be overridden when cells mechanically sense the surface.

By controlling the fluid flow in the microchannel, we find that a drag force of about 20 pN is sufficient to induce $> 50\%$ of the 'newborn' swarmer cells to attach immediately after the division. This surface mediated attachment is strongly dependent on pilli, active flagellum, intact holdfast production and cyclic di-GMP concentration. High speed imaging studies show that swarmer cells, which do not attach immediately, have a tendency to rotate $(20 - 30$ Hz) just before they separate from the stalked cell. Immediately attaching swarmers do not rotate but show a directional creeping suggesting surface attachment.

BP 1.8 Mon 11:45 H43

Search patterns of human T-cells — •Marc Neef[1], Hélène Lyrmann[2], Carsten Kummerow[2], Markus Hoth[2], and Karsten Kruse[1] — [1]Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken — [2]Biophysik, Universität des Saarlandes, 66421 Homburg

At the start of immune response, the T-cells have no detailed information about the locations of their target cells, so they have to perform a random search. The effectiveness of this search depends on the geometry of the search area as well as on the type of the random search. We track primary human T-lymphocytes using in vitro time-lapse microscopy and compare the experimental tracks to theoretical models like Lévy-Walks, persistent random walks and more complex models. We analyse displacements, gyration and velocity auto correlation of experimental and theoretical tracks and find, that these features are best fitted with a model, that alternates between persistent motion and a resting phase.

Furthermore we test the effectiveness (i.e. average search time) of different search models in simple geometries. We find that the most effective model as well as the optimal parameters for this model strongly depend on the system size.

BP 1.9 Mon 12:00 H43

Modelling malaria parasite motility in heterogeneous environments — •Anna Battista[1], Friedrich Frischknecht[2], and Ulrich Schwarz[1] — [1]ITP, Heidelberg University, Germany — [2]University Clinics Heidelberg, Germany

Plasmodium sporozoites are the parasites responsible for malaria transmission from a mosquito to a vertebrate host. The movement of a sporozoite in the skin of the host appears to be irregular, whereas the same parasite describes a roughly circular trajectory on a flat substrate and a roughly helical trajectory in an unstructured 3D environment [1, 2]. Experiments performed in the Frischknecht group at Heidelberg University focused on the motion of sporozoites within regularly patterned micropillar arrays [3], corroborating the idea that the movement of the parasite is strongly determined by the nature of the surrounding environment. It is expected that the parasite has evolved a strategy to cope with irregularities in its environment, because malaria can develop only if a sporozoite reaches a blood vessel within a relatively short time after injection. We present a first theoretical model which predicts trajectories based on geometrical and energetic considerations. In particular, we discuss different scenarios for the interaction with obstacles and how these change the circular/helical path in 2D/3D environments. [1] S. Muenter et al., Cell Host & Microbe Vol. 6, 2009. [2] R. Amino et al., Nat. Med. Vol. 12, 2006. [3] J.K. Hellmann et al., Plos Pathogens Vol. 7, 2011.

BP 1.10 Mon 12:15 H43

Swimming mechanism of the African trypanosome using mesoscale hydrodynamics simulations — •Davod Alizadehrad and Holger Stark — ITP, TU Berlin

The African trypanosome is a microswimmer with a unique morphology that migrates through the blood-brain barrier and causes the devastative sleeping sickness. The trypanosome has a single flagella, which is firmly attached along its length to the membrane of the elongated cell body and has a free anterior part beyond the cell body [1]. A bending wave propagating along the flagellum pulls the cell body forward [1].

We simulate the swimming behavior of the trypanosome using a mesoscale particle base model with parallel computing on supercomputers. Our simulation reproduces the swimming dynamics of the trypanosome perfectly. The numerical results demonstrate that the free anterior part of the flagella together with its helical attachment to the cell body determines the swimming behavior and dynamics of the trypanosome. Simulation results for the swimming velocity and the ratio of the body rotational frequency to the propogating wave frequency agrees very well with experimental observations [1]. The simulations predict how the mechanical properties of the flagella, the cell body and the surrounding fluid affect the trypanosome locomotion and morphology. Furthermore we study the trypanosome locomotion within a crowded environment containing red blood cell sized particles.

1. Heddergott N, et al. (2012) PLoS Pathog 8(11): e1003023.

BP 1.11 Mon 12:30 H43

Analyzing the mechanics and energetics of motile bacteria with object-adapted optical traps — •Julian Roth, Matthias Koch, and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

The spread of bacterial diseases and their pathogenicity can often be directly linked to their ability to move under different environmental conditions. In order to understand the basic locomotion principles of single helical bacteria, we use the recently developed object-adapted optical trapping and shape-tracking technique [1] to analyze their complex movements. In particular, we investigate Spiroplasma melliferum and the Spirochetes Borrelia japonica. Spiroplasma belong to the smallest and simplest forms of life, they cause tremendous agricultural damage, but their motility is not completely understood so far. As we show, Spiroplasma can rapidly undergo continuous transitions between different states of mechanical energy during motility. These transitions are related to conformational changes of the molecular subunits of their unique fibril-like cytoskeleton. We track their shape with nm precision at rates up to 1 kHz and estimate the energetics and forces involved in this process. In this project, we develop a model describing the potential landscape of the cytoskeletal ribbon and try to link it to different environmental influences, which we control by the addition of drugs, changes of the viscosity or the pH value of the surrounding medium. First experimental and computational results are presented.

[1] Koch, M. & A. Rohrbach (2012). Nature Photonics 6(10): 680-686

BP 1.12 Mon 12:45 H43

The Physical Bounds of In Vivo Cell Motility — •Josef A. Käs — Division of Soft Matter Physics, Institute for Experimental Physics I, University of Leipzig

Migration of cells through tissues is quintessential for wound healing, neuronal plasticity, and the functioning of the immune system. In disease it is also a key determinant of cancer metastasis and nerve regeneration. Mammalian tissues are a new state of active fluid matter. A broad range of different cell types demix like non miscible fluids building natural boundaries for migrating cells. At least to some extent the cells are hold back by an effective surface tension, which is determined by cell-cell adhesion and cell contractility. Individual cells in tissues behave very much like active soft colloids. Thus, cells have

a high probability to get jammed when moving through tissues and collective cell assemblies are close to be frozen by the glass transition. Cells that effectively move through tissues and are able to transgress tissue boundaries are softer and more contractile than cells that stay local in tissues. Soft and contractile avoids jamming and is optimal to overcome boundaries. Naturally, softness has to have its limits. So neuronal growth cones are too soft to carry large loads and thus excessively weak to move efficiently e.g. through scar tissue, which is required for nerve regeneration. Whereas cancer cells optimize their biomechanical and contractile properties for metastasis during tumor progression. In synopsis, the physical bounds that the functional modules of a moving cell experience in tissues may provide an overarching motif for novel approaches in diagnosis and therapy.

BP 2: Proteins

Time: Monday 9:30–12:45 Location: H44

Topical Talk BP 2.1 Mon 9:30 H44

Energy conversion mechanisms of heat shock proteins — •Thorsten Hugel — Physik Department and IMETUM, Technische Universität München, Boltzmannstr.11, 85748 Garching, Germany

Single molecule methods allow real time observation of molecular machines at work. We have utilized single molecule Förster Resonance Energy Transfer (smFRET) to decipher the mechano-chemical cycle of the heat shock proteins yeast Hsp90 [1] and bacterial Hsp90 [2]. Although they are homolog we observe significant differences in domain movement and in their mechanism of energy conversion.

To further elucidate the structure-function relationship in these Hsp90s we use optical tweezers and a smFRET based nanopositioning system. Our in vitro results are mostly consistent with the crystal structure of yeast Hsp90 [3], but show some significant deviations in the N-terminal domain.

Finally, these methods are not only suited to determine the structure and function of isolated single proteins, but yield valuable insights into their interplay with other proteins.

[1] Ratzke et al., PNAS (2012) [2] Ratzke et al., JMB (2012) [3] Ali et al., Nature (2006)

BP 2.2 Mon 10:00 H44

Peptide with a trigger: The aggregation and refolding of pH sensitive peptide GALA in solution and at interfaces — •Denise Schach, Christoph Globisch, Adrian Fuchs, Clemens K. Weiss, Christine Peter, Mischa Bonn, and Tobias Weidner — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz

GALA is a 30 amino acid synthetic peptide consisting mainly of the Glu-Ala-Leu-Ala repeat motif. Originally it was designed to act as a shuttle across lipid membranes in drug or gene delivery systems. Importantly, structure and function can be triggered by pH. The triggering mechanism relies on the conversion from a random coil to an amphipathic α-helix when decreasing the pH from 7 to 5. The helix formation is driven by protonation, i.e. neutralization, of the Glu side at pH 5, which makes a folded structure energetically more favorable. The repetition of hydrophobic and hydrophilic residues is responsible for the amphipathic peptide properties in the helical state. In its amphipathic state, GALA is also likely to aggregate. Near a lipid membrane the aggregation leads to cell penetration, pore formation and membrane leakage. To better understand the fundamental mechanisms of refolding and aggregation in bulk solution and at interfaces, we probe structural details with Fourier-transform infrared spectroscopy and sum frequency generation. Moreover, we apply Brewster angle microscopy and light scattering to follow aggregation. The interpretation of the experiments is complemented by molecular dynamics simulations of GALA refolding and aggregation.

BP 2.3 Mon 10:15 H44

Structure and dynamics of the iron binding protein Lactoferrin studied with neutron scattering — •Clemens Sill[1], Ralf Biehl[1], Bernd Hoffmann[2], and Dieter Richter[1] — [1]JCNS-1 & ICS-1: Neutron Scattering, Forschungszentrum Jülich, Germany — [2]ICS-7: Biomechanics, Forschungszentrum Jülich, Germany

The understanding of the functionality of proteins started with a rigid model, namely the Lock and Key analogy. Meanwhile, a more dynamic and flexible picture of these macromolecules has evolved to explain protein function. The importance of thermodynamically driven, internal motions for the functioning of proteins is subject of ongoing research.

Lactoferrin is an iron-binding protein with antimicrobial activity as a part of the innate immune system. It consists of two binding sites located in a cleft of the two main domains, each is capable of binding and releasing one iron ion. A combined approach of Small Angle Neutron Scattering for structural characterization and Neutron Spin Echo spectroscopy to elucidate the dynamic properties of different binding states was undertaken to enlighten the influence of iron binding on large scale protein dynamics. A comparison of the SANS data with 3D structures (crystallography and homology models) proved that the binding sites are closed when occupied by iron and open otherwise. In combination with normal mode analysis it was found from the NSE measurements that the internal dynamics are dominated by fluctuations of the main domains relative to each other. Stretching and twisting motions can describe the found dynamics, and their occurrence is independent whether the domains are open or closed.

BP 2.4 Mon 10:30 H44

Influence of surface and subsurface properties on the structure and activity of adsorbed lysozyme — •Christian Spengler[1], Stéphane Mesnage[2], Hendrik Hähl[1], Peter Loskill[1], Simon J. Foster[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, 66041 Saarbrücken — [2]University of Sheffield, The 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 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 and effectivity of adsorbed proteins are also influenced by the properties of the underlying material. In this study, we investigate how the activity -the bactericidal effect- of adsorbed lysozyme is affected by surface and subsurface 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 2.5 Mon 10:45 H44

Integrating Genomic Information with Molecular Simulation for Protein Dynamics — •Alexander schug[1], Hendrik Szurmant[2], Martin Weigt[3], and Abhinav Verma[1] — [1]Karlsruhe Institute of Technology — [2]The Scripps Reserach Institute — [3]Université Pierre et Marie Curie

Protein function often requires a protein to form a complex or adopt multiple conformations during its function cycle. Structural characterization of these states is experimentally difficult as they are typically stabilized by transient interactions. Here, we demonstrate how a mixed theory approach can predict such structures on the example of two-component signal transduction systems (TCS), a ubiquitous signal response system. We predicted the TCS complex structure in high agreement (3.5 RMSD) with concurrent experimental work [1] by combining molecular dynamics [2] and statistical genomic analysis [3]. Similarly, we were able to predict the active conformation occurring during autophosphorylation by identifying co-evolving interdomain amino acid pairs in agreement with biochemical mutagenesis data [3]. We can now simulate the conformational transition between active and inactive conformations, quantify its free-energy barrier and its change as reaction to transmembrane forces exercised by the sensor domain. [unpublished data]

[1] Schug A et al., PNAS (2009) 106, 22124-22129
[2] Schug A and Onuchic J, Curr Opin Pharm (2010) 10, 709-714
[3] Weigt M et al., PNAS (2009) 106, 67-72

[4] Dago A et al., PNAS (2012), 109, E1733-42

15 min break

BP 2.6 Mon 11:15 H44

Urea's effect on protein secondary structures — •Beate Moeser and Dominik Horinek — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg

Proteins in cells are surrounded by a large variety of chemical compounds (as e. g. metabolites, messenger substances, and osmoregulators). Some of these cosolutes denature proteins and others (over-)stabilize their native fold. This is due to the fact, that they interact differently with different protein secondary structures. The molecular origin thereof, however, is not yet fully understood.

We developed a simulation setup [1] for molecular dynamics simulations, which allows us to quantitatively investigate cosolute effects on various secondary structural elements and provides insight into the molecular forces at play.

Here, we present the influence of the denaturant urea on homopeptides in four distinct conformations: extended strand, 3_{10}-helix, α-helix, and β-sheet. Furthermore, we check, whether the strength of urea's effect on a given structure is proportional to the solvent accessible surface area of the conformation. This is one of the main assumptions of the group transfer model (TM), which is widely used to predict cosolute effects on proteins. Our quantitative checks allow for a detailed validation and assessment of implementations of the TM and its conclusions concerning the role of the backbone and sidechains in urea denaturation.

[1] Horinek, D., Netz, R.R. 2011. *J Phys Chem A 115(23)*, 6125-6136

BP 2.7 Mon 11:30 H44

Internal protein dynamics - a study on fully deuterated cyano phycocyanin by 2H NMR experiments and random-walk simulations — •Kerstin Kämpf, Beke Kremmling, and Michael Vogel — TU Darmstadt

Although possessing an ordered structure, proteins exhibit a versatile but common internal dynamics. The precise nature and geometry of this motion remains, however unclear. In order to investigate this, a combined approach of solid state 2H NMR and random-walk simulations (RWS) is used. Solid state 2H NMR is sensitive to the time scale as well as the geometry of motion[1]. It has been applied to samples of fully deuterated c-phycocyanin (hydration h= 0 g/g,h= 0.3 g/g). Suppressing the contribution of the fast methyl groups, we find that the protein backbone exhibits a temperature dependent small amplitude motion. The NMR parameters of the backbone motion are calculated by RWS for two limiting cases: A heterogeneous scenario with temperature dependent correlation times and a homogeneous scenario, in which the amplitude of motion increases with temperature. The RWS show that the existence of a T dependent amplitude of the motion is a main feature of internal protein dynamics. Nevertheless a single T dependent angle, increasing from 0°-15° for 200<T<300 K, cannot explain all experimental observations. A distribution of angles is required for a good description of the observations in 2H NMR. Thus, the present study reveals that internal protein dynamics is a complex motion with an amplitude that strongly depends on temperature.

[1]Lusceac, BBA, (2010), 1804, 41-48.

BP 2.8 Mon 11:45 H44

Effects of ligand binding on the mechanical properties of ankyrin repeat proteins — •Giovanni Settanni[1], David Serquera[2], Piotr Marszalek[3], Emanuele Paci[4], and Laura Itzhaki[5] — [1]Physics Department, Johannes Gutenberg University, Mainz, Germany — [2]Hutchison/MRC Research Centre, Cambridge, UK — [3]Duke University, Durham, NC, USA — [4]University of Leeds, UK — [5]University of Cambridge, UK

Ankyrin repeat proteins are elastic materials that unfold and refold repeat by repeat, under force. Herein we use atomistic molecular dynamics to compare the mechanical properties of the 7-repeat protein Gankyrin in isolation and in complex with its binding partner S6-C. We show that the bound S6-C greatly increases the resistance of Gankyrin to mechanical stress. The effect is specific to those repeats of Gankyrin directly in contact with S6-C. A consequence of the localized nature of ligand binding is that it impacts on all aspects of the protein's mechanical behavior, including the order of repeat unfolding, the diversity of unfolding pathways, the nature of partially unfolded intermediates, the forces required and the work transferred to the system to unfold the whole protein and its parts. Stepwise unfolding thus provides the means to buffer repeat proteins and their binding partners from mechanical stress in the cell. Our results illustrate how ligand binding can control the mechanical response of proteins. The data also point to a cellular mechano-switching mechanism whereby binding between two partner macromolecules is regulated by mechanical stress.

BP 2.9 Mon 12:00 H44

Regulatory mechanism of the light-activable DNA-binding switch LOV-TAP : A computer simulation study — Emanuel Peter, Bernhard Dick, and •Stephan A Baeurle — Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany

The spatio-temporal control of gene expression is fundamental to elucidate cell proliferation and deregulation phenomena in living systems. Novel approaches based on light-sensitive multi-protein complexes have recently been devised, showing promising perspectives for the reversible modulation of the DNA-transcriptional activity in vivo. This has lately been demonstrated in a striking way through the generation of the artificial protein construct light-oxygen-voltage (LOV)-tryptophan-activated protein (TAP), in which the LOV2-Jalpha photoswitch of phototropin1 from Avena sativa (AsLOV2-Jalpha) has been ligated to the tryptophan-repressor (TrpR) protein from Escherichia coli. Here, we elucidate the early stages of the light-induced regulatory mechanism of LOV-TAP at the molecular level, using the non-invasive molecular dynamics simulation technique [1]. More specifically, we find that Cys450-FMN-adduct formation in the AsLOV2-Jalpha-binding pocket after photoexcitation induces the flexibilization through unfolding of a hairpin-like helix-loop-helix region interlinking the AsLOV2-Jalpha- and TrpR-domains, ultimately enabling the condensation of LOV-TAP onto the DNA surface.

[1] E. Peter, B. Dick, S.A. Baeurle, Prot. Struct. Funct. Bioinf., in press (2012); doi:10.1002/prot.24196

BP 2.10 Mon 12:15 H44

Zinc Finger Proteins and the 3D Organization of Chromosomes — •Dieter Heermann[1], Christoph Feinauer[1], Sebastian Goldt[2], Andreas Hofmann[1], Lei Liu[1], and Gabriell Mate[1] — [1]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg — [2]Fitzwilliam College, Cambridge University, Cambridge, England

Zinc finger domains are one of the most common structural motifs in eukaryotic cells. These DNA-binding proteins contain up to 37 zinc finger domains connected by flexible linker regions. They have shown to be important organizers of the 3D structure of chromosomes and as such are called the master weaver of the genome.

Our results indicate that the binding affinity is increased by the flexible linkers by several orders of magnitude. Moreover, the binding map for proteins with more than one domain exhibits interesting structures which, having been neither observed nor described before can be interpreted to fit very well with existing theories of facilitated target location.

We have developed a methodology to characterize these flexible proteins. Employing the concept of barcodes we propose a measure to compare such flexible proteins in terms of a similarity measure. This measure is validated by a comparison between a geometric similarity measure and the topological similarity measure that takes geometry as well as topology into account.

BP 2.11 Mon 12:30 H44

Stochastic dynamics of direct and hierarchical virus capsid assembly — •Heinrich Klein[1], Johanna Baschek[1], and Ulrich S. Schwarz[1,2] — [1]Institute of Theoretical Physics, University of Heidelberg — [2]Bioquant, University of Heidelberg

In order to replicate within their host, many viruses have developed self-assembly strategies for their capsids which are sufficiently robust as to be reconstituted in vitro. Models for virus self-assembly usually assume that the bonds leading to cluster formation have constant reactivity over the time course of assembly (direct assembly). In some cases, however, binding sites between the capsomers have been reported to be activated during the self-assembly process (hierarchical assembly).

Here we present a computational approach to study assembly of icosahedral viruses based upon the overdamped Langevin equation (Brownian dynamics)[1]. Hard spheres covered by reactive patches (patchy particles) serve as fundamental building units for the capsid.

Hierarchical assembly is implemented by a switching in reactivity upon the formation of pentameric and hexameric rings. These substructures are considered key intermediates during the assembly.

Using computer simulations, we compare the efficiency of direct versus hierarchical assembly as function of association and dissociation rates. Our analysis shows for which molecular parameters hierarchical assembly schemes can outperform direct ones and suggests that viruses with high bond stability might prefer hierarchical assembly schemes.

[1] Johanna E. Baschek, Heinrich C. R. Klein and Ulrich S. Schwarz. BMC Biophysics 5:22, 2012.

BP 3: Statistical Physics in Biological Systems I (joint with DY)

Time: Monday 9:30–11:30 Location: H47

BP 3.1 Mon 9:30 H47

Cardiorespiratory data segmentation during sleep — •Sabrina Camargo[1], Maik Riedl[1], Celia Anteneodo[2], Thomas Penzel[3], and Niels Wessel[1] — [1]Department of Physics, Humboldt Universität zu Berlin, Berlin, Germany — [2]Department of Physics, PUC-Rio, Rio de Janeiro, Brazil — [3]Sleep Center, Charité University Hospital, Berlin, Germany

The variability in cardiorespiratory data is closely related to the regulation of sleep. When the brain is very active as in the REM sleep stage, heart rate as well as respiration have long-range correlations, while, in contrast, in deep sleep those correlations vanish after a few seconds, indicating that cardiovascular data can be useful to reflect sleep disturbances. But physiological data usually display a highly nonstationary behavior, caused by either environmental conditions or the inherent complexity of the underlying dynamics of the biological rhythms. Considering that the signal is composed of stationary segments, we apply a nonparametric segmentation approach in order to detect such locally stationary segments, where statistical measures of first and second order, for example, mean and variance, are more likely to remain constant. Thus, segmentation provides a picture of the nonstationarity of a time series, in particular, the intrinsic time scales. Moreover, by finding the stationary regimes, we are able to identify changes in time series, as those coming from the cyclic reduction of the airflow. We compare the segmentation outcomes in the presence and the absence of respiratory induced sleep disturbances and we verify an increased variability in blood pressure in patients suffering from this events.

BP 3.2 Mon 9:45 H47

Extended diffusion models for sleep stage switching — Anna Barkentien and •Jens Christian Claussen — INB, University of Lübeck, Germany

Short awakening periods especially occuring during the second half of the night follow a peculiar power law [1] for which 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. In contrast to an Ornstein-Uhlenbeck process the restoring force is inversely proportional (or a power law with negative exponent) to the excursion distance from the sleep/wake border. 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].

[1] C.-C. Lo, L. A. Nunes Amaral, S. Havlin, P. Ch. Ivanov, T. Penzel, J.-H. Peter, and H. E. Stanley. Dynamics of sleep-wake transitions during sleep. Europhysics Letters, 57, 631, 2002.
[2] J. W. Kim, J. -S. Lee, P. A. Robinson, D. -U. Jeong, Markov Analysis of Sleep Dynamics. Phys. Rev. Lett. 102, 2009.
[3] A. Barkentien and J.C. Claussen (in preparation).

BP 3.3 Mon 10:00 H47

Caveats in Modelling Coarse-Grained Descriptions of a Bistable Frustrated Unit — •Darka Labavić[1], Hannes Nagel[2], Wolfhard Janke[2], and Hildegard Meyer-Ortmanns[1] — [1]School of Engineering and Science, Jacobs University Bremen — [2]Institut für Theoretische Physik, Universtät Leipzig

From a coarse-grained perspective the motif of a self-activating species, activating a second species which acts as its own repressor, is widely found in biological systems. In [1] we studied this model on the proteonic level in a fully stochastic version. In [2] we zoom into the level of genes which are described as directly producing proteins. We focus on the effect that inherent time scales of the underlying scale of this genetic circuit can have on the bifurcation patterns on the coarser scale of proteins. Depending on the ratio of binding and unbinding rates of the transcription factors to the decay times of the proteins, the appropriate averaging procedure for obtaining a coarse-grained description changes and leads to sets of deterministic equations, which considerably differ in their bifurcation structure. In particular, the desired intermediate range of regular limit cycles fades away when the binding rates of genes are not fast as compared to the decay time of the proteins. Our analysis illustrates that the common topology of the widely found motif alone does not imply universal features in the dynamics.

[1] Garai A, Waclaw B, Nagel H, and Meyer-Ortmanns H, J. Stat. Mech. (2012) P01009;
[2] Labavić D, Nagel H, Janke W, and Meyer-Ortmanns H, submitted

BP 3.4 Mon 10:15 H47

DNA denaturation in correlated environments — Viktoria Blavatska[1], •Christian von Ferber[2], and Yurij Holovatch[1] — [1]Institute for Condensed Matter Physics, NAS Ukraine, Lviv — [2]Applied Mathematics Research Centre, Coventry University, UK

We revisit the problem of DNA denaturation in the frames of the Poland-Scheraga model. This model predicts a first or second order transition depending on the value of the loop exponent.

Usually an unperturbed background is assumed within this model. However, in a biologically relevant environment correlated structures are prevalent and the transition may change due to the influence of this environment.

Applying renormalisation group methods we determine the loop exponent in higher orders up to the fourth order in the ϵ-expansion. In the absence of disorder this allows us to determine the numerical value of the exponent using resummation techniques.

Performing corresponding calculations for the situation of correlated environments we find strong disorder effects.

BP 3.5 Mon 10:30 H47

Simulations of aggregation in homopolymer systems — •Johannes Zierenberg and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Germany

We investigate the aggregation transition of a coarse-grained many-polymer system. To this end we apply parallel multicanonical simulations for different system sizes and densities. Our data suggests that the aggregation process in the simple model is a first-order phase transition. We investigate the dependence of the transition temperature on the density and size of the system and look at generic properties.

BP 3.6 Mon 10:45 H47

Collective behaviour of competing, coupled particles on a 1d chain — •Ines Weber[1], Ludger Santen[1], and Martin Evans[2] — [1]Department of Theoretical Physics, Saarland University, 66041 Saarbrücken, Germany — [2]Department of Physics & Astronomy, University of Edinburgh, Edinburgh EH9 3JZ, UK

Biopolymers are dynamic filaments involved in a wide variety of biological processes such as intracellular transport. Experiments have shown them to exhibit non-equilibrium fluctuations and deformations induced by molecular motors. I will present a simple model of such processes, which comprises competing species of interacting particles on a lattice. They perform a 'tug-of-war' and induce deformation and drift on a 1d chain. Constraints given by hard core coupling to next-neighbour sites influence the system's dynamics and result in collective particle behaviour.

BP 3.7 Mon 11:00 H47

Coexistence and survival in conservative Lotka-Volterra networks — •Johannes Knebel[1], Torben Krüger[2], Markus Weber[1], and Erwin Frey[1] — [1]Arnold-Sommerfeld Center for Theo-

retical Physics and Center for NanoScience, Theresienstraße 37, 80333 München — [2]Department of Mathematics, Ludwig-Maximilians-Universität München, Theresienstraße 38, 80333 München

Conservative Lotka-Volterra (LV) models play a fundamental role in many fields of science such as population dynamics. New insights into the maintenance of biodiversity can be gained by understanding the long-term behavior of complex LV interaction networks and by revealing their coexistence and survival scenarios.

Here we present a classification scheme for coexistence scenarios in well-mixed, conservative LV networks. Our theoretical approach to study global stability properties builds on a deterministic analysis by using the Pfaffian of the interaction matrix, a simpler form of the determinant for skew-symmetric matrices. We find that the classification of conservative LV dynamics on the basis of their interaction topology is incomplete and that non-cyclic networks can also maintain coexistence of all species. The deterministic analysis also leads to a deeper understanding of the stability of ecological networks in finite populations as is reflected by a generalized scaling law for the extinction time in the vicinity of critical reaction rates. Our general results are illustrated for systems composed of four and five species.

BP 3.8 Mon 11:15 H47

Evolutionary game dynamics between random mutants — •Weini Huang[1], Bernhard Haubold[2], Christoph Hauert[3], and Arne Traulsen[1] — [1]Evolutionary Theory Group, Max Planck Insitute for Evolutionary Biology, August-Thienemann-Straße 2, 24306, Plön,Germany — [2]Bioinformatics Group,Max-Planck-Insitute for Evolutionary Biology, August-Thienemann-Straße 2, 24306, Plön,Germany — [3]Department of Mathematics, The University of British Columbia, 1984 Mathematics Road, Vancouver V6T1Z2, British Columbia, Canada

Polymorphism occurs when more than one genotype or phenotype exist in the same population. Although polymorphisms are often observed in populations, the emergence and maintenance of polymorphsims remain unclear.We investigate this question by introducing a new model, named as mutant games. In evolutionary game theory, the interactions of different types in a population are described by payoff matrices. However, the number of types is usually fixed and payoff matrices are typically predefined. This can be a limit to model a biological population with random mutations. In our mutant games, the interactions of mutants and resident types are represented by a dynamical payoff matrix. The resulting dynamics caused by random mutants under frequency dependent selection, leads to a remarkably higher diversity, compared to the mutants under constant selection. Interestingly, although arbitrary number of mutants are allowed in mutant games, an intermediate level of diversity is maintained.

BP 4: Symposium Charge Transfer Effects in Molecular Materials (SYCT, joint with CPP, HL and DS)

Time: Monday 9:30–12:00 Location: H1

Invited Talk BP 4.1 Mon 9:30 H1

A coarse grained QM/MM approach for the description of charge transfer in complex systems — •Marcus Elstner — Karlsruhe Institute of Technology, Karlsruhe, Germany

Charge transfer in DNA has received much attention in the last years due to its role in oxidative damage and repair in DNA, but also due to possible applications of DNA in nano-electronics. Despite intense experimental and theoretical efforts, the mechanism underlying long range hole transport is still unresolved. We present a new computational strategy to evaluate the charge-transfer (CT) parameters for hole transfer in DNA. Based on a fragment orbital approach, site energies and coupling integrals for a coarse grained tight binding description of the electronic structure of DNA can be rapidly calculated using the approximate Density Functional method SCC-DFTB. Environmental effects are captured using a combined quantum mechanics/molecular mechanics (QM/MM) coupling scheme and dynamical effects are included by evaluating these CT parameters along extensive classical molecular dynamics (MD) simulations. The fluctuations of the counterions, strongly counterbalanced by the surrounding water, leads to large fluctuations of the site energies, which govern the hole propagation along the DNA strand, while the electronic couplings depend strongly on DNA conformation and are not affected by the solvent (2) . Using this methodology, the time course of the hole can be followed by propagating the hole wave function using the time dependent Schrödinger equation for the coarse grained Hamiltonian (5,6).

Invited Talk BP 4.2 Mon 10:00 H1

Identifying and resolving charge separation in organic solar cells — •Eberhard Riedle — BioMolekulare Optik, LMU München

The charge separation and the charge mobility are essential factors for efficient solar devices. Time resolved spectroscopy can resolve these processes completely. We use sub-50 fs resolution, fully tunable pump pulses, and continuum probing from 300 to 1700 nm. Since solar cells are intended to absorb visible light, particularly probing in the NIR allows to differentiate between the excitonic and polaron states. We show that the primary excitation in P3HT-Si hybrid cells are excitons located on the polymer. They dissociate to polarons in 140 fs. A significant part of the excitation is lost at this early stage due to internal conversion back to the ground state [1]. Using the knowledge from the transient measurements, we optimize the composition and preparation of the cells to an efficiency of 1.1 % [2]. The character and mobility of the polarons is determined by excitation fluence dependent measurements. In a series of polymers - mixed with C_{60} - with increasing conjugation length, the highly structured transient spectra do not allow the easy identification of polarons. The analysis shows that the spectrum is closely related to the electroabsorption spectrum of the polymer, i.e. the derivative of the absorption spectrum. In this way we can conclude that indeed charge separation and an electric field is generated in the thin film solar cells by the visible excitation.

[1] D. Herrmann et al., J. Am. Chem. Soc. **133**, 18220 (2011).
[2] S. Niesar et al., Green **1**, 339 (2011).

Invited Talk BP 4.3 Mon 10:30 H1

Quantifying the energy of charge transfer states: From molecular crystals to donor-acceptor blends — •Reinhard Scholz — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden, Germany

In molecular crystals, exciton models accounting for neutral molecular excitations and charge transfer (CT) allow to deduce their energy alignment from measured spectra.[1] Donor-acceptor blends may reveal weak CT absorption and photoluminescence spectra below the main absorption bands, and for polymer-fullerene solar cells, the respective energies correlate with the open circuit voltage.[2] Calculations of CT energies in these materials require computational methods with the correct asymptotics of the mutual Coulomb interaction between pairs of ionized donor and acceptor molecules like constrained DFT schemes.[3] Moreover, the solvation energy arising from the embedding polarizable medium and the screening of the Coulomb interaction result in substantial deviations from the interaction between oppositely charged donor and acceptor molecules in vacuum. Based on a constrained DFT scheme and an embedding scheme accounting for the polarizable medium, calculated CT energies for selected donor-acceptor pairs are compared to available spectroscopic data and the open circuit voltage of photovoltaic devices.

[1] L. Gisslén and R. Scholz, Phys. Rev. B **80**, 115309 (2009).
[2] K. Vandewal *et al.*, Adv. Funct. Mater. **18** 2064 (2008).
[3] M. Rapacioli, F. Spiegelman, A. Scemama, and A. Mirtschink, J. Chem. Theory Comput. **7**, 44 (2011).

Invited Talk BP 4.4 Mon 11:00 H1

Efficient Exciton Generation and Collection in Organic Solar Cells — •Mark Thompson[1], Cong Trinh[1], Steve Forrest[2], and Jeramy Zimmerman[2] — [1]University of Southern California, Los Angles, CA, USA — [2]University of Michigan, Ann Arbor, MI, USA

The exciton is a critical part of each of the processes leading to photocurrents in Organic PhotoVoltaics (OPVs), and being able to control the location, lifetime and energy of the exciton is essential to achieving high efficiency. We have investigated methods for tuning exciton energies and controlling their migration paths within a thin film. I will discuss our most recent work with both organic dyes, such as squaraines

and dipyrrins as well as metallo-porphyrin materials for OPVs. This involves a careful materials design study that leads to both low energy absorption (into the nearIR) and the efficient use of multiple absorbers to efficiently harvest photons through the entire visible spectrum.

A key limiter of OPV performance is the open circuit voltage, Voc. A number of parameters control the Voc, including the energetics of the donor and acceptor, the energy of the charge transfer exciton formed at the D/A interface and the structure of the materials at the D/A interface. We have investigated methods to tailor the interfacial structure at the D/A interface, leading to improved Voc. We have investigated thermal and solvent annealing, as well as a process we call chemical annealing, where the thin film is exposed to an external agent, which is incorporated into the film stoichiometrically. I will discuss each of these methods and how they affect the device performance.

Invited Talk BP 4.5 Mon 11:30 H1

Electron transport in organic single-crystal transistors and Schottky-gated heterostructures — •Alberto Morpurgo — University of Geneva, Geneva, Switzerland

Organic single-crystal transistors have unprecedented quality and enable the investigation of several interesting phenomena (band-like transport in, the Hall effect, interfacial polarons, etc.). So far, virtually only p-type devices have been studied. Here, I will discuss electron transport in single-crystal FETs and heterostructures, showing how the best n-type devices perform at the level of their p-type counterparts. I will first focus on PDIF-CN2 single-crystal FETs, in which we observe the characteristic signatures of band-like transport (electron mobility increasing upon cooling and of Hall effect). The experimental results, and a comparison with p-type materials in which band-like transport in FETs is observed, suggest that the coupling of the charge carriers to the polarizability of the organic semiconductor plays a key role in determining which organic materials are more likely to exhibit band-like transport. Next, I will discuss new Schottky-gated heterostructures based on rubrene and PDIF-CN2 crystals, in which a conducting 2D layer forms spontaneously due to charge transfer. Gate-dependent transport and Hall measurements show that electrons are responsible for the conductivity, and that their density decreases linearly with decreasing temperature. We understand this behavior in terms of the heterostructure band-diagram, which quantitatively captures the slope of the linear temperature dependence. In the best devices, the electron mobility remains as high as ~ 1 cm2/Vs at T=30 K.

BP 5: Cytoskeleton

Time: Monday 15:00–17:00 Location: H43

Topical Talk BP 5.1 Mon 15:00 H43

Cytoskeletal pattern formation: Self organization of driven filaments — •Andreas Bausch — Technische Universität München

Living cells rely on the self organization mechanisms of cytoskeleton to adapt to their requirements. Especially in processes such as cell division, intracellular transport or cellular motility the controlled self assembly to well defined structures, which still allow a dynamic reorganization on different time scales are of outstanding importance. Thereby, the intricate interplay of cytoskeletal filaments, crosslinking proteins and molecular motors a central role. One important and promising strategy to identify the underlying governing principles is to quantify the physical process in model systems mimicking the functional units of living cells. Here I will present in vitro minimal model systems consisting of actin filaments, crosslinking molecules and myosin II exhibiting collective long range order and dynamics. I will discuss how a balance of local force exertion, alignment interactions, crosslinking and hydrodynamics affect the evolving dynamic structures.

BP 5.2 Mon 15:30 H43

Time dependent irreversible bundling of actin filaments with magnesium ions — Timo Maier[1,2], •Tamás Haraszti[1,2], and Joachim P. Spatz[1,2] — [1]New Materials and Biosystems group, MPI for Intelligent Systems, Heisenbergstr. 3, 70569-Stuttgart, Germany — [2]Biophysical Chemistry, University of Heidelberg, Im Neuenheimerg Feld 253, 69120-Heidelberg, Germany

Actin, an abundant protein in eukaryotic cells, forms filamentous structures playing critical roles in cellular adhesion, motility and determining the elastic properties and the shape of cells. Mixed with divalent cations, bundles were observed above a critical electrolyte concentration, e.g. $27\,mM$ for Mg^{2+}. The process is driven by counter ion condensation, but there are still unclear details. We have investigated two of these details using 2-dimensional networks of prepolymerized actin filaments, following the bundling process by the thermal motion of tracer particles attached to the bundles and fluorescence microscopy. Our results indicate, that the filaments preferentially adsorb the divalent magnesium ions, resulting in crosslinking down to $5 - 8\,mM$ background concentration when the solution is provided by a mediate ($0.4\,\mu l/min.$ loading rate) flow. While the driving forces are in the order of $0.1 - 0.25\,pN$, as we have reported earlier in single actin experiments, the resulted bundling is not reversible by thermal motion even after removing the magnesium and adding EGTA to the solution for several hours.

BP 5.3 Mon 15:45 H43

The dynamical cytoskeleton regulates morphogenesis in rod-like bacteria — •Sven van Teeffelen — Department for Molecular Biology, Princeton University, Princeton, USA

Bacteria were long regarded as unstructured bags of freely diffusing proteins and DNA. Contrary to this view, bacterial cells are now known to display intricate sub-cellular localization and dynamics of their constituents, which is required for a variety of processes including cellular morphogenesis. Biophysically, one mechanism for achieving macroscopic order relies on the bacterial cytoskeleton. Here we report a quantitative study of the dynamics of the Escherichia coli actin homolog MreB, which is essential for the maintenance of rod-like cell shape in bacteria. We found that MreB rotates around the long axis of the cell in a persistent manner and that this rotation depends on the assembly of the peptidoglycan cell wall. Biophysical modeling suggests that MreB and cell-wall synthesis are physically coupled. Thus, the MreB motion observed constitutes a reporter of the local insertion of cell-wall material. In agreement with recent experiments on macroscopic twisting of the cell envelope during growth we find that peptidoglycan is deposited in the cell wall in a helical manner. The cell wall in turn ultimately determines bacterial cell shape. Semi-atomistic computational simulations suggest that one function of MreB is to ensure a uniform distribution of new peptidoglycan insertion sites, a necessary condition to maintain rod shape during growth. Based on the same computational framework we hypothesize that MreB governs bacterial cell shape in a non-trivial manner.

BP 5.4 Mon 16:00 H43

Super-resolution imaging of dynamic MreB filaments in B. Subtilis - a multiple motor driven transport? — Philipp von Olshausen[1,2] and •Alexander Rohrbach[1,2] — [1]Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany — [2]Centre for Biological Signalling Studies (bioss), University of Freiburg

The cytoskeletal protein MreB is an essential component of the bacterial cell shape generation system. By a super-resolution variant of total internal reflection microscopy using structured illumination and by 3D stacks of deconvolved epi-fluorescence microscopy, we found that inside live Bacillus subtilis cells MreB forms filamentous structures of variable lengths, typically not longer than one micrometer. These filaments move mainly perpendicular to the long bacterial axis revealing a maximum velocity at an intermediate length and a decreasing velocity with increasing filament length. Filaments move along straight trajectories, but can reverse or alter their direction of propagation. Based on our measurements, we provide a model being able to explain all observations. In this model MreB filaments mechanically couple several motors that putatively synthesize the cell wall, whereas the filaments traces mirror the trajectories of the motors. Based on this idea, we developed a mathematical model that can explain the nonlinear velocity length dependence. We deduce that the coupling of cell wall synthesis motors determines the MreB filament transport velocity, whereas the filament mechanically controls a concerted synthesis of parallel peptidoglycan (PG) strands to improve cell wall stability.

BP 5.5 Mon 16:15 H43

Mechanochemical patterning of the PAR system in *C. elegans* — •Vijay Krishnamurthy[1,2], Justin Bois[3], Frank Jülicher[1], and Stephan Grill[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany. — [2]Max Planck Institute for Molecular Cell Biology and Genetics, Pfotenhauer Straße 108, 01307 Dresden, Germany. — [3]UCLA Department of Chemistry and Biochemistry, Los Angeles, CA 90095, USA.

The polarization of partitioning defective (PAR) proteins into anterior and posterior domains is a conserved mechanism in the zygotes of *Caenorhabditis elegans*. This segregation is driven by flows established in the actomyosin cortex. Passive advection of the PARs by these flows is known to lead a transient segregation of the PAR system. However, the mechanism by which the PAR proteins regulate the cortical flows is unclear. We present a model which incorporates the feedback of the PAR concentration fields into cortical flows, via a coupling to the local myosin concentration. This leads to stable segregated states of the PAR system. Our model provides a self-consistent and closed mechanism for the polarization of the PAR-actomyosin system which compares well with the known experimental facts.

BP 5.6 Mon 16:30 H43

Cell membrane deformation and its role during cytokinesis — •Jochen A. M. Schneider[1], Andrea M. Pereira[2], Ewa Paluch[2], and Guillaume Salbreux[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Cell Biology and Genetics, Dresden, Germany

Cytokinesis, the process of physically dividing the cell at the end of mitosis, is achieved through the regulated variations of forces within the cell. A key player in this process is the cell cortex, a thin layer of actin filaments and myosin molecular motors. Recently, Sedzinski *et al.* have introduced a mathematical model to describe the role of the cell cortex in cytokinesis. The model has shown that because of the contractile behavior of the cell cortex, the cell shape can be unstable with respect to symmetry breaking, and that cell elasticity is required for cell shape stability. We present here a potential role of the cell membrane in contributing to cell elasticity. The membrane is attached to the cell cortex and has to mechanically balance the difference between extracellular and intracellular pressure. Under simple hypothesis on the membrane mechanical behavior and its area regulation by the cell, we investigate how its interaction with the cortex influences cell shape.

BP 5.7 Mon 16:45 H43

Chromosome oscillations in mammalian cells — •Federica Tavano[1], Nenad Pavin[2], and Iva M. Tolic-Norrelykke[1] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany — [2]Department of Physics, Faculty of Science, University of Zagreb, 10002 Zagreb, Croatia

Mitosis is the process by which eukaryotic cells replicate chromosomes into two identical sets that segregate to the nuclei of the two daughter cells. During mitosis, sister chromatids connect to mitotic spindle microtubules via protein complexes called kinetochores, and oscillate around the equatorial plane of the spindle. These oscillations are correlated with the microtubule plus-end dynamics. However, the mechanism of the oscillations is not known. Here we show that kinetochores in mammalian epithelial cells move roughly with a constant velocity until they switch the direction of movement. During the movement, the distance between sister kinetochores increases. During directional switches, sister kinetochores are not synchronized: The leading kinetochore stops while the trailing one continues moving, decreasing the distance between the sister kinetochores. These results suggest that the sister kinetochores are under tension during their movement, whereas they get compressed when they switch direction. Moreover, these data imply that the microtubules on the leading side undergo rescue before the microtubules on the trailing side undergo catastrophe. We propose that forces on the kinetochores synchronize microtubule dynamics, which is required for chromosome oscillations.

BP 6: Publishing in the Age of the Internet (joint with jDPG)

The two talks by the editors of Physical Review Letters and New Journal of Physics, respectively, will be followed by a general discussion. Organized by Stephan Köhler (jDPG) and Ulrich Schwarz (BP).

Time: Monday 15:30–17:30 Location: H44

Topical Talk BP 6.1 Mon 15:30 H44

Publishing in Physical Review Letters — •Karsten Kruse — Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany

Physical Review Letters (PRL) is the world's foremost physics letters journal, providing rapid publication of short reports of significant fundamental research in all fields of physics. Every year we receive around 12000 manuscripts out of which about 3500 get eventually published in PRL. This talk is intended to provide young scientists a guide for publishing in PRL. I will start by explaining the editorial process and give some practical tips on how to prepare a manuscript for PRL. Finally, I will provide an overview of features that have been put into place during the last years to make PRL's content readily available to the community. These include, for example, the option of open access, support of ORCID, "Suggestions" highlighting articles of special interest, and coverage of selected articles in "Physics", a platform notably designed for young scientists.

Topical Talk BP 6.2 Mon 16:00 H44

The Opportunities of Open Access Publishing — •Eberhard Bodenschatz — MPI Dynamics and Self-Organization, Goettingen, Germany

In my talk I shall give a review of OA as it has developed over the past years. Then I shall address future opportunities. I shall give special attention to video abstracts, to 'living paper' and novel possibilities for quality control. I shall also discuss the impact factor and other developments one may consider. I shall close my talk with a request for input and suggestions from the audience.

up to 60 min of discussion

BP 7: Symposium Magnetic Nanoparticles in Biomedical Diagnostics and Therapy (SYBD, joint with MA, CPP and ST)

Time: Monday 15:00–17:30 Location: H1

Invited Talk BP 7.1 Mon 15:00 H1

Functionalization and Pharmaceutical Aspects of Magnetic Nanoparticles (Magnetic Carriers) — •Urs O. Häfeli — University of British Columbia, Faculty of Pharmaceutical Sciences, Vancouver, BC, Canada

This presentation will review the properties and applications of modern magnetic nanoparticles and microspheres for application as nanomedical agents, both for diagnosis and therapy of different diseases. Basic applications in biomedicine and industry, clinical applications, as well as open questions regarding risk and economy will be discussed.

Important features make nanoparticles and microspheres interesting for in vitro and in vivo applications: biocompatibility, biodegradability, transport capacity, surface functionalization with biological active molecules, binding of fluorescent and radioactive markers, increasing surface area with decreasing size, organ-specific targeting.

To further increase the particles efficiency, further work is necessary

in the design of effective magnetic targeting systems, the coatings for optimized particles, the choice of targeting ligands, as well as the maximization of the particles* magnetic moment. Altogether, exciting in vivo applications are possible in magnetic guidance and controlled delivery of drugs, genetic material, and stem cells, in addition to their current use for the contrast enhancement in magnet resonance imaging and local hyperthermia treatment of cancer.

For additional information about the scientific field of magnetic particles, please check out www.magneticmicrosphere.com.

Invited Talk BP 7.2 Mon 15:30 H1

Fluid mechanical aspects of therapeutic application of suspensions of magnetic nanoparticles — •Stefan Odenbach — TU Dresden, Chair of Magnetofluiddynamics, Measuring and Automation Technology, Dresden, Germany

One of the promising approaches for the use of magnetic nanoparticles in cancer therapy is a technique called magnetic drug targeting. Here a chemotherapeutic agent is attached to the surfactant of the magnetic particles and a water based suspension of these drug carrying particles is injected into a supplying artery of the tumour. Using appropriate magnetic fields magnetic forces can be generated targeting the particles towards the tumour. As a result chemotherapy without side effects is envisaged.

Within the talk some of these aspects resulting from fluid mechanics will be highlighted and discussed. On the one hand we'll have a look on model experiments studying the targeting process for the magnetic fluid and its dependence on magnetic field configuration. The respective experiments presented will be accompanied by numerical simulations which are intended to provide a tool for future clinical applications allowing an optimal field control on the basis of angiographic data.

The second part of the talk will focus on magnetic field effects concerning the viscosity of ferrofluids for biomedical applications as well as on changes of the flow behaviour of blood with suspended magnetic particles in a field and will thus highlight investigations on fundamental fluid properties being important for experiments as well as simulations.

Invited Talk BP 7.3 Mon 16:00 H1

Magnetic Particle Imaging: A new Medical Imaging Modality — •Thorsten Buzug — Institute of Medical Engineering, University of Lübeck, Germany

Recently, magnetic particle imaging (MPI) has been introduced as a novel method for direct measurement of the spatial distribution of superparamagnetic iron oxide nanoparticles (SPIOs) that are used as tracer material. The SPIOs are subjected to a sinusoidally oscillating magnetic field and respond with a nonlinear change in magnetization. The acquired induction signal contains harmonics of the fundamental excitation frequency, which are subsequently used for determination of the spatial particle distribution and concentration. For spatial encoding a magnetic gradient field (the selection field) is superimposed onto the sinusoidal excitation field (the drive field) such that a field-free point (FFP) is established at a desired location within the field of view. Nanoparticles located near the FFP contribute to the signal generation, whereas particles that are far from the FFP are in saturation and cannot contribute. Image reconstruction from the measured induction signals can be seen as the solution for the corresponding inverse problem. In this talk, the state of the art in magnetic coil design for MPI is discussed. With a new symmetrical arrangement of coils, a field-free line can be produced that promises a significantly higher sensitivity compared with the standard arrangement for an FFP. Additionally, an alternative single-sided coil assembly is presented for the use in hand-held applications.

Invited Talk BP 7.4 Mon 16:30 H1

Superparamagnetic iron oxide nanoparticles for MR-visible mesh implants and novel drug targeting models — •Ioana Slabu[1,2], Anjali Roeth[3], Christiane Kuhl[4], Thomas Schmitz-Rode[1], and Martin Baumann[1] — [1]Applied Medical Engineering, Medical Faculty, Helmholtz Institute, RWTH Aachen University, Germany — [2]II. Physical Institute, RWTH Aachen University, Germany — [3]Department of Surgery, University Hospital, RWTH Aachen University, Germany — [4]Department of Radiology, University Hospital, RWTH Aachen University, Germany

Two major medical applications of superparamagnetic iron oxide (SPIO) nanoparticles are presented, exploiting their physical and magnetic properties to combine diagnostic and therapeutic functionalities. First, the concept and realization of a (magnetic resonance) MR-visible mesh implant is described which facilitates an accurate determination of complications after mesh implantation by means of MR imaging. The visual investigation of the implant helps to reduce the exposure of the patient to redundant surgery interventions. Second, magnetic drug targeting approaches based on numerical simulations for cancer therapies are developed. A new concept of placing an array of permanent magnets and coils inside hollow organs of the body very close to tumors is described. In this way, a stronger magnetic field and its higher gradient are achieved in the tumor. This allows a local accumulation of administrated SPIO nanoparticles with bounded drugs and enhances the efficiency of the therapy. First simulation results are already applied and validated in animal trials.

Invited Talk BP 7.5 Mon 17:00 H1

Magnetic measurement techniques assisting biomedical applications of magnetic nanoparticles — •Lutz Trahms — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, D-10587 Berlin, Germany

Due to their biocompatibiliy and their small size, magnetic nanoparticles (MNP) made of iron oxide can be guided to virtually every biological environment. MNP are susceptible to external magnetic fields and can be used, e.g., for drug transportation, heat generation or as contrast agents for MRI. All these applications require knowledge about the magnetic properties and, when applied in-vivo, quantitative knowledge about the spatial distribution in the living tissue. In this contribution, I will report on a number of magnetic measurement techniques that provide such information, i.e. in particular on conventional susceptibility measurements M(H), magnetorelaxometry, and magnetic particle spectroscopy. In addition, I will give examples how these analytical or spectroscopic techniques can be modified to obtain quantitative spatial information.

BP 8: Posters: Proteins

Time: Monday 17:30–19:30 Location: Poster B2

BP 8.1 Mon 17:30 Poster B2

Effects of ligand binding on cyclophilin A: experimental and computational studies — •Jack Heal[1], Stephen Wells[2], Claudia Blindauer[3], Rudolf Römer[2], and Robert Freedman[4] — [1]MOAC Doctoral Training Center, University of Warwick, Coventry, UK, CV4 7AL — [2]Department of Physics, University of Warwick, Coventry, UK, CV4 7AL — [3]Department of Chemistry, University of Warwick, Coventry, UK, CV4 7AL — [4]Department of Life Sciences, University of Warwick, Coventry, UK, CV4 7AL

Cyclophilin A is an enzyme which plays a role in the folding of proteins. It also binds to and aids the function of the immunosuppressant drug cyclosporin A as well as binding to the HIV-1 capsid protein. We use the computational tools FIRST and FRODA to model the flexibility and motion of cyclophilin A in order to predict the results of hydrogen-deuterium exchange NMR (HDX) experiments. The rigidity analysis software FIRST can be used to predict the 'folding cores' of proteins identified as slowly exchanging residues in HDX. This prediction is improved using the protein mobility software FRODA. We are using these methods to investigate the effect of ligand binding on cyclophilin A computationally and experimentally.

BP 8.2 Mon 17:30 Poster B2

Peptide interactions with metal surfaces — •Isidro Lorenzo[1], 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

Understanding and controlling protein-surface interactions is gaining increasing fundamental scientific interest, such as in medical, diagnostic and biotechnology applications.

In this work we want to provide a characterization of peptide / gold interactions at a molecular level in order to explain and interpret recent

surface experiments [1].

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. We have employed a recently developed force field which has been extensively tested in biomolecular-inorganic interactions [3]. This has permitted to identify the most favorable binding modes on the different surfaces. Both neutral and zwitterionic forms for each peptide are analyzed .

[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

[3] Heinz H, Farmer BL, Pandey RB, Slocik JM, Patnaik SS, Pachter R, Naik RR. J. Am. Chem. Soc. 2009, 131, 9704-9714

BP 8.3 Mon 17:30 Poster B2

Time-Resolved FTIR Difference Spectroscopy of Vibrational Control Experiments on Bacteriorhodopsin — •Christian Bauer[1,2], Michael Gensch[2], and Joachim Heberle[1] — [1]Freie Universität Berlin — [2]HZDR

We aim at investigating how photoreactions of proteins can be controlled by means of intense THz radiation tuned in resonance to specific vibrational modes, much in analogy to coherent control experiments conducted by fs NIR laser pulses [1]. Bacteriorhodopsin is the sole protein of the purple membrane of the archaebacterium Halobacterium salinarum [2]. Upon illumination, its chromophore retinal isomerizes around the C13-C14 double bond [3] and the protein undergoes a sequence of intermediate states which is called a photocycle. For investigation of this photocycle we combined a time-resolved IR difference spectroscopic setup using the step-scan technique [4] with intense, tunable narrow bandwidth THz radiation at the ps beamline of the THz free electron laser FELBE [5]. In our experiments, the photoreaction is initiated by a visible laser pulse as in standard experiments, but then the sample will be irradiated by a THz pulse from the free electron laser tuned into resonance with low-energy vibrational modes which is supposed to influence the photoreaction [1].

[1] Prokhorenko V.I. et al. Science 313, 1257 (2006) [2] Oesterhelt D. et al. PNAS 70, 2853 (1973) [3] Stoeckenius W. et al. Biophys. Struct. Mech. 3, 65 (1977) [4] Radu I. et al. Photochem. Photobiol. Sci. 8, 1517 (2009) [5] Bauer, C. et al. Journal of Physics Conference Series, 359, 012011 (2012)

BP 8.4 Mon 17:30 Poster B2

Dual-Color Fluorescence Cross-Correlation Spectroscopy of the macromolecular spliceosomal complex — •Mira Prior[1], Thomas Ohrt[2], Julia Dannenberg[2], Ingo Gregor[1], Reinhard Lührmann[2], and Jörg Enderlein[1] — [1]Drittes Physikalisches Institut-Biophysik, Göttingen — [2]Max Planck Institut für Biophysikalische Chemie, Göttingen

The spliceosome is the cellular machinery responsible for removing non-coding introns from precursor mRNA. During its catalytic action the spliceosome undergoes compositional and conformational changes. We are investigating the conditions for recruitment and release of particular proteins during the splicing steps. We determine how the changes occur (stepwise or in a correlated manner) and the roles of certain spliceosomal RNA helicases in the restructuring of the complex. The spectroscopic method we use is Dual-Color-Fluorescence Cross-Correlation Spectroscopy (2-color-FCCS) which allows for studying structural and dynamical properties of proteins. We observed the thermally stable splicing factor Cwc25. We could determine, under which conditions it binds to the complex, when it is released and the conditions for stable binding of Cwc25 to the spliceosome. By measuring several mutants we could answer the question whether Cwc25 is released before or during the second catalytic step. Furthermore, we detected the binding of the proteins Slu7 and Prp16. These proteins are necessary for the second catalytic step and are involved in the binding behavior of Cwc25.

BP 8.5 Mon 17:30 Poster B2

Tip-Enhanced Raman Spectroscopy on Membrane Proteins — •Elmar Hassan Hubrich and Joachim Heberle — Freie Universität Berlin, Department of Physics, Exp. Molecular Biophysics, Arnimallee 14, 14195 Berlin, Germany

Membrane proteins are essential parts of organisms and involved in cell processes such as transport, signal transmission, catalysis, cell adhesion and (photo-)synthese. Obtaining information on molecular level of such proteins is one of the major tasks in modern biophysics.

In these research, we attempt to develop tip-enhanced Raman spectroscopy (TERS), as a tool to study structure and function of single proteins. TERS combines high spatial resolution of AFM with structural sensitivity of surface-enhanced Raman spectroscopy (SERS). Using a gold-coated AFM tip, it is possible to measure Raman signals with a spatial resolution up to 20 nm.

Additionally to imaging a SERS probe (=TERS), AFM can be used induce and messure physical force. The force is used to achieve structural changes or even unfolding of a protein, namely single-molecule force spectroscopy (SMFS).

SERS can be used to achieve molecular level information while AFM applies a physical force. In order to detect single proteins we use the enhancement of SERS. The Raman signal is enhanced in the vicinity of silver- or gold-coated surfaces (here: the AFM tip).

Up to now, this technique is mainly applied to inorganic samples. Here, we introduce the experimental setup and discuss the application of TERS to the investigation of membrane proteins.

BP 8.6 Mon 17:30 Poster B2

Dynamic force spectroscopy on the binding of monoclonal antibodies to tau peptides — •Carolin Wagner[1], David Singer[2], Tim Stangner[1], Christof Gutsche[1], Ralf Hoffmann[2], and Friedrich Kremer[1] — [1]Leipzig University, Department of Molecular Physics, Leipzig, Germany — [2]Leipzig University, Institute for Bioanalytical Chemistry, Leipzig, Germany

Optical tweezers-assisted dynamic force spectroscopy (DFS) is employed to investigate specific receptor/ligand bindings on the level of single binding events [1]. Here, the binding of the phosphorylation-specific antibody HPT-101, to synthetic tau-peptides with two potential phosphorylation sites (Thr231 and Ser235) is analyzed. According to ELISA-measurements, the antibody binds only specificly 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 like the lifetime of the bond without force, the characteristic length and the free energy of activation are determined for all interactions. The longest lifetime is obtained for the specific binding to the double-phosphorylated peptide. Furthermore we introduce a method to estimate the relative affinity of the bonds from dynamic single-molecule experiments. The result is in accordance with the ELISA measurements.

[1] C. Wagner et al., Soft Matter, 2011, 7 (9), 4370 - 4378

BP 8.7 Mon 17:30 Poster B2

Hydrophobin adsorption to the air/water interface: Unusual adsorption kinetics and their origin — •Jonas Raphael Heppe[1], Sebastian Backes[1], Hendrik Hähl[1,2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, 66041 Saarbrücken, Germany — [2]University of Zurich, Institute of Physical Chemistry, 8057 Zürich, Switzerland

Adsorption of proteins to the interface between water and other liquids (e.g. oil) or air is of major technological interest. Adsorbed proteins stabilize this interface and hence serve as emulsifying or foaming agent. In food industry, this characteristic is used for products such as milk, beer, or coffee. To optimize production sequences and to be able to give predictions, a deeper understanding of the competitive processes leading to the final adsorbate is necessary. Hydrophobins are a class of proteins that have emerged to have a high technological potential and may also serve as ideal model candidates. Produced by filamentous fungi, hydrophobins are extremely conformationally stable, particularly amphiphilic, highly surface active, and form ordered layers at the water surface [1,2]. We studied wild types and specifically designed mutants of hydrophobins featuring different properties, sizes, and forms. To access the processes involved in the adsorption, we used ellipsometry to record in situ the adsorbed amount at different ambient and solution conditions. Our results reveal adsorption kinetics that significantly differ from that of other systems and cannot be explained by conventional theoretical models. [1] S. Varjonen et al., Soft Matter 7 (2011) 2402 [2] T. Hakala et al., RSC Advances 2 (2012) 9867

BP 8.8 Mon 17:30 Poster B2

Demonstration of catch bonds between glycosaminoglycan and positively charged hydrophilic domain from the cell surface sulfatase Sulf1 — •A.-K. Möller, A. Harder, F. Milz, P. Neuhaus, V. Walhorn, Th. Dierks, and D. Anselmetti — Bielefeld University, Germany

The unique hydrophilic domain (HD) found in the human sulfatases

Sulf1 and Sulf2 is responsible for targeting Sulf1 to the cell surface by interacting with its substrate. The enzymatic activity of Sulf1 is known to be specifically directed towards the 6-O-sulfation sites of heparan sulfate (HS) within highly sulfated regions of the glycosaminoglycan. Since the function of many growth and differentiation factors is regulated by HS, which acts as an essential cofactor for the interaction with cell surface localized receptors, these molecular and cellular interactions have great influence on embryogenesis and homeostasis. We used single-molecule AFM force spectroscopy (SMFS) to investigate the specificity of the interaction between HD and the glycosaminoglycans dermatan sulfate (DS) as well as heparin (Hep), the latter serving as model for the interacting regions of HS due to its high sulfation. Thereby we found an increased binding probability by increasing pulling velocity which is similar to experiments on P-selectin and its counterligand PSGL-1. We additionally applied AFM force clamp experiments to measure the force-dependent lifetimes of the interaction. We observed prolonged bond lifetimes under higher tensile forces between 10-20 pN, which we will discuss within the framework of molecular catch bonds.

BP 8.9 Mon 17:30 Poster B2

Investigation of enzyme complex dynamics via atomic force microscopy — •Mitja Platen[1], Sabin Prajapati[2], Kathrin Schröder-Tittmann[2], Kai Tittmann[2], and Iwan Schaap[1] — [1]III. Physikalisches Institut, Georg August Universität Göttingen, Germany — [2]Albrecht-von-Haller-Institut, Georg August Universität Göttingen, Germany

The pyruvate dehydrogenase multienzyme complex (PDHc) links glycolysis to the citric acid cycle by converting central metabolite pyruvate into acetyl-CoA, a building block for many fundamental metabolic pathways. The core of the human PDHc consists of 60 dihydrolipoamide acetyltransferase enzymes (E2), which assemble into a 50 nm diameter dodecahedral structure. A key trait vital to PDHc function is the flexibility of the N-terminal "swinging lipoyl domain" of E2, which is capable of reaching the active sites of all proximal enzyme components. Although low resolution structural information about the PDHc is available, the underlying dynamics of catalysis, in particular substrate channeling, is not understood.

To be able to observe the structure of single PDH complexes we are applying AFM in liquid. Ultimately, we aim to observe the core dynamics at real-time via optimization of imaging techniques by exploring the limits of amplitude and frequency modulation as well as jumping mode AFM. We will present our approach to maximize the spatial and temporal resolution and will present our first results on this enzyme complex.

BP 8.10 Mon 17:30 Poster B2

Self-diffusion of proteins in solution close to a salt-induced phase transition — •Marco Grimaldo.[1], Vincent Glenisson[1,2], Marcus Hennig[1], Felix Roosen-Runge[1], Fajun Zhang[1], Tilo Seydel[2], and Frank Schreiber[1] — [1]Fakultät für Physik - Universität Tübingen, Auf der Morgenstelle 10, D-72076 Tübingen, Germany — [2]Institut Laue-Langevin, B.P. 156, F-38042 Grenoble, France

A reentrant phase diagram is observed in aqueous solutions of Bovine Serum Albumin (BSA) upon addition of a trivalent salt (Yttrium Chloride) at concentration c_s . In particular, increasing c_s for a certain protein concentration c_p, a phase transition occurs at a characteristic concentration c_s^*. For $c_s > c_s^*$ macroscopic aggregates form [1]. Measurements on the neutron backscattering spectrometers IN10 and IN16 at the Institute Laue-Langevin have shown that the short time self-diffusion of the proteins in such system decreases when c_s approaches c_s^*. For a better understanding of this phenomenon, data has been collected also with the backscattering spectrometer BASIS (SNS, ORNL) in order to increase the accessible time scales. In presenting the data analysis we will also discuss the method adopted to obtain consistent results from different quasi-elastic neutron scattering (QENS) instruments.

[1] Zhang et al. PRL 101 (2008) 148101
[2] Roosen-Runge et al. PNAS 108 (2011) 11815

BP 8.11 Mon 17:30 Poster B2

Biophysical Characterization of the Platelet Factor 4-Heparin Complex Responsible for Heparin-induced Thrombocytopenia — •Martin Kreimann[1], Werner Weitschies[2], Andreas Greinacher[3], and Mihaela Delcea[1] — [1]ZIK HIKE, University of Greifswald, Greifswald, Germany — [2]Department of Biopharmaceutics and Pharmaceutical Technology, University of Greifswald, Greifswald, Germany — [3]Institute for Immunology and Transfusion Medicine, University of Greifswald, Greifswald, Germany

The human protein Platelet Factor 4 is known to form complexes with the polysaccharide heparin when the latter is administered as an anticoagulant during cardiac surgery. This complex is responsible for the fatal adverse effect known as heparin-induced thrombocytopenia. The study of the PF4-heparin complex is primordial because heparin remains one of the most frequently used anticoagulants. To determine the biophysical basis of the PF4-heparin complexes, the binding interaction between PF4 and heparin was investigated by Isothermal Titration Calorimetry and Quartz Crystal Microbalance and the formed complexes were imaged by Atomic Force Microscopy. Our data shows that the binding of PF4 to heparin is mainly driven by electrostatic interactions. Hydrophobic interactions and conformational restrictions only play a minor role in the energetics of the process. AFM imaging shows that the height of PF4 molecules appearing as single features is reduced when complexed with heparin.

BP 8.12 Mon 17:30 Poster B2

The dynamics and flexibility of protein disulphide-isomerase (PDI): simulations predict experimentally-observed domain motions — J Emilio Jimenez-Roldan[1], Moitrayee Bhattacharyya[2], Stephen A Wells[1], •Rudolf A Römer[1,4], Saraswathi Vishweshwara[2], and Robert B Freedman[3] — [1]Department of Physics, The University of Warwick, Coventry, UK — [2]Department of Biochemistry, IISc, Bangalore, India — [3]School of Life Sciences, The University of Warwick, Coventry, UK — [4]Centre for Scientific Computing, The University of Warwick, Coventry, UK

We simulated the mobility of the folding catalyst, protein disulphide-isomerase (PDI), by molecular dynamics and by a rapid approach based on flexibility analysis. We analysed our simulations using measures of backbone movement, relative positions and orientations of domains, and distances between functional sites. Despite their different assumptions, the two methods are surprisingly consistent. Both methods show that motion of domains is dominated by hinge and rotation motion of the a and a' domains relative to the central b-b' domain core. Both methods identify the a' domain as showing the greatest intra-domain mobility. However, only the flexibility method, which requires 10^4-fold less computer power, predicts some large-scale features of inter-domain motion that have been observed experimentally. We conclude that the methods provide complementary insight into the motion of this large protein and detailed structural models that characterise its functionally-significant conformational changes.

BP 8.13 Mon 17:30 Poster B2

Proteinfoldingdynamics of hPin1 WW domain studied by single molecule FRET. — •Phillip Kroehn and Jörg Enderlein — Universität Göttingen, Deutschland

Georg-August-Universität Göttingen, Friedrich-Hundt-Platz 1, 37077 Göttingen

Förster resonance energy transfer (FRET) is the commonly used method to study fast molecular dynamics in a scale of 1-10 nanometer.

The energy transfer between a donor molecule and an acceptor molecule e.g. organic fluorophore by dipole interaction depends strongly on the distance between them.This phenomenon offers the possibility to use FRET as a nonoscopic ruler.

The primary structure of small soluble proteins is believed to contain all chemical information necessary for proper folding to its native state.The hPin1 WW Domain is a 40 Amino acid all beta sheet protein that consist of three strands. It can be seen as a simple model system to investigate the formation of beta fold secondary structures.

The hPin1 is involved in cell cycle regulation, the WW domain at the N terminal site of hPin1 is able to bind to proline rich ligands. Due to its high thermal stability the hPin1 WW domain is suitable for folding/unfolding studies.

BP 8.14 Mon 17:30 Poster B2

Reaction mechanism of the enzyme PHM: quantum tunneling and origin of kinetic isotope effects — •Enrique Abad, Judith Rommel, and Johannes Kästner — Computational Biochemistry Group, Institut für Theoretische Chemie, Universität Stuttgart, Stuttgart, Germany

Copper proteins catalyze important biochemical reactions, in particular in the nervous system of higher eukaryotes. PHM is a binuclear Cu protein that stereospecifically hydroxylates one C-H bond of small

peptides (such as oxytocin), as a intermediate step for its later amidation.

The reaction mechanism of PHM is still not understood. Several proposals have been made [1, 2], but they have not taken explicitly into account the strong kinetic isotope effects (KIE) present in this reaction [3]. In this work, we perform QM/MM calculations at the DFT level, and tunneling rates for a set of possible reaction paths. We suggest a new reaction mechanism in which tunneling of a H atom is crucial for explaining the KIE.

[1] A. Crespo, et al. (2006) J. Am. Chem. Soc. 128, 12817
[2] P. Chen and E. I. Solomon (2004) J. Am. Chem. Soc. 126, 4991
[3] W. A. Francisco, et al. (2002) J. Am. Chem. Soc. 124, 8194

BP 8.15 Mon 17:30 Poster B2

Intracellular crowding effects on cellular metabolism — •Florencia Noriega[1], Márcio Argollo[2], and Alexei Vázquez[3] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]UFF, Niterói, Brazil — [3]UMDNJ-Robert Wood Johnson Medical School, New Brunswick, USA

70 to 90% of the dry weight in the cell is occupied by the 3 types of macromolecules: DNA, RNA and proteins. The high density levels of macromolecular components in the cellular cytoplasm, also known as molecular crowding, is important for the development of many cellular functions like protein folding, protein protein association and dissociation, biochemical reactions rates, molecular diffusion within the cell, among others. It has been shown that molecular crowding acts also at a global scale limiting the cytoplasm solvent capacity [1], due to the limited available volume in the cell. To estimate the molecular crowding global effect on a simple cellular metabolic network we develop a flux balance model considering the macromolecular concentrations at different growth rates and determine the metabolic steady states, given by the fluxes of the metabolic reactions. We found a metabolic switch, activation and inactivation of the fluxes, in a simple cell model, when is shifted from low to high growth rates. Such behavior is observed in yeast cells and is called crabtree effect, where at high growth rates acetate compound is secreted by the cell, indicating the activation of the fermentation pathway of glucose consumption.

[1] Beg QK, et al.(2007) PNAS 104: 12663-12668. Vázquez A, et al. (2008) BMC Systems Biol 2: 7.

BP 8.16 Mon 17:30 Poster B2

Robust signatures in the current-voltage characteristics of DNA molecules oriented between two graphene nanoribbon electrodes — Carlos J. Paez[1], Peter A. Schulz[1,2], Neil Wilson[3], and •Rudolf A. Römer[3,4] — [1]Instituto de Fisica Gleb Wataghin, Universidade Estadual de Campinas, 777 Cidade Universitaria 13083-859 Campinas, SP Brazil — [2]Faculdade de Ciencias Aplicadas, Universidade Estadual de Campinas, 13484-350 Limeira, SP Brazil — [3]Department of Physics, University of Warwick, Coventry, CV4 7AL, UK — [4]Centre for Scientific Computing, University of Warwick, Coventry, CV4 7AL, United Kingdom

In this work we numerically calculate the electric current through three kinds of DNA sequences (telomeric, λ-DNA, and p53-DNA) described by different heuristic models. A bias voltage is applied between two zig-zag edged graphene contacts attached to the DNA segments, while a gate terminal modulates the conductance of the molecule. We show that a telomeric DNA sequence, when treated as a quantum wire in the fully coherent low-temperature regime, works as an excellent semiconductor. Clear steps are apparent in the current-voltage curves of telomeric sequences and are present independent of lengths and sequence initialisation at the contacts. independent of length and sequencing initialisation at the contacts. The difference between telomeric DNA and other DNA, such as λ-DNA and DNA for the tumour suppressor p53, is particularly visible in the length dependence of the current.

BP 8.17 Mon 17:30 Poster B2

Video-based and interference-free axial force detection and analysis for optical tweezers — •Sebastian Knust, Andre Spiering, Andy Sischka, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

For measuring the minute forces exerted on single molecules during controlled translocation through nanopores with sub-piconewton precision, we have developed a video-based axial force detection and analysis system for optical tweezers [1].

As the bandwidth of the system is not as high as in backscattered light based systems, we integrated Allan variance analysis [2] for trap stiffness calibration.

Upon manipulating a microbead in the vicinity of a weakly reflecting surface with simultaneous axial force detection, interference effects have to be considered [3]. We measured and analyzed the backscattering light properties of polystyrene and silica microbeads with different diameters and propose distinct and optimized experimental configurations (microbead material and diameter) for minimal light backscattering and virtually interference-free microbead position detection.

As a proof of principle, we investigated the nanopore threading forces of a single dsDNA strand attached to a microbead with an overall force resolution of ± 0.5 pN at a sample rate of 123 Hz.

[1] S. Knust et. al., Rev. Sci. Instrum. **83**, 103704 (2012)
[2] B. Lansdorp, O. Saleh, Rev. Sci. Instrum. **83**, 025115 (2012)
[3] A. Sischka et. al., Rev. Sci. Instrum. **79**, 63702 (2008)

BP 8.18 Mon 17:30 Poster B2

Mechanical properties of sister chromatids studied by a polymer model — •Sebastian Isbaner, Yang Zhang, and Dieter W. Heermann — Institute for Theoretical Physics, Heidelberg University, Germany

A chromosome in metaphase consists of two highly condensed sister chromatids forming a chromosome. In experiments, chromosomes show characteristic force-extension curves with a linear region followed by a plateau. However, where and how exactly sister chromatids are linked to each other and how these links influence their overall organization and mechanical properties is still not well understood. In this work, we use a dynamic folding model for mitotic chromatids and investigate the influence of dynamic cross-links between two model sister chromatids. Our results show that the number of sister links has severe influence on the overall organization of the model chromatids. Too few cross-links cause the model chromatids to drift apart due to entropic repulsion, whereas many links result in an agglomeration. We characterize these different states in a phase diagram. We further investigate the force-extension behavior and find that it qualitatively reproduces experimental results. Our results also demonstrate that inter sister cross-links decrease the elasticity compared to isolated model chromatids. In summary, we show that only a limited range for the concentration of inter sister chromatid cross-links can exist to result in observed chromosome shapes and our model is able to reproduce experimental findings for the elasticity of chromosomes.

BP 8.19 Mon 17:30 Poster B2

Computational Analysis of Co-transcriptional Riboswitch Folding — •Benjamin Lutz[1,2], Abhinav Verma[1], and Alexander Schug[1] — [1]Steinbuch Centre for Computing (SCC), Karlsruher Institut für Technologie (KIT), 76128 Karlsuhe, Germany — [2]Fakultät für Physik, Karlsruher Institut für Technologie (KIT), 76128 Karlsruhe, Germany

Structured RNA in non-coding regions often plays crucial regulatory roles. Riboswitches are an important example that can prevent expression of the downstream gene by terminating transcription or translation. Typically, one out of two distinct conformations is formed depending on ligand binding. The extrusion out of RNA polymerase (RNAP) takes place at time scales comparable to those of folding and binding. We investigate these interdependent processes by simulating the extrusion out of RNAP and concurrent folding for the SAM-I and adenine riboswitches with molecular dynamics. Atomically resolved structure-based models reduce the computational effort sufficiently to simulate different extrusion velocity scenarios. Depending on the scenario, we observe and quantify different pathways in structural formation. Considering the inherent link of folding and binding, this underlines modulation of extrusion velocity as another degree of freedom in genetic evolution. Our simulational findings therefore complement experimental measurements to understand the dynamic behavior of nascent RNA.

BP 8.20 Mon 17:30 Poster B2

Ubiquitin dynamics in complexes investigated using Molecular Dynamics simulations — •Jan Henning Peters and Bert de Groot — Max Planck lnstitute für Biophysikalische Chemie, Göttingen, Germany

Protein-protein interactions play an important role in all biological processes. However, the principles underlying these interactions are only beginning to be understood. Ubiquitin is a small signalling protein that is covalently attached to different proteins to mark them for degradation, regulates transport and other functions. As such, it in-

teracts with and is recognised by a multitude of other proteins. We have conducted molecular dynamics simulations of ubiquitin in complex with several different binding partners on a microsecond timescale and compared them with ensembles of unbound ubiquitin to investigate the principles of their interaction and determine the influence of complex formation on the dynamic properties of this protein. Along the main mode of fluctuation of ubiquitin, binding in most cases reduces the conformational space available to ubiquitin to a subspace of that covered by unbound ubiquitin. This behaviour can be well explained using the model of conformational selection. For lower amplitude collective modes, a spectrum of zero to almost complete coverage of bound by unbound ensembles was observed. The significant differences between bound and unbound structures are exclusively situated at the binding interface.

BP 8.21 Mon 17:30 Poster B2

Discerning overall and internal motion of flexible molecules — •Florian Sittel and Gerhard Stock — University of Freiburg

Classical molecular dynamics (MD) simulations allow us to study the structure and dynamics of biomolecules in microscopic detail. To extract the internal molecular motion from an MD trajectory, first the overall motion of the molecule needs to be removed. This procedure is well established in the case that the molecule is almost rigid, i.e. if the vibrational dynamics is well described by small-amplitude motion around an equilibrium structure. In the case of a flexible molecule, however, the transformation does not completely decouple internal and rotational motion due to rotovibrational coupling. In this work, we study the range of validity and applicability of commonly used rotational fitting techniques. To this end, we adopt previously performed MD simulations of polyalanine and villin and compare their conformational distribution in internal and Cartesian coordinates. The study reveals that the free energy landscape of a Cartesian PCA can exhibit remarkable artifacts. Cartesian coordinates on the other hand, may be superior for the study of small-amplitude functional motions in proteins.

BP 8.22 Mon 17:30 Poster B2

Langevin simulations of proteins using models in generalized coordinates — •Sina Zendehroud, Anne Müller, and Martin E. Garcia — Theoretische Physik, Fachbereich 10, Universität Kassel. Kassel, Germany

Using the the coarse-grained protein model developed by Nan-Yow Chen et al. [Phys. Rev. Lett. 96, 078103 (2006)], we derived the Langevin equation of motion in generalized coordinates, namely the Ramachandran angles. We developed a code to integrate the aforementioned equation for small real proteins. The interaction potential does not need any a priori information about the native conformation. We have studied the folding behavior of different proteins.

BP 8.23 Mon 17:30 Poster B2

Langevin simulations of conformational changes in proteins under non-equilibrium conditions — •Anne Müller, Bernhard Reuter, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Fachbereich 10, Kassel, Germany

Using the potential of a coarse-grained model of proteins developed by Nan-Yow Chen et al. [PhysRevLett.96.078103(2006)], we developed a program to simulate the folding dynamics of small, real proteins through integration of the Langevin equation of motion. The force field does not need any a priori information about the native state and is known to be able to describe the folding of proteins to both alpha-helices and beta-sheets. We have studied the folding behavior of proteins which present both secondary structures in their native state. In particular we investigated the influence of temperature gradients on the dynamics of the proteins during conformational changes.

BP 8.24 Mon 17:30 Poster B2

Adjusting a Langevin model to Molecular Dynamics — •Norbert Schaudinnus[1], Andrzej Rzepiela[1], Rainer Hegger[2], and Gerhard Stock[1] — [1]Biomolecular Dynamics, Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freibur — [2]J.W. Goethe University, Institute for Physical and Theoretical Chemistry, Max-von-Laue-Str. 7, 60438 Frankfurt/Main

Molecular Dynamics simulations (MD) are nowadays routinely used to investigate the behaviour of proteins, employing huge amounts of resources to propagate the Newtonian equations of motion for each atom. The Langevin formalism provides a method to recover those dynamics, based on a reduced subset of collective coordinates. Describing the time evolution as a superposition of drift and diffusive motion, the Langevin approach has been shown to correctly reproduce the conformational dynamics of polyalanines [1]. Using local estimates to compute the corresponding fields from MD trajectories, the method contains parameters, which determine the accuracy of the Langevin approach. We investigate this dependence providing a strategy to optimize the Langevin technique. We further demonstrate a method to reduce the amount of underlying data used to compute our estimates in a reliable way to further increase the efficiency of our method. We show the application of our method for various peptide systems. [1] R. Hegger and G. Stock, J. Chem. Phys. 130, 034106 (2009)

BP 8.25 Mon 17:30 Poster B2

Thermal, Autonomous Replicator Made from Transfer RNA — Hubert Krammer, •Friederike M. Möller, and Dieter Braun — Systems Biophysics, Physics Department, Center for Nanoscience, Ludwig Maximilians Universität München, Amalienstrasse 54, 80799 München, Germany

Evolving systems rely on the storage and replication of genetic information. Here we present an autonomous, purely thermally driven replication mechanism. A pool of hairpin molecules, derived from transfer RNA replicates the succession of a two-letter code. Energy is first stored thermally in metastable hairpins. Thereafter, energy is released by a highly specific and exponential replication with a duplication time of 30 s, which is much faster than the tendency to produce false positives in the absence of template. Our experiments propose a physical rather than a chemical scenario for the autonomous replication of protein encoding information in a disequilibrium setting.

BP 8.26 Mon 17:30 Poster B2

Analyzing protein folding by high-throughput simulations — •Claude Sinner[1,2], Benjamin Lutz[1,2], Abhinav Verma[1], and Alexander Schug[1] — [1]Steinbuch Centre for Computing (SCC),Karlsruher Institut für Technologie (KIT), 76128 Karlsuhe, Germany — [2]Fakultät für Physik, Karlsruher Institut für Technologie (KIT), 76128 Karlsruhe, Germany

Molecular Dynamics allows investigating the dynamical properties of biomolecules. Protein folding simulations are computationally challenging when simulating all involved (solvent) atoms considering timescales of ms or slower. Native structure based models (SBM,'Go-models') reduce computational complexity and have shown to be a robust and efficient way for exploring the protein folding process. They are based on energy landscape theory and the principle of minimal frustration. Using this framework, we simulate protein folding for a large set ($\sim$ 200) of non-homologous monomeric proteins sized from 50-150 amino acids in coarse-grained simulations. A fully automatized workflow implemented with the help of ESBMTools guides these simulations. From the simulations, we extract typical folding properties like phi-values, folding free energy landscape and transition state ensembles. We repeat the simulations for a variant SBM with flavored contact strengths pending on amino acid composition. The resulting database estimates the robustness of folding parameters, quantifies the folding behavior, compares the behavior to existing experimental data and can serve as a baseline for comparison to future experiments or simulations of protein folding.

BP 8.27 Mon 17:30 Poster B2

Inhibition of HIV-1 protease: the rigidity perspective — •Jack Heal[1], Emilio Jimenez-Roldan[2,3], Stephen Wells[2], Robert Freedman[3], and Rudolph Römer[2] — [1]MOAC Doctoral Training Center, University of Warwick, Coventry, UK, CV4 7AL — [2]Department of Physics, University of Warwick, Coventry, UK, CV4 7AL — [3]Department of Life Sciences, University of Warwick, Coventry, UK, CV4 7AL

HIV-1 protease is a key drug target due to its role in the life-cycle of the HIV-1 virus. There are more than 200 high resolution ($\leq$ 2 Å) X-ray crystal structures of the enzyme in complex with a variety of ligands. We have carried out a broad study of these structures using the rigidity analysis software FIRST. This approach allows us to make inferences about the effect of ligand binding upon the rigidity of the protein. The protease inhibitors currently used as part of antiretroviral treatments can be split into two categories, which may offer an explanation for the efficacy of particular combination therapies.

BP 8.28 Mon 17:30 Poster B2

Distance Dependency And Minimum Amino Acid Alphabets

for Decoy Scoring Potentials — •Kay Hamacher — TU Darmstadt

Protein scoring potentials are a valuable tool in molecular biophysics to assess the quality of, e.g., a protein structure. Among those several knowledge-based potentials were developed in the past. However, continuous distance information have not been suggested yet. Here, we propose to close this methodological gap. This becomes possible as the parametrization problem can be formulated as a linear program, for which even large-dimensional instances can be solved efficiently. This allowed us to extended the study into assessing the usability of reduced amino acid alphabets.

[1] S. Pape, F. Hoffgaard, M. Dür, K. Hamacher, "Distance Dependency And Minimum Amino Acid Alphabets for Decoy Scoring Potentials", J. Comp. Chem., 34: 10-20, 2013.

BP 8.29 Mon 17:30 Poster B2

Non-Equilibrium MD simulations of intramolecular signaling in allosteric proteins — •Sebastian Waltz — Biomolecular Dynamics Physik Institut Uni-Freiburg

The interaction of a protein with another protein or ligand causes local energetic and or conformational changes of the protein around the binding side. This structural changes may propagate through the protein and produce functional changes at the distant side. This process is often referred to as allostery. There is an ongoing discussion about the signaling pathway and on the timescale on which the information travels along the protein. To resolve this open question, we perform intensive Non-equilibrium molecular dynamic simulations of a photoinduced conformational change and intramolecular signaling, that allow us to observe the functioning of the protein in real time. The goal is to directly prove the existence of dynamically driven pathways of intramolecular signaling.

BP 8.30 Mon 17:30 Poster B2

Pitfalls and artifacts in two-focus fluorescence fluctuation spectroscopy — •Andreas Veres and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Fluorescence fluctuation spectroscopy is a powerful technique to quantify intracellular transport on the almost single-molecule scale. Going beyond a single observation volume, temporally cross-correlating the fluorescence from two separated foci can be exploited to obtain large-scale transport coefficients, and to detect transport barriers or directed flow. Using mean-field theory and simulations in combination with experiments on a laser scanning microscope (LSM), we have investigated which artifacts and pitfalls may hamper this promising approach. We find that the unavoidable bleaching of fluorophores only has a minor influence on the results, whereas the typically poor statistics in commercial LSMs severely limits the applicability of the approach to in vitro systems.

BP 9: Posters: Membranes

Time: Monday 17:30–19:30 Location: Poster B2

BP 9.1 Mon 17:30 Poster B2

Simulation of supported lipid bilayer formation — •Marc Fuhrmans and Marcus Müller — Theoretische Physik, Universität Göttingen, Göttingen, Deutschland

Exposition of unilamellar vesicles to attractive surfaces is a frequently used way to create supported lipid bilayers. Although this approach is known to produce continuous supported bilayers, the mechanism of their formation and its dependence on factors like surface roughness or membrane tension as well as the interplay between neighboring vesicles or the involvement of pre-adsorbed bilayer patches are not understood very well.

We have used dissipative particle dynamics simulations to assess different mechanisms of vesicle spreading on attractive surfaces, placing special emphasis on the orientation of the resulting bilayer. Making use of the universality of lipid-associated phenomena, we employed a solvent-free coarse-grained model, enabling us to cover the relatively large system sizes and time scales required. Our results indicate that, depending on the strength and range of the interactions with the substrate as well as the surface's roughness, different mechanisms of vesicle spreading occur, resulting in a switch from a predominant inside-up to an outside-up orientation of the created supported bilayer.

BP 9.2 Mon 17:30 Poster B2

Lattice-based Monte Carlo simulations of lipid membranes: Correspondence between triangular and square lattices — •Anastasiia B. Artemieva, Eugene P. Petrov, and Petra Schwille — Max Planck Institute of Biochemistry, Department of Cellular and Molecular Biophysics, 82152 Martinsried, Germany

We have recently demonstrated [1, 2] that lattice-based Monte Carlo (MC) allows one to study the structure and dynamics of membranes on experimentally relevant spatial scales and time intervals with moderate computational expenses. To date, most of lattice-based MC simulations of lipid membranes have been carried out on triangular lattices. Previously we have argued [1, 2] that the particular lattice geometry in MC simulations should not matter for reproducing the properties of the membrane at scales larger than the lattice unit, provided that the lipid–lipid interaction parameters are properly rescaled. Still, it remained an open question whether there exists a single conversion factor for all lipid–lipid interaction parameters to achieve identical results on triangular and square lattices, or the different interaction parameters have to be adjusted individually. Here, based on the properties of the Ising model, we demonstrate that one can indeed choose a single numerical coefficient to rescale all lipid–lipid interaction parameters depending on the lattice type, which provides one-to-one correspondence of thermodynamics properties of lipid membranes in lattice-based MC simulations on triangular and square lattices.

[1] J. Ehrig, E. P. Petrov, P. Schwille, *Biophys. J.* **100** (2011) 80

[2] J. Ehrig, E. P. Petrov, P. Schwille, *New J. Phys.* **13** (2011) 045019

BP 9.3 Mon 17:30 Poster B2

Cytoskeletal pinning prevents large-scale phase separation in model membranes — •Eugene P. Petrov[1,2], Senthil Arumugam[1], Jens Ehrig[1], and Petra Schwille[1,2] — [1]Biophysics, BIOTEC, Technische Universität Dresden, 01307 Dresden, Germany — [2]Max Planck Institute of Biochemistry, Department of Cellular and Molecular Biophysics, 82152 Martinsried, Germany

One important feature of cell membranes, which has been difficult to recapitulate in the artificial bilayer systems, is the membrane-associated cytoskeleton, which is considered to be one of the reasons for the sub-resolution size of membrane domains. Here we describe a minimal model cytoskeletal network formed by the prokaryotic tubulin homologue, FtsZ. Using giant unilamellar vesicles formed from a quaternary lipid mixture, we demonstrate that, on the one hand, the artificial membrane-associated cytoskeleton suppresses large-scale phase separation below the phase transition temperature, and, on the other hand, preserves phase separation above transition temperature. Our experimental observations support the ideas put forward in our previous simulation study [1]: In particular, the picket-fence effect on phase separation explains why micrometer-scale membrane domains are observed in isolated, cytoskeleton-free giant plasma membrane vesicles, but not in intact cell membranes. The experimentally observed suppression of large-scale phase separation much below the transition temperatures also serves as an argument in favor of the cryoprotective role of the cytoskeleton.

[1] J. Ehrig, E. P. Petrov, P. Schwille, *Biophys. J.* **100** (2011) 80.

BP 9.4 Mon 17:30 Poster B2

A physical description of actin-driven filopodia growth — •Denis Johann and Karsten Kruse — Uni Saarland, Postfach 151150, 66041 Saarbrücken, Germany

Filopodia are cytoskeleton-driven fingerlike protrusions of eukaryotic cells that are filled with actin filaments. Motivated by these structures, we investigate the length distribution of membrane protrusions driven by treadmilling filaments growing at the tip and disassembling at the base. To this end we use a continuum mean-field equation for the treadmilling filaments and their constituting subunits as well as for the membrane that is characterized by its surface tension and its bending rigidity. The coupling between the membrane and the cytoskeleton is mediated by an effective potential. Using a GPU-based

parallelized algorithm, we find that this system can create stationary filopodia lengths. This length increases linearly with the concentration of free monomers at the bottom of the filopodia, but also depends on the kinetic parameters governing filament assembly and disassembly as well as the mechanical properties of the membrane. Finally, we characterize the filament length distribution in steady state.

BP 9.5 Mon 17:30 Poster B2

Single lipid molecule tracking on suspended lipid membranes — •Jens Ehrig[1], Susann Spindler[1], Cornelia Becker[1], Chia-Lung Hsieh[2], and Vahid Sandoghdar[1] — [1]MPI for the science of light, Erlangen, Germany — [2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

We study the diffusion of single lipid molecules in free-standing lipid membranes by means of interferometric scattering microscopy (iSCAT)[1]. Free-standing aperture-spanning membranes are obtained by bursting giant unilamellar vesicles on a holey Si_3N_4 support[2]. The diffusion of lipids is studied by recording the scattering signal from gold nanoparticles (AuNP) bound to various molecules in the membrane including the ganglioside GM1 as well as phospholipids with a biotinylated headgroup. The AuNP are bound to GM1 via cholera toxin subunit B (CTxB) or antibodies. In case of the biotinylated phospholipids the biotin directly binds to the streptavidin-covered AuNP. Using the iSCAT technique we are able to resolve the motion of single lipid molecules at a high spatial and temporal resolution of below $\sim$2 nm and $\sim$1 μs, respectively. The results from measurements on free-standing membranes are compared to the ones obtained on supported lipid bilayers.

[1] K. Lindfors et al. *Phys Rev Lett* **93** 2004; P. Kukura et al. *Nat Methods* **6** 2009; [2] F. Heinemann and P. Schwille *ChemPhysChem* **12** 2011

BP 9.6 Mon 17:30 Poster B2

Optical force induced phagocytic particle binding and uptake by Giant Unilamellar Vesicles — •Andreas Meinel and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Germany

Phagocytosis is a central cellular mechanism in order to engulf particles into the cell membrane. Due to the complex interplay between active and passive cellular components, this mechanism is still not fully understood. A better investigation of the uptake process can be reached by reducing the system's complexity through using biomimetic systems. We utilize a Giant Unilamellar Vesicle (GUV) as a model for the cell membrane and a photonic force microscope (PFM) to induce and characterize the phagocytic particle uptake.

The PFM allows the trapping and tracking of a micron sized bead in all three dimensions with a high temporal resolution and a spatial precision in the nanometer range. In this study we focus on the acting forces between the particle and the cell membrane during the uptake process. Furthermore, the GUV-bead interaction is described by a theoretical model and compared with experimental results. The proposed methodology initiates a way to get access to the underlying energetical and mechanical concepts of the phagocytic particle uptake process.

BP 9.7 Mon 17:30 Poster B2

The interaction between polyproline containg cell-penetrating peptides and a lipid bilayer — •Johannes Franz, Kalina Peneva, Mischa Bonn, and Tobias Weidner — Max Planck Institute for Polymer Research, 55118 Mainz, Germany

Cell-penetrating peptides (CPPs) are membrane-permeable, short amino acid sequences that can be used to deliver covalently and non-covalently bound cargoes, i.e. drugs, into cells without damaging the cell membrane. However, the mechanism for CPP internalization is still subject of ongoing research. CPPs are divided into different subfamilies, depending on their chemical properties. They differ not only in their primary structure and overall charge, but also in their local folding. We used a modified form of SAP (sweet arrow peptide), an anionic CPP containing repetitive polyproline motifs, as a model peptide. The secondary structure of SAP(E), polyproline II (PPII), allows aggregation and could contribute to the peptides membrane permeability. Membrane models omit the complexity of the natural cell membrane while ensuring the full functionality of embedded peptides. We built up a polymer-assisted lipid bilayer to enable an unimpeded translocation of CPPs across the model membrane. Sum frequency generation (SFG) vibrational spectroscopy was used to investigate molecular interactions between SAP(E) and the tethered lipid bilayer during membrane translocation.

BP 9.8 Mon 17:30 Poster B2

Evaluation of methods for membrane preparations. — •Patrick Paul[1], Ulla Nolte[1], Reinhard Fässler[2], and Kay E. Gottschalk[1] — [1]Institute of Experimental Physics, Ulm University, Ulm, Germany — [2]Max Planck Institute of Biochemistry, Department of Molecular Medicine, Martinsried, Germany

The interaction of proteins with the intracellular side of cell membranes is important for a variety of cellular functions. To study these interactions, we try to prepare cell membranes of adherent cells such that the intracellular side is exposed. We characterize different membrane preparation methods with light microscopy and high resolution atomic force microscopy.

BP 9.9 Mon 17:30 Poster B2

Laser-spectroscopic Characterization of the Interaction between fluorescent Molecules and nano-sized Lipid Vesicles — •Alice Wilking, Idir Yahiatène, and Thomas Huser — Universität Bielefeld, Abteilung für Experimentalphysik, 33605 Bielefeld, Germany

Nanolipoproteins (NLPs) play an important role in the transport of bioactive compounds (e.g. cholesterol) through the blood. This work addresses the synthesis of NLPs and the investigation of their diffusion characteristics by Fluorescence Correlation Spectroscopy (FCS) to determine their size and shape in solution. We show the fabrication of 100 nm lipid vesicles using a mini-extruder. To make them visible the lipid vesicles were labeled with the lipid-intercalating fluorophore Di-I.

Di-I changes its photophysical character with its chemical environment. We also characterized Di-I by FCS, absorption and emission spectra in different solvents (changes in central wavelengths, dimer formation) and used dSTORM (direct Stochastical Optical Reconstruction Microscopy) to directly image and quantify the photophysical character of the dye; in its free and intercalated state. We found that Di-I is more photostable while it is intercalated. We also synthesized NLPs by mixing lipid vesicles with the protein ApoA-1. These NLPs are synthetic lipoproteins and as already demonstrated they portray a mean diameter of 7 nm - 15 nm. We have been able to confirm these values by FCS measurements.

BP 9.10 Mon 17:30 Poster B2

Pore-spanning lipid bilayers on microchips — •Theresa Kaufeld and Christoph F. Schmidt — Drittes Physikalisches Institut, Biophysik Universität Göttingen

Several methods exist for artificial membrane formation, e.g. membranes on a solid hydrophilic support, or the classical BLM, a free-standing lipid bilayer formed across hydrophobic apertures. We have here focused on the reconstitution of lipid bilayers on porous substrates, combining the stability of solid supports and the accessibility of both sides of the bilayer of the classical BLM which is necessary for electrical recordings of membrane channels. We have designed microsubstrates with individually addressable arrays of micrometer-sized apertures for electrical experiments and fluorescence microscopy, which are also suitable for other techniques such as mechanical manipulation of lipid bilayers. The substrates were characterized in terms of surface roughness and pore geometry by SEM and AFM. Impedance spectroscopy was used to characterize the substrate electrically and showed a resistance in the kilo-Ohm range, which is clearly distinguishable from the Giga-Ohm seal. Solvent-free lipid bilayers were formed by GUV-spreading and imaged with fluorescence microscopy. Electric experiments using Gramicidin D as a test ion channel showed suitability for single channel resolution.

BP 10: Posters: Imaging

Time: Monday 17:30–19:30 Location: Poster B2

BP 10.1 Mon 17:30 Poster B2

Distinguishing immature and mature HIV-1 particles by superresolution optical fluorescence microscopy — •Viola Mönkemöller[1], Benjamin Dale[2], Wolfgang Hübner[1], Benjamin Chen[2], and Thomas Huser[1] — [1]Biomolecular Photonics, Universität Bielefeld, Germany — [2]Immunology Institute, Mount Sinai School of Medicine New York, NY, USA

The human immunodeficiency virus (HIV) is the agent of the global epidemic of the immune disease AIDS (acquired immunodeficiency syndrome). Therefore further investigations on the viral structure and molecular mechanisms are of particular importance in the search for medical therapies. HIV-1 is assembled in infected cells and buds out as an immature particle. The uncleaved major structural polyprotein Gag defines the immature non-infectious state of the virus. HIV-1 has to undergo maturation to become infectious. During the maturation process Gag is cleaved which leads to a different structure in the infectious HIV-particle. We are interested in characterizing the immature and mature virus particles by superresolution fluorescence microscopy. The size of HIV-1 particles is approx. 130nm in diameter and is therefore below the diffraction limit of conventional fluorescence light microscopy. Techniques such as PALM (Photoactivated Localization Microscopy) and STORM (Stochastic Optical Reconstruction Microscopy) should allow us to resolve structures down to 20nm spatial resolution.

We plan to utilize this and other superresolution approaches to track the position and state of individual HIV virions in 4D, which will be very useful for future studies on HIV infection mechanisms.

BP 10.2 Mon 17:30 Poster B2

Monitoring early embryogenesis with single-plane illumination microscopy — •Philipp Struntz, Rolf Fickentscher, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Single-plane illumination microscopy (SPIM) is a fluorescence-imaging technique that combines rapid widefield detection with optical sectioning. Due to a reduced phototoxicity induced by bleaching, SPIM is capable of providing a long-term, three-dimensional time-resolved in vivo imaging of specimen. We have built and automated a SPIM-setup specifically designed for imaging eggs of the nematode Caenorhabditis elegans in the early stages of embryogenesis. With the obtained time-lapse images it is possible to track cell positions within the developing embryo to get information about the spatiotemporal development of tissues. Based on this, we have designed a simple model that is capable of explaining experimental observations during the first stage of embryogenesis.

BP 10.3 Mon 17:30 Poster B2

On the role of Sec16 in the self-organization of exit sites in the endoplasmic reticulum — •Julia Hoffmann and Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

The endoplasmic reticulum (ER) is the first station of newly synthesized proteins in eukaryotic cells. The export of properly folded proteins occurs almost exclusively at specialized membrane domains, so-called ER exit sites (ERES). Protein export at ERES but also the self-organization of ERES themselves are still poorly understood. Sec16 is a large peripheral protein that plays an important role in both processes. However, its precise function has remained elusive so far. Here we present an investigation of Sec16 dynamics in vivo by means of quantitative fluorescence microscopy techniques. As a result, we have found that Sec16 rapidly cycles between an ER-bound and a cytoplasmic state (ratio about 1:1) while being mobile in both states. Moreover, our data indicate a role of Sec16 as a metastable platform for the self-assembly of ERES.

BP 10.4 Mon 17:30 Poster B2

PyCorrFit - a versatile tool for FCS data analysis — •Paul Müller — Biotechnology Center of the TU Dresden, Germany

We present the general-purpose fluorescence correlation spectroscopy (FCS) evaluation software PyCorrFit. PyCorrFit supports various commercially available FCS setups (e.g. ConfoCor3, Zeiss), and offers several built-in model functions, exploiting a wide range of applications. The program comes with several features for data manipulation, permits the import of external model functions that do not require prior programming skills, and can be expanded to fit the needs of the more versed user. We demonstrate the implementation of PyCorrFit in current research, such as diffusional measurements in lipid monolayers or protein affinity assays in free solution. PyCorrFit is free, open-source and available at http://fcstools.dyndns.org/pycorrfit.

BP 10.5 Mon 17:30 Poster B2

SOFI of GABA-B neurotransmitter receptors in hippocampal neurons elucidates intracellular receptor trafficking and assembly — •Anja Huss[1], Omar Ramírez[2], Felipe Santibáñez[2], Andrés Couve[2], Steffen Härtel[2], and Jörg Enderlein[1] — [1]III. Institute of Physics: Biophysics, Georg-August-University Göttingen, Germany — [2]Institute of Biomedical Sciences, Faculty of Medicine and Nucleus of Neural Morphogenesis (NEMO), Universidad de Chile, Santiago, Chile

The synaptic efficacy of neurons depends on the availability of neurotransmitter receptors and is controlled by their intracellular trafficking routes. GABA-B receptors (GABA-BRs) are heteromeric proteins found at the plasma membrane of dendritic postsynaptic sites. Detailed insights of trafficking routes and thus the assembly of the subunits are still missing.

To address this question we have studied the distribution and colocalization of the GABA-BR subunits in the plasma membrane and in the intracellular compartments in hippocampal neurons with dual-color, 3D Stochastic Optical Fluctuation Imaging (SOFI). SOFI is a fluorescence imaging modality which yields super-resolved spatial resolution, 3D-sectioning and high image contrast.

BP 10.6 Mon 17:30 Poster B2

Researches on iron containing bacteria with PEEM — •Christoph Keutner[1], Ulf Berges[1], Philipp Espeter[1], Alex von Bohlen[2], David J. Keavney[3], Claus M. Schneider[4], and Carsten Westphal[1] — [1]DELTA/Experimentelle Physik I, TU Dortmund — [2]ISAS Dortmund — [3]APS, Argonne National Laboratory — [4]PGI-6, FZ Jülich

Members of the polyphyletic group of magnetotactic bacteria (MTB) are forming chains of membrane-encapsulated particles by the natural process of biomineralisation. These so-called magnetosome chains consist of greigite or iron oxides, and are used for an oriented navigation along the Earth's magnetic field. This is very important for the bacteria since they seek the oxic-anoxic transition zone which is their optimal living environment. In technological, medical, and environmental applications these magnetosomes are considered as a perspective material due to their narrow size and shape distribution.

In this work experiments on imaging the MTB species *Magnetospirillum magnetotacticum* with photoemission electron microscopy (PEEM) were continued. Now, an improved preparation procedure yielded a significantly higher MTB concentration on the sample surface. At the same time the residuals of the culture medium could drastically be decreased by this new procedure. We present first photoelectron emission microscopy data recorded at the Advanced Photon Source, Chicago (USA). The measurements show an element-specific detailed structure of the bacteria, including a clear signature of the iron oxides within the bacteria.

BP 10.7 Mon 17:30 Poster B2

Wide-field magnetometry imaging using nitrogen-vacancy centers — Steffen Steinert[1], •Nicolas Götz[1], Florestan Ziem[1], Andrea Zappe[1], Liam Hall[2], Lloyd Hollenberg[2], and Jörg Wrachtrup[1] — [1]3 Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart Germany — [2]2School of Physics, University of Melbourne, Victoria 3010, Australia

Imaging of weak electromagnetic signals with sub-cellular resolution under life sustaining conditions is of great importance in the context of life science, but could not be achieved yet. A diamond doped with a shallow layer of nitrogen-vacancy centers (NV) potentially fulfills this requirements. The spin state of a single negatively charged NV center can be optically polarized and read out. Measuring the local Zeeman shift and spin state lifetime of several NVs enables to determine the magnetic fields in the vicinity of the Diamond. Using a wide-field microscopy technique, we can simultaneously capture the signal of a 60*m

x 60*m area of the diamond surface on a CCD camera with diffraction limited resolution. Here we present the investigation of different magnetic species as marker for magnetic cell imaging via microfluidic detection. We also evaluate the feasibility of label-free imaging using this technique.

BP 10.8 Mon 17:30 Poster B2

Non-Invasive Imaging and Quality Assessment of Artificial Cartilage — •Lena Nolte[1], Iwan Schie[2], and Thomas Huser[1,2] — [1]Universität Bielefeld — [2]University of California, Davis

More than five million people in Germany are currently suffering from osteoarthritis. Due to the daily stress placed in our joints the cartilage between the bones wears off. Once the cartilage is damaged it cannot recover by itself which leads to little treatment options. New approaches in tissue engineering provide promising results in the development of artificial cartilage that could be transplanted to a patient. Nevertheless, the quality of this artificial cartilage must be assessed in order to prevent further issues for the patient. The challenge, however, is to investigate the cartilage at a microscopic scale without influencing it as otherwise with fluorescence microscopy. Here, we developed a combination of several optical techniques to analyze the cartilage without special preparation or labeling. We demonstrate how cartilage cells (chondrocytes) can be visualized by coherent anti-Stokes Raman scattering (CARS), and the extracellular matrix (ECM) using Second Harmonic Generation (SHG). Images of a size of up to 1.5 cm x 7.5 cm with a spatial resolution down to 1 μm can be reconstructed. Furthermore, spontaneous Raman scattering can be applied to obtain Raman spectra from specific points of interest. This provides molecular information about the cartilage composition within these specific regions. We believe this novel multiphoton microscopy system is a powerful device which enables us to expose the similarity and differences between natural and artificial cartilage.

BP 10.9 Mon 17:30 Poster B2

High Harmonic Generation For Coherent Diffractive Imaging — •Sergey Zayko[1], Eike Mönnich[1], Murat Sivis[1], Tobias Mey[3], Dong-du Mai[2], Klaus Mann[3], Tim Salditt[2], and Claus Ropers[1] — [1]Materials Physics Institute and Courant Research Centre, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institute fo X-ray Physics. University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [3]Laser-Laboratorium Göttingen e.V. (LLG) Hans-Adolf-Krebs-Weg 1 37077 Göttingen

Light sources based on high harmonic generation (HHG) open up the possibility to achieve coherent ultra-short high energy pulses up to the soft x-ray regime in a tabletop setup. Here, we present an implementation and characterization of a compact HHG setup to perform coherent diffractive imaging (CDI) and pump-probe spectroscopy with femtosecond temporal resolution. Coherent pulses up to the 51st harmonic order corresponding to 80 eV photon energy have been obtained.

The degree of spatial coherence and the optical wavefront of high harmonics were characterized. As a proof-of-concept, a test pattern with 170 nm feature size structured by focused ion beam milling was imaged by CDI at a wavelength of 32 nm.

BP 10.10 Mon 17:30 Poster B2

Chasing the next level in molecular sensitivity — •Henning Hachmeister, Michael Stührenberg, Lena Nolte, Christian Pilger, Gerd Wiebusch, and Thomas Huser — Biomolecular Photonics, Universität Bielefeld, Germany

Fluorescence microscopy is a well-established, molecularly specific imaging technique in the life sciences which continues to gain popularity due to the ongoing development of novel fluorescent probes and superresolution imaging techniques. The use of fluorescent probes, however, is potentially detrimental to biological activity and requires careful controls. Rapid photobleaching and the toxicity of many of these probes greatly limit their use in physiological studies of cells.

A new way to image the structure of cells is the use of vibrational spectroscopy as a microscopic imaging technique. In vibrational spectroscopy, vibrations of molecular bonds inside a molecule are excited using laser beams. Within the last decade the nonlinear optical imaging of molecular modes by coherent anti-Stokes Raman scattering (CARS) has been developed to the point where it can now be routinely use to image e.g. lipid structures within cells within the need for fluorescent probes.

Here, we demonstrate a versatile, new technique called doubly-resonant CARS (DR-CARS) which can enhance weak CARS signals by up to 1000x to enable the detection and analysis of other molecular bonds besides aliphatic C-H groups.

BP 10.11 Mon 17:30 Poster B2

Broadening the applications of vibrational spectroscopy in microscopy with super resolution techniques — •Christian Pilger, Henning Hachmeister, Michael Stührenberg, Lena Nolte, Gerd Wiebusch, and Thomas Huser — Biomolecular Photonics, Universität Bielefeld, Germany

In vibrational spectroscopy coherent anti-Stokes Raman scattering (CARS) is an established method for imaging biological samples on the microscopic scale. This process results in the specific excitation of molecular bonds. Utilizing a four-wave mixing process the Raman signal is strongly enhanced, and can now be used e.g. for imaging inner cell structures.

In comparison to fluorescence microscopy, CARS requires no organic fluorophores to highlight cellular structures of interest. Thereby the biological structures and processes are unaltered and the signal is persistent.

This type of laser scanning microscopy is, however, still limited in its spatial resolution by the diffraction limit. We are exploring a number of potential ways that will enable us to overcome the diffraction limit in nonlinear optical microscopy. Ultimately, we hope to be able to image individual viral particles in vivo during their entire life cycle from the assembly of new virions to the infection of new cells.

BP 10.12 Mon 17:30 Poster B2

Stimulated Raman Scattering for noninvasive live imaging — •Michael Stührenberg, Henning Hachmeister, Lena Nolte, and Thomas Huser — Biomolecular Photonics, Universität Bielefeld, Germany

A common method for the visualisation of biological molecules is fluorescence microscopy. By using a fluorescent dye, the molecules of interest can be made visible. Fluorescence microscopy covers a wide range of techniques and continues to gain popularity in respect to i.e. superresolution and 3D live cell imaging. Nevertheless, these techniques have some major disadvantages. Amongst other things there is no guarantee that the probes won't affect certain characteristics of the molecule, such as motility or binding capability. Therefor, the use of fluorescent probes requires careful controls in order for it to not be detrimental to biological processes. To overcome these drawbacks, we demonstrate a rapid noninvasive imaging technique based on Raman scattering. In Stimulated Raman Scattering (SRS) the molecule of interest is excited to a specific vibrational mode. This is achieved by the application of 2 different confocal laserbeams overlapping in time and space. Through excitation in a vibrational mode, one beam loses intensity, while the other one experiences, through induced stimulation, an intensity gain. The probability for this is small compared to a fluorescent signal and requires a lock-in based detection system. Yet this results in a nearly background free noninvasive imaging technique, which can be tuned to a wide range of molecules. The ultimate goal is live imaging for which we apply a homebuilt lock-in amplifier with a high temporal resolution.

BP 10.13 Mon 17:30 Poster B2

Sample preparation and delivery at the European XFEL Facility — •Sadia Bari[1], Charlotte Uetrecht[1,2], and Joachim Schulz[1] — [1]European XFEL GmbH, Notkestraße 85, 22607 Hamburg, Germany — [2]Molecular Biophysics, Uppsala University, Husargatan 3, 75124 Uppsala, Sweden

The ultrashort, high-intensity X-rays of the European XFEL will enable new science with a wide range of potential samples delivered in various forms into diverse environments. Providing the delivery methods and target systems that allow such a variety of samples to be studied using the fast repetition rate and high peak intensity of the European XFEL is the job of the Sample Environment group.

Sample delivery methods that are planned and in preparation will be introduced and discussed; for example a liquid jet primarily used in nano-crystallography and an aerodynamic lens optimised for single particle imaging of e.g. aerosols and viruses. But also the options for fixed targets and their challenges like fast sample exchange, control of temperature and sample orientation will be presented.

BP 10.14 Mon 17:30 Poster B2

Scanning X-Ray Nano-Diffraction on Hydrated Cells in Microfluidic Devices — •Britta Weinhausen, Christian Dammann, Oliva Saldanha, Robin Wilke, Christian Olendrowitz, Jens-Friedrich Nolting, Tim Salditt, and Sarah Köster — Institute

for X-Ray Physics, University of Göttingen, Germany

The combination of X-ray scattering techniques with sample chambers based on microfluidics allows for studying biological samples in a well-controlled and adaptable environment. However, bio- as well as X-ray compatibility of the materials, the device geometry and the sample environment is a challenging issue during device fabrication. Especially when using high-flux synchrotron radiation sources, material degradation or strong background scattering is observed for most materials that are commonly used for microfluidic experiments in combination with visible light microscopy.

We develop a novel type of X-ray compatible microfluidic device, which is based on silicon nitride membranes as window material and allows for studies on hydrated biological samples. As sample we choose adherent eukaryotic SK8K18-2 cells, exhibiting a pronounced keratin network structure. Scanning nano-diffraction experiments using hard X-rays are performed on fixed (hydrated) as well as living cells in these flow chambers at different synchrotron set-ups. Different contrast mechanisms are employed to generate real-space images of the cells with a resolution on the order of the beam size.

BP 10.15 Mon 17:30 Poster B2

New Developments in Laboratory SAXS Instruments — •Bastian Arlt[1] and Andreas Keilbach[2] — [1]Anton Paar Germany GmbH, Hellmuth-Hirth-Straße 6, D-73760 Ostfildern — [2]Anton Paar GmbH, Anton-Paar-Straße 20, A-8054 Graz

Surfactants, dispersions, polymer or protein solutions and (micro-) emulsions are intensively investigated systems in current science. Consequently, an essential point is the careful characterization of these systems in-situ. The small angle X-ray scattering (SAXS) technique offers precise and fast measurements to investigate parameters such as size, shape, interaction effects of particles in solution. Thus, SAXS is a complementary method to TEM, AFM, or NMR techniques. SAXS measurements are performed at synchrotron facilities or, thanks to recent developments, using laboratory instruments which have become an excellent alternative.

We are going to present the latest developments and trends in the field of laboratory SAXS instruments. Thanks to high-flux X-ray sources, short exposure times are possible. Additionally, Anton Paar has explored novel techniques in sample positioning which are commonly known from synchrotron measuring stations and allow extending the available detection range and resolving smallest dimensions.

BP 10.16 Mon 17:30 Poster B2

Raman spectroscopic characterization of sepsis relevant bacteria appearing in urinary tract infections on a dielectrophoresis chip — •U.-Ch. Schröder[1,2], C. Assmann[1], A. Ramoji[1], U. Glaser[1,2], U. Hübner[2], Ch. Leiterer[2], A. Csáki[2], W. Fritzsche[2], M. Bauer[1], J. Popp[1,2,3], and U. Neugebauer[1,2] — [1]Center for Sepsis Control and Care, Jena University Hospital — [2]Institute of Photonic Technology Jena e.V. — [3]Institute for Physical Chemistry and Abbe Center of Photonics, University Jena

Sepsis reflects a dysregulated response of the immune system due to the invasion of pathogens characterized by high mortality rates. Due to the requirement for overnight cultivation steps the standard microbiological diagnostic methods are too slow for an early start of tailored therapy. To make things worse bacteria are getting more and more resistant towards antibiotics. We have combined direct dielectrophoretic capturing of bacteria in dilute suspensions above a quadrupol microelectrode array with using micro-Raman spectroscopy to achieve a novel rapid, highly specific, label-free and culture-independent lab on chip method. As a proof-of-principle study two commonly participating bacterial strains in urinary tract infections, Escherichia coli and Enterococcus faecalis, are respectively captured, and are classified with respect to their molecular signature. To demonstrate rapid antibiotic susceptibility testing, the differentiation of antibiotic treated and non-treated Enterococcus faecalis strains has been carried out. With the help of multivariate statistical analysis a robust classification model has been established. Acknowledgement: BMBF (FKZ 01EO1002)

BP 10.17 Mon 17:30 Poster B2

Characterization of Caco-2 cells via confocal Rama Microscopy — •Susanne Kimeswenger[1,2], Krisztina Vincze-Minya[1], Mohammad-Reza Lornejad-Schäfer[2], Klaus Schröder[2], and Sabine Hild[1] — [1]Institute of Polymer Science, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria — [2]Biomed-zet Life Science GmbH, Industriezeile 36/I, 4020 Linz, Austria

Eucaryotic cells consist of 60-70 % water, the rest is bioorganic material, which is highly heterogenous: lipids, peptides, carbohydrates and nucleic acids. The distribution of these components varies in different cell types and cell states. Over the past few years Raman spectroscopy got more and more interesting for the characterization of cells, as Raman spectroscopy is a non-destructive, non-contact in vitro method to analyze cells providing information about their viability, differentiation status and tumorigenicity. The human carcinoma cell line Caco-2 has the special characteristic to showing a small intestine enterocyte phenotype when cultured for 21 days. Caco-2 cells seeded on different substrates (silicium, calcium fluoride) were tested. Confocal Raman microscopy reveals the differences between vital and fixated cells. As correlation of Raman spectra and different cell components in fixated cells was not possible, characterization of Caco-2 cells was performed in vital cell status; the identification of Raman spectra of cell components was promising. Furthermore we have revealed differences between differentiated and proliferated Caco-2 cells regarding to their Raman spectra, reflecting differences in bio-molecular composition.

BP 11: Posters: Statistical Physics in Biological Systems (joint with DY)

Time: Monday 17:30–19:30 Location: Poster B2

BP 11.1 Mon 17:30 Poster B2

Perturbed self-organized critical networks as a sleep model — li chen[1] and •christian meisel[1,2] — [1]Max-Planck-Institut for Physik komplexer Systeme, Noethnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Neurology, University Clinic Carl Gustav Carus, Fetscherstr. 74, 01307 Dresden, Germany

Why do we need sleep is a long mystery for centuries. Here, we propose a perturbed self-organized critical binary networks as a possible model to mimic the whole processes for the brain during awake time and sleep. By systematically characterizing the network activity, our results shows that the input received in awake time always derivates our brains from critical state, with decreasing computational power, shorter effective response range, worse p-values etc. That is the reason why we need sleep to recover these brain functions by self-organizing back to critical networks by turning off all input from surroundings. An observation of the probability distribution of phase-lock interval from EEG data during growing sleep deprivation is given.

BP 11.2 Mon 17:30 Poster B2

Information filtering by synchronous spikes in a neural population — •Nahal Sharafi — Bunsenstrasse 10, 37073 Goettingen

Information about time-dependent sensory stimuli is encoded by the spike trains of neurons. Here we consider a population of uncoupled but noisy neurons (each subject to some intrinsic noise) that are driven by a common broadband signal. We ask specifically how much information is encoded in the synchronous activity of the population and how this information transfer is distributed with respect to frequency bands. In order to obtain some insight into the mechanism of information filtering espects found previously in the literature, we develop a mathematical framework to calculate the coherence of the synchronous output with the common stimulus for populations of simple neuron models. Within this frame, the synchronous activity is treated as the product of filtered versions of the spike trains of a subset of neurons. We compare our results for the simple cases of (1) a Poisson neuron with a rate modulation and (2) an LIF neuron with intrinsic white current noise and a current stimulus. For the Poisson neuron, formulas are particularly simple but show only a low-pass behavior of the coherence of synchronous activity. For the LIF model, in contrast, the coherence function of the synchronous activity shows a clear peak at high frequencies, comparable to recent experimental findings. We uncover the mechanism for this shift in the maximum of the coherence and discuss some biological implications of our findings.

BP 11.3 Mon 17:30 Poster B2

Modelling of rhythmic patterns in hippocampus — •Anastasia Lavrova[1], Michael Zaks[2], and Lutz Schimansky-Geier[2] — [1]Immanuel Kant Baltic Federal University, Kaliningrad, Russia — [2]Humboldt University at Berlin, Berlin, Germany

The hippocampal circuit can exhibit network oscillations in different frequency ranges (gamma - 30-80 Hz; theta - 4-12 Hz; as well as theta/gamma or a bursting regime) both in vivo and in vitro and switch between them.

Our goal is to investigate how coupling strength and delayed propagation influence synchronization and switching between different oscillatory states in minimal neuronal networks. To this end, we constructed a simple model of neurons comprising two fast-spiking and two slow-spiking cells, respectively. The network is described by coupled FitzHugh-Nagumo equations that well reproduce the dynamical behavior of different cells types: their periods, amplitudes, and phase shifts.

The model allows us to analyze the influence of synaptic strengths on the network synchronization and dynamical switching between theta, gamma, and bursting regimes. In particular, we perform a thorough bifurcation analysis and identify parameters of synaptic connections that can efficiently induce switches in the network activity.

BP 11.4 Mon 17:30 Poster B2

Interaction between Looped-Star Polymers — •Dieter Heermann and Benoit Knecht — Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg

We study the properties of looped star polymers, in which each arm is a ring that can be over- or underwound and compare them to the classic linear-arm star polymer. Looped star polymers are more compact and overwounding increases their density. The effective repulsion between looped stars is similar to that of linear star polymers with twice as many arms half the length, following a logarithmic–Gaussian potential. The force pushing the arms outwards is more than twice as strong for looped star polymers than it is for linear star polymers for a number of arms f>2.

BP 11.5 Mon 17:30 Poster B2

Collective behavior and structure formation of hydrodynamically interacting active particles — •Marc Hennes, Katrin Wolff, and Holger Stark — Institut für Theoretische Physik TU Berlin

Lattice Boltzmann simulations of active run-and-tumble particles (RTPs) subject to an external trapping force have shown the emergence of a self-assembled pump in the presence of hydrodynamic interactions[1]. Here, we extend these results to active Brownian particles (ABPs), simulated by means of Brownian Dynamics simulation including hydrodynamic interactions. ABPs, in contrast to RTPs, do not tumble but reorient smoothly due to thermal noise, external torques, and vorticity fields in the fluid. Here, we clarify that the pump is a dynamic cluster of ABPs which only forms above a threshold value for the swimming speed. We assign an effective dipole moment to the pump and show that in this non-equilibrium situation the orientations of the particles are Boltzmann-distributed around the pump direction. We also consider bottom-heavy particles in an external gravitational field. Without hydrodynamic interactions and at sufficiently large swimming speeds, these particles accumulate at the top of the simulation box. However, when they interact hydrodynamically, we find this steady state to be unstable and observe the emergence of spatially separated, dynamical toroidal structures, reminiscent of classical bioconvection.

[1] M.E.Cates et al., Phys.Rev.Lett. 104, 258101 (2010)

BP 11.6 Mon 17:30 Poster B2

Evolutionary food web model on a set of patches coupled by migration — •Eva Marie Weiel, Korinna T. Allhoff, and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt

Ecological food webs in a heterogeneous environment can be modelled by a complex network with two different types of connections. The local connections of these "networks on networks" represent the interaction through predation and competition of ecological populations in each habitat. The second type of connections represents migration between the habitats. Understanding how the spatial dimension affects the structure and stability of these complex networks is of large interest in ecological theory. We investigate the emergence, dynamics and interaction of food webs in a small set of patches. The dynamics in each patch is based on the often-cited evolutionary model introduced by Loeuille and Loreau in 2005. In addition to local evolution we include different types of migration between the patches and analyse their influence on the structure of the emerging food webs.

BP 11.7 Mon 17:30 Poster B2

Effects of a stage structure in a population dynamics model to explain cyclic dominance of pacific sockey salmon — •Fabian Fertig[1], Christoph Schmitt[1], Christian Guill[2], and Barbara Drossel[1] — [1]Institut für Festkörperphysik, TU Darmstadt — [2]Institut für Zoologie and Anthropologie, Georg-August-Universität Göttingen

The number of sockeye salmon that return from the ocean to their lakes of birth in the Fraser River basin in Canada shows a remarkably strong and regular four-year oscillation. This so-called cyclic dominance phenomenon is reproduced as a stable attractor by a recently introduced predator-prey model for salmon fry and their main predator in the rearing lakes, rainbow trout. However, rainbow trout is known to prey also strongly on kokanee salmon, which spend all their life in the lakes. Including kokanee in the model typically leads to a breakdown of cyclic dominance and often also to the extinction of one of the salmon species. This means either that the observed coexistence of the two species together with the occurence of cyclic dominance in the sockeye population is a transient phenomenon, or that the model is not detailed enough. In order to explore the conditions under which cyclic dominance could persist in the presence of both salmon species, we investigate various models that take the stage structure of trout and the different preference of adult and juvenile trout for kokanee and sockeye salmon into account. We show that the parameter range for cyclic dominance can be increased in stage structured models.

BP 11.8 Mon 17:30 Poster B2

Simple models for generation cycles — •Torsten Pfaff[1], Barbara Drossel[1], and Christian Guill[2] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt — [2]Institut für Zoologie und Anthropologie, Georg-August-Universität Göttingen

Many biological species show population oscillations due to density dependent competition. The periods of the oscillations are related to the life cycle of the species, and they have been used to classify the oscillating systems.

We present three simple models consisting of a one dimensional time delay equation with only two parameters. These models show all essential properties of generation cycles. Due to their simplicity, they are helpful for obtaining a mechanistic understanding of the population oscillations, and they give new insights into the origin of the periods and into the size of the intervals that are covered by these periods. Based on the insights gained from our simple models, we also obtain a better understanding of the more complex models presented in the classical paper by Gurney & Nisbet 1985, and we can extend their results.

As an outlook, we argue that the simple models are useful for investigating generation effects in many species food webs.

BP 11.9 Mon 17:30 Poster B2

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

Domains of aligned filaments play an important role in solutions of semiflexible biopolymers. For instance, they occur as a consequence of shear induced ordering upon sample preparation or as a precursor of bundle formation. 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 filament by surrounding filaments. It is represented through a cylindrical confinement potential that is self-consistently determined. In particular, we analyze the effect of local nematic order on the micro-structure in terms of the tube radius distribution [2], which can experimentally be measured with high accuracy for F-actin solutions [3], allowing for a precise quantitative comparison of theory and experiment.

[1] Morse, D. C., Phys. Rev. E 63, 031502 (2001)

[2] Glaser, J. et al., Phys. Rev. E 84, 051801 (2011)

[3] Glaser, J. et al., Phys. Rev. Lett. 105, 037801 (2010)

BP 11.10 Mon 17:30 Poster B2

Stochastic tug-of-war model with symmetric motor properties does not provide processive cargo movement. — •Sarah Klein[1], Cecile Appert-Rolland[2], and Ludger Santen[1] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken — [2]Laboratory of Theoretical Physics, Paris-Sud University, Orsay

Many different types of cellular cargos are transported bidirectionally along microtubules by teams of molecular motors. The motion of this object has been experimentally characterized *in vivo* as processive with rather persistent directionality. By means of an effective theoretical approach, introduced by Lipowsky *et al.* [1], it has been argued that the dynamics of these object are the result of a tug-of-war between different kinds of motors. This picture has been questioned in a recent article by Kunwar *et al.* [2], who considered the coupling between motor and cargo in more detail. In this contribution we discuss possible scenarios within this framework that eventually lead to the observed dynamic patterns of bidirectional cargo transport.

[1] M. J. I. Müller, S. Klumpp, R. Lipowsky, PNAS 105, 4609 - 4614 (2008)
[2] A. Kunwar, S. K. Tripathy, J. Xu, PNAS 108(47), 18960-18965 (2011)

BP 11.11 Mon 17:30 Poster B2

Modeling diversity of immune genes in host-parasite coevolution — •Yixian Song and Arne Traulsen — Max Planck Institute for Evolutionary Biology Plön

We investigate an individual based stochastic model of host-parasite co-evolution. The model is made to simulate the origin and maintenance of the major histocompatibility complex (MHC) polymorphism, i.e., coexistence of diverse genetic variants in a population. In the genes of the MHC, the key component of adaptive immunity, very high levels of allelic diversity are observed. MHC molecules are essential in antigen presentation process by T-cells. The high polymorphism of MHC genes has drawn attention of evolutionary biologists and population geneticists. Our model is focused on one locus with two alleles. Thereby the dynamics of coexisting parasites and alleles are explored. The goal of this model is to develop a theoretical understanding of the dynamic equilibrium in which the MHC diversity in a population approximately remains from generation to generation, but changes in composition.

BP 11.12 Mon 17:30 Poster B2

Interaction Dynamics of Colloidal Particles in an Optical Light Tube — •Benjamin Tränkle and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Germany

Specific reactions of Brownian particles are often affected by long and short ranging forces, such as hydrodynamic, entropic and steric forces. An example is the fusion of vesicles within a living cell. Colloidal particles can serve as a model system for the investigation of such interaction events. We trap two particles in a single potential, which is generated by an oscillating optical line trap. In this geometry, the reaction rate is increased due to the confined space, while rotational and translational degrees are preserved. An accousto-optic deflector (AOD) is used to steer the optical trap and therefore achieve kHz scanning rates. The spheres' positions are tracked simultaneously in 3 dimensions with back focal plane interferometry [1]. With this method we can measure the interaction dynamics of spheres diffusing in a single optical potential with a spatial precision in the nanometer range at kHz rates. Static and dynamic interaction information is gained by analyzing the particle trajectories. The AOD is also used to control the line potential, by steering the laser power during the scanning process. Thereby, we are able to change the reaction volume and investigate its effect on the reaction rate and interaction duration [2].

[1] Speidel et al., Interferometric 3D tracking of several particles in a scanning laser focus. Optics Express, 17(2):7-9, 2009.
[2]Tränkle et al., Interaction dynamics of two colloids in a single optical potential. Physical Review E, 86(2):1-5

BP 11.13 Mon 17:30 Poster B2

A simple polymer in a spherical cage — •Martin Marenz, Johannes Zierenberg, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, D-04009 Leipzig, Germany

We study the change of the pseudo phase transition of a simple homopolymer inside a spherical confinement. Of particular interest is the shift of the collapse and freezing transitions with shrinking radius of the sphere. The polymer is a simple bead-stick model, where the distance between neighboring monomers is fixed, between three monomers in a row acts a bending potential and all non neighboring monomers interact via a Lennard-Jones potential. We use modern Monte Carlo methods to investigate the phase space of this model. Most of the results are obtained by parallel tempering simulations followed by a multi-histogram reweighting method combining a direct and a recursive procedure. To crosscheck our results, especially near the pseudo phase transition, we used a parallelized kind of the multicanonical simulation.

To characterize the pseudo phase transition we analyse fluctuations of energetic and conformational observables. As zero order case the spherical cage is modeled only as a geometrical constraint without any interaction with the polymer. In further simulations we switched on a interaction between the polymer and the surface of the sphere and looked for effects induced by this interaction.

BP 11.14 Mon 17:30 Poster B2

Hybrid simulation model for spatiotemporal intracellular calcium signals — •Martin Rückl[1], Nagaiah Chamakuri[2], and Sten Rüdiger[1] — [1]Humboldt-Universität, Berlin — [2]RICAM, Linz, Austria

Calcium induced calcium release (CICR) from IP3R channels on the ER membrane and the interplay with calcium buffers can result in complex spatiotemporal calcium distributions in the cytosol which play an important role in intra- and extracellular signaling.

To model those patterns, we solve the coupled reaction diffusion and master equations for both the DeYoung-Keizer [1] and the four state [2] stochastic IP3R gating models, using an interplay between a 3D finite element method and the Gillespie algorithm. We investigate the impact of the local calcium decay after a channel closing and the diffusive coupling of clustered channels on the collective stochastic behaviour of the channels. To obtain different calcium decays we performed simulations for different buffer configurations while the diffusive coupling is altered by means of a larger inter channel distance within a channel cluster. Our results can also be used to assess the reliability of different computationally cheaper approximations frequently used in other works.

[1] D.W. DeYoung and J. Keizer, Proc. Natl. Acad. Sci. U.S.A 89, 9895 (1992).
[2] G. Ullah, I. Parker, D.D. Mak, J.E. Pearson, Cell Calcium, 52(2):152-160, 2012

BP 11.15 Mon 17:30 Poster B2

Measuring structural changes in chromatin induced by ionizing radiation: an analysis of localization microscopy images — •Yang Zhang[1], Gabriell Máté[1], Sabina Hillebrandt[2], Patrick Müller[2], Michael G. Hausmann[2], and Dieter W. Heermann[1] — [1]Institute for Theoretical Physics, Heidelberg University, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg University, Germany

The elaborate cell response to the arising of DNA double-strand breaks caused by ionizing radiation (IR) involves local remodeling and structural changes of the surrounding chromatin. In particular, experiments indicate different repair characteristics in heterochromatin (HC) and euchromatin (EC). However, there is still no detailed understanding of these changes of the genome organization. In this work we analyzed localization microscopy images by means of statistical physics and graph theory to provide a quantitative description of structural changes induced by IR. HeLa cells were exposed to different doses of IR. Positions of fluorescence stained nucleosomes were determined using localization microscopy. Simultaneously, markers of modified histones indicating HC or EC were localized. We then calculated the pair correlation functions as well as edge length distributions and mean coordination numbers for graphs obtained by triangulations of the marker positions. Our results show that HC regions undergo a relaxation immediately after exposure to ionizing radiation while EC regions show the opposite behavior. We further demonstrate that at later times after irradiation these alterations become less pronounced.

BP 11.16 Mon 17:30 Poster B2

Pulling experiments on biological molecules: model analysis and simulation — •Katharina Wenzel and Andreas Heuer — Westfälische Wilhelms Universität Münster

The implementation of AFM-pulling routines by Steered Molecular Dynamics (SMD) has created a powerful tool to provide information of the unfolding and refolding process of biological molecules. Here, a molecule is stretched under pulling with the help of an umbrella po-

tential where the choice of pull speed and cantilever stiffness can play a critical role in the unfolding pathway. To investigate the influence of these parameters several pull experiments under the same circumstances are simulated with the Trp-cage Miniprotein TC5b in vacuo. It can be shown that simulations can lead to very unstable behaviour, especially for higher force speed and stiff cantilever.

To get a more general understanding a basic setup for pulling experiments with one particle under Brownian motion is implemented. Likewise the chosen pathway over the energy barrier as well as the degree of fluctuations strongly depend on the chosen speed and stiffness.

BP 11.17 Mon 17:30 Poster B2

Mutation and Migration in Structured Populations — •Matthias Lechner, Jonas Cremer, Anna Melbinger, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Despite the risk of exploitation, altruistic individuals are a common phenomenon in nature. The solution to this so called Dilemma of Cooperation is the purpose of many models in the field of evolutionary dynamics. A recent approach to explain this dilemma is to combine population dynamics with evolutionary game theory in a stochastic description, which shows a transient initial increase of cooperation [1]. This model was then extended by a group-structured population that is subject to repetitive regrouping events, giving rise to a long-term maintenance of cooperation under certain initial conditions [2].

Here, we study the consequences of introducing mutation and migration to this model. With the use of numerical simulations we show that both have similar effects on the system's dynamics. The evolution of purely cooperative groups turns out to be pivotal in the explanation of these changes. For mutation, we support this claim by an analytical approximation, which reproduces our numerical results. In summary, we find that although mutation and migration eventually inhibit cooperation in this model, cooperative behavior is still maintained for a wide range of parameters.

[1] A. Melbinger et al., PRL 105, 178101 (2010)
[2] J. Cremer et al., Scientific Reports, 2, 281 (2012)

BP 11.18 Mon 17:30 Poster B2

Swimming patterns of bacteria in confined microchannels with obstacles — •Michael Raatz, Matthias Theves, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

Depending on environmental conditions, single bacteria can irreversibly attach to a solid-liquid or liquid-air interface and form the cores for surface associated growth into aggregates, where cells are embedded in a polymer matrix and become resistive to antibiotic treatment (biofilms). We use microfluidic channels and high-speed time lapse microscopy to investigate the movement of cells which are swimming in close proximity to the wall interface and interact with various arrangements of circular obstacles. Motility statistics show that in the presence of obstacles, the average run length of a bacterium and the probability distribution of turn angles changes when compared to an obstacle-free channel. At small collision angles with the obstacle, the cell trajectory is slightly deflected while large angle collisions can induce reversals in the direction of propagation of a cell. Furthermore, we observe cases where cells move around the obstacle in a circular path, maintaining a stable 'orbit' at a distance of one or two cell diameters from the obstacle surface.

BP 11.19 Mon 17:30 Poster B2

Evolution of increasingly complex filamentous molecules — •Philipp Zimmer[1], Emanuel 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

On the young earth, molecules with increasing complexity evolved under prebiotic conditions. How the interplay of different, competing molecular species and the spontaneous generation of new ones eventually led to the formation of cells remains poorly understood. Here we investigate a mechanism of "biased variation" and show that it provides a way to generate more complex structures. In this mechanism certain variations of existing molecular species are more likely to occur than others. Combined with an exponential amplification, this process can generate increasing complexity. We investigate this mechanism using a stochastic model for the evolution of linear molecules and we present a DNA-based experimental realization.

BP 11.20 Mon 17:30 Poster B2

In-phase and anti-phase synchronization in noisy Hodgkin-Huxley neurons — •Xue Ao, Peter Hänggi, and Gerhard Schmid — Institut für Physik, Universitätsstr. 1, 86159 Augsburg, Germany

We numerically investigate the influence of intrinsic channel noise on the dynamical response of delay-coupling in neuronal systems. The stochastic dynamics of the spiking is modeled within a stochastic modification of the standard Hodgkin-Huxley model wherein the delay-coupling accounts for the finite propagation time of an action potential along the neuronal axon. We quantify this delay-coupling of the Pyragas-type in terms of the difference between corresponding presynaptic and postsynaptic membrane potentials. For an elementary neuronal network consisting of two coupled neurons we detect characteristic stochastic synchronization patterns which exhibit multiple phase-flip bifurcations: The phase-flip bifurcations occur in form of alternate transitions from an in-phase spiking activity towards an anti-phase spiking activity. Interestingly, these phase-flips remain robust in strong channel noise and in turn cause a striking stabilization of the spiking frequency.

BP 11.21 Mon 17:30 Poster B2

Inverse statistical analysis in heart rate variability — •Haleh Ebadi — Bioinformatics Group, Department of Computer Science, University of Leipzig, Germany

This poster presents an investigation on heart cycle time series, using the inverse statistical analysis, a concept borrowed from turbulence. By inverse statistics, also sometimes called exit time statistics, we turn the variables around such that the fluctuating variable becomes the fixed variable, while the fixed variable becomes fluctuating. Using this approach, we studied the distribution of the exit time needed to achieve a predefined level of heart rate alteration. Such analysis uncovers the most likely waiting time needed to reach a certain change in the rate of heart beat. This analysis showed a significant difference between the raw data and shuffled data, when the heart rate accelerates or decelerates to a rare event. We also report that inverse statistical analysis can distinguish between the electrocardiograms taken from healthy volunteers and patients with heart failure.

BP 11.22 Mon 17:30 Poster B2

Bifurcation analysis of a thalamocortical mean field model — •Michael Schellenberger Costa, Thomas Martinetz, and Jens Christian Claussen — INB, University of Lübeck, Germany

Multiple studies have shown the importance of slow wave sleep for the development of memories. Furthermore slow oscillatory activity can be modulated by non-invasive stimulation, which leads to an enhancement of memory consolidation [1]. In order to optimize the experimental procedures and thereby further improve the memory consolidation, a detailed knowledge of the cortical response to the applied stimuli is essential. Mean field models of the cortex have been extensively studied [2], however the interplay between the thalamus and the cortex is know to be crucial for both slow wave sleep and the processing of sensory stimuli. Therefore we investigate the dynamic properties of an extended phenomenological mean field model of the thalamocortical system, that is able to resemble the EEG signal during slow wave sleep.

[1] L. Marshall et al, Nature 444, 610 (2006).
[2] M. Ursino, F. Cona and M. Zavaglia, Neuroimage 52, 1080 (2010).

BP 11.23 Mon 17:30 Poster B2

Limitations on entrainment frequency in cortical slow wave stimulation — •Arne Weigenand[1], Lisa Marshall[2], Thomas Martinetz[1], and Jens Christian Claussen[1] — [1]INB, University of Lübeck — [2]Neuroendocrinology, University of Lübeck, Germany

Stimulation of cortical slow waves during sleep has recently raised considerable attention due to enhancement of memory consolidation [1]. We consider the question how slow waves, comprised by bursty up and quiescent down states, can be entrained or strengthened by external stimulation. In a purely cortical model no limitation within the relevant frequency range occurs [2]. Stimulation by TMS or optogenetic methods [3,4] hint at an upper entrainment frequency of 4 Hz. In contrast, our optical stimulation experiments [5] revealed that entrainment is only possible up to 1 Hz. We account thalamic gating for this difference. Hence we consider the inclusion of thalamic feedback loops

into generic cortical network models, for adaptation of parameters in a phenomenological mean-field model. We optimize pulse length and frequency to obtain an optimized stimulation protocol.
[1] L. Marshall et al, Nature 444, 610 (2006). [2] Weigenand, Martinetz, Claussen, Cogn. Neurodyn. 6, 367 (2012); Schütt, Claussen, Cogn. Neurodyn. 6, 343 (2012). [3] Massimini et al., PNAS 104, 8407 (2007). [4] Kuki et al, Frequency-dependent entrainment of neocortical slow oscillation to repeated optogenetic stimulation in the anesthetized rat, Neurosci. Res. (2012, in press). [5] Weigenand et al (in preparation).

BP 11.24 Mon 17:30 Poster B2

Approach for automated sleep stage classification from spectral data — •Stephan Volkland and Jens Christian Claussen — INB, University of Lübeck, Germany

Manual scoring of sleep stages according to the Rechtschaffen-Kales rule catalogue (or the only simplified AAMS rules) is done on 30s epochs and requires extensive manual labor. Further the inter-rater and intra-rater reliabilities are not fully satisfactory for subsequent quantitative analysis. Hence it would be desired to develop and use automatic methods: attempts in this direction have been tried numerously but not paved their way to clinical practice as the EEG signatures of the sleep stages differ between subjects even in a qualitative way. Furthermore it would be desired to detect and resolve sub-stages as well as acheive a higher time resolution; both is unfeasible for manual scoring which would then be slower than real time. Here we refer and compare to an approach by [1] where three quantitative indexes are derived from EEG and EMG and broken down to 8 possible states. Our approach also is based on EMG and EEG, whereby we also use EOG, and use full information from five physiological EEG bands as input for unsupervised clustering (k-means) of data where clusters then are assigned to sleep stages [2]. We observe that the known difficulties to reliably distinguish S1, REM and wake stages persist. For the range between stages S2 and S4, we however can obtain a reliable interpolation between the sleep stages even for 16s or shorter time intervals.
[1] B. Müller, W.D. Gäbelein, H. Schulz, Sleep 29, 967 (2006).
[2] Stephan Volkland, BA thesis, INB, Lübeck (2012).

BP 12: Molecular Motors

Time: Tuesday 9:30–11:45 Location: H43

Invited Talk BP 12.1 Tue 9:30 H43

Motor and Track Systems for Navigating the Cytoskeleton — Joanna Kalita[1,2] and •Ronald Rock[1] — [1]The University of Chicago, Chicago, USA — [2]University of Wrocław, Wrocław, Poland

An emerging paradigm in motility is the notion of "specialized" motors, or motors that are fine-tuned to perform a specific function. Rather than merely traveling anywhere and everywhere, such motors are programmed to select certain tracks, to respond to forces in a defined way, or to actively remodel their tracks. Here, we further develop the ex vivo motility assay to determine how cells remodel their actin tracks and redirect myosin V traffic in response to Rho GTPase signaling. We transfected 3T3 cells with constitutively active or dominant negative forms of Rac1, RhoA, or CDC42, triton extracted the cells to expose the cytoskeletons, and applied labeled myosin V for single molecule tracking. We find that all Rho constructs increase myosin V activity. Remarkably, only a small fraction of actin filaments are used by myosin V, as we find that motors repeatedly travel in limited zones while ignoring nearby regions of high actin density.

BP 12.2 Tue 10:00 H43

Bi-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], Olga Zaitsava[3], Marcel E. Janson[3], Larisa Gheber[2], and Christoph F. Schmidt[1] — [1]Georg-August-Universität, Göttingen, DE — [2]Ben-Gurion University of the Negev, Beer-Sheva, IL — [3]Wageningen University, Wageningen, NL

The tetrameric yeast Kinesin-5 Cin8 can switch from a fast minus-end to a slow plus-end-directed motion. We found evidence that binding between two microtubules switches the motor to plus-end motility. We hypothesized that the tail domains of Cin8 influence the adjacent motor domains, depending on the binding state between microtubules. We designed two different motor constructs to test our hypothesis. To rule out any head-tail-interactions we removed the tail domains of Cin8 (Cin8Δtail). This construct retained its ability to link and slide apart two microtubules. Its motility on single microtubules, however, was under all conditions slow, intermittent, and mostly plus end directed. We also constructed a stably dimeric Cin8/Kinesin-1 chimera (Cin8Kin), consisting of head and neck linker of Cin8 fused to the stalk of Kinesin-1. This chimera showed a similar motility as Cin8Δtail. We therefore conclude that the Cin8 head domains are inherently bidirectional and that the interaction between tail and motor domains of Cin8 are responsible for stably switching the motility to either plus- or minus-end directed motion.

BP 12.3 Tue 10:15 H43

Passive and active cross-linkers can conjointly generate a stable finite overlap between antiparallel polar filaments — Debajit Goswami and •Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Saarbrücken, Germany

During cell division, pairing of sister chromosomes and their segregation is driven by the mitotic spindle. This bipolar structure microtubules consists mostly of microtubules, motor proteins and further associated proteins regulating microtubule dynamics and cross-linking. Through their combined action, a stable structure of overlapping antiparallel microtubules is generated. How this state is maintained is currently unknown. Recently, a possible mechanism based on passive cross-linkers and molecular motors was studied experimentally in vitro. We present a stochastic model for a pair of antiparallel polar filaments that interact via active and passive cross-links. We investigate in detail the dependence of the overlap region's size on parameters. We then apply our system to the specific cases of the active cross-linkers Eg5 and Ncd, respectively, as well as the passive cross-linker Ase1.

BP 12.4 Tue 10:30 H43

Positioning of microtubule organizing centers by cortical pushing and pulling forces — •Nenad Pavin[1,2], Liedewij Laan[3], Rui Ma[1,4], Marileen Dogterom[3], and Frank Jülicher[1] — [1]MPI-PKS, Dresden, Germany — [2]University of Zagreb, Zagreb, Croatia — [3]AMOLF, Amsterdam, The Netherlands — [4]Tsinghua University, Beijing, China

Positioning of microtubule organizing centers (MTOC) with respect to the confining geometry of cells depends on pushing and/or pulling forces generated by MTs that interact with the cell cortex. How, in living cells, these forces lead to proper positioning is still largely an open question. Using in vitro experiments in artificial microchambers it was shown that in a square geometry, MT asters center more reliably by a combination of pulling and pushing forces than by pushing forces alone. Theoretically, we show that pulling and pushing forces acting on the MTOC in different geometries depend on orientations of MTs. We find that these forces can have centering or off-centering behavior in different geometries. Pushing forces center in a one-dimensional and a square geometry, but lead to off-centering in a circle if reorientation is sufficiently pronounced. Pulling forces, however, do not center in a one-dimensional geometry, but improve centering in a circle and a square. In an elongated stadium geometry, positioning along the short axis depends mainly on pulling forces, while positioning along the long axis depends mainly on pushing forces. Our theoretical results suggest that different positioning strategies could be used by different cell types (Laan et al 2012 Cell, Pavin et al NJP 2012).

BP 12.5 Tue 10:45 H43

Theory of Microtubule Length Regulation by Molecular Motors — •Louis Reese[1], Anna Melbinger[2], and Erwin Frey[1] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München — [2]Institut Pasteur, Paris, France

Important players in microtubule length regulation are depolymerizing motor proteins. The accumulation of kinesin-8 along a microtubule provides sensitive regulation of the microtubule's length [1,2]. However, cellular mechanisms of length regulation are still obscure. This

is due to the complicated dynamics of microtubule assembly and disassembly and the presence of a multitude of regulatory proteins. We develop a theoretical framework that allows to address this problem systematically [2]. Employing analytic methods and stochastic simulations, different regimes of motor traffic are identified. With these results at hand it is possible to infer for which parameter regimes depolymerizing motor molecules regulate microtubule length. The resulting microtubule dynamics is analyzed with respect to fluctuations and the microtubule length. We find that particular molecular interactions between kinesin-8 and the microtubule enhance fluctuations such that they are reminiscent of microtubule dynamic instability.

[1] L. Reese, A. Melbinger, E. Frey, Biophys. J. 101 (2011)
[2] A. Melbinger, L. Reese, E. Frey, Phys. Rev. Lett. 108 (2012)

BP 12.6 Tue 11:00 H43

Efficiencies of a molecular motor with application to the F_1-ATPase — •Eva Zimmermann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

In experiments, the properties of a molecular motor are often inferred by measuring the stochastic trajectory of an attached probe particle. Recently, Toyabe et al. measured the heat dissipated by the probe particle to investigate the efficiency of the F_1-ATPase and found values for this efficiency close to 1 [1].

We discuss a simple model consisting of two degrees of freedom representing the motor and the probe which are elastically coupled. In this model, the motor protein hydrolyzes (or synthesizes) one ATP molecule per mechanical step which represents tight mechanochemical coupling. We apply the model to the F_1-ATPase and investigate three types of efficiencies both in simulations and in a Gaussian approximation [2]. In particular, we clarify the conditions under which the definition of efficiency used in [1] can become even larger than 1 and should therefore not be interpreted as efficiency in the thermodynamic sense. Overall, we obtain good quantitative agreement with the experimental data.

[1] S. Toyabe et al., Phys. Rev. Lett. 104, 198103 (2010)
[2] E. Zimmermann and U. Seifert, New J. Phys. 14, 103023 (2012)

Invited Talk BP 12.7 Tue 11:15 H43

Molecular Motors from DNA — •Andrew Turberfield — University of Oxford, Department of Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, U.K.

DNA is a wonderful material for nanoscale construction: its self-assembly can be programmed by making use of its information-carrying capability, and its hybridization or hydrolysis can be used as to provide energy for synthetic molecular machinery. With DNA it is possible to design and build three-dimensional scaffolds, to attach molecular components to them with sub-nanometre precision and then to make them move. I shall describe our work on autonomous, biomimetic molecular motors powered by chemical fuels and the use of synthetic molecular machinery to control covalent chemical synthesis. I shall demonstrate bipedal motors whose operation depends on the coordination of the chemomechanical cycles of two separate catalytic centres and burnt bridges motors that can be programmed to navigate networks of tracks. I shall also discuss the use of kinesin motor proteins to power synthetic devices.

BP 13: Imaging

Time: Tuesday 9:30–12:00 Location: H44

Topical Talk BP 13.1 Tue 9:30 H44

Ultrasensitive detection, microscopy, tracking, and manipulation of nano-objects — •Vahid Sandoghdar — Max Planck Institute for the Science of Light, Erlangen, Germany

The advent of fluorescence microscopy and spectroscopy in the 1990s ushered in single molecule detection as a powerful tool for a wide range of studies, ranging from biophysics to quantum optics. Since then a number of techniques have pushed the limits of spatial resolution and detection sensitivity for the visualization of matter down to the single molecule level. In our laboratories, we have approached these issues in two different ways. First, we have developed extinction detection and spectroscopy for investigating nonfluorescent single nano-objects such as metallic nanoparticles, viruses, quantum dots, and organic molecules [1-6]. In particular, I will present measurements of single virus motion and its interaction with receptor lipids [4], studies of nanoparticle fast motion on artificial membranes, and very recent detection of unlabeled single proteins [7]. In the second approach, we exploit cryogenic single molecule detection to push localization microscopy to the angstrom precision level [8].

[1] K. Lindfors, et al, Phys. Rev. Lett. 93, 037401 (2004). [2] P. Kukura, et al, Nano Lett. 9, 926 (2009). [3] P. Kukura, et al, Nature Methods 6, 923 (2009). [4] P. Kukura, et al, J. Phys. Chem. Lett. 1, 3323 (2010). [5] M. Celebrano, et al, Nature Photonics 5, 95 (2011). [6] M. Krishnan, et al, Nature 467, 692 (2010). [7] M. Piliarik and V. Sandoghdar, in preparation. [8] S. Weisenburger, et al, in preparation.

BP 13.2 Tue 10:00 H44

Probing Transcription Factor DNA Binding at the Single Molecule Level in Live Mammalian Cells — •J. Christof M. Gebhardt[1,4], David M. Suter[1,4], Rahul Roy[1,2], Ziqing W. Zhao[1], Alec Chapman[1], Srinjan Basu[1,3], Tom Maniatis[3], and X. Sunney Xie[1] — [1]Harvard University, Cambridge MA, USA — [2]Indian Institute of Science, Bangalore, India — [3]Columbia University Medical Center, New York NY, USA — [4]equal contribution

Imaging single fluorescent proteins in living mammalian cells is challenging due to out-of-focus fluorescence excitation by common microscopy schemes. We report the development of a novel fluorescence microscopy method, reflected light sheet microscopy (RLSM), which allows selective plane illumination throughout the nucleus of living mammalian cells, for reducing out-of-focus fluorescence signal. Generation of a thin light sheet parallel to the imaging plane and close to the sample surface is achieved by reflecting an elliptical laser beam incident from the top by 45° with a small mirror. The thin light sheet allows for an increased signal-to-background ratio superior to previous illumination schemes and enables imaging of single fluorescent proteins with up to 100 Hz time resolution. We demonstrate the sensitivity of RLSM by measuring the DNA-bound fraction of glucocorticoid receptor (GR) and determine the residence times on DNA of various oligomerization states and mutants of GR and estrogen receptor (ER), enabling us to resolve different modes of DNA binding of GR. Finally, we demonstrate two-color single molecule imaging by observing the spatio-temporal co-localization of interacting protein pairs.

BP 13.3 Tue 10:15 H44

STED Microscope with Spiral Phase Contrast — •Marcel Andreas Lauterbach[1], Marc Guillon[1], Asma Soltani[2], and Valentina Emiliani[1] — [1]University Paris Descartes, Paris Sorbonne Cité, Neurophysiology and New Microscopies Laboratory, Paris, France — [2]University Paris Descartes, Paris Sorbonne Cité, Laboratory of Membrane Dynamics and Neurological Diseases, Paris, France

We present a STED (STimulated Emission Depletion) microscope with phase contrast imaging capabilities. Phase contrast permits the visualization of weak phase objects without any labeling. It is implemented without extra optical elements in the STED light path, which would compromise STED imaging capabilities. Scanning phase contrast allows for registration with the fluorescence images and principally for simultaneous recording of phase contrast and STED images.

Phase contrast images of objects as thin as a few nanometers in optical path mismatch are obtained. The method provides a second imaging channel in a STED microscope for phase contrast imaging even in index-matched mounted cell cultures. This allows for correlation of morphological structures with high-resolution fluorescence images.

BP 13.4 Tue 10:30 H44

Object-adapted optical trapping and shape-tracking of helical bacteria — •Matthias Koch and 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. Therefore, advanced photonic measurement techniques are needed which are also capable of extracting forces and energetics on a broad temporal bandwidth.

We show how the trapping potential of an optical tweezers setup

can be adapted to the shape of a tiny elongated helical bacterium (Spiroplasma melliferum - SM) in order to hold and orient it in the focal plane of a microscope [1]. Further, the coherently scattered laser light is used to analyse its fast and complex cellular shape changes with nm precision at rates up to 1 kHz. By localizing each slope of the only 200nm thin bacterium we generate high contrast, super-resolution movies in three dimensions - without any object staining.

To demonstrate this method, we analysed SM bacteria and show how temporal changes in the transition between different energetic modes during external disturbances can be identified and imaged in 3D. As a response to an external perturbation, the minute long death of the bacterium is recorded and analysed by decaying energy fluctuations, which represents a novel approach in bacteriology.

[1] Koch, M. and A. Rohrbach (2012). "Object-adapted optical trapping and shape-tracking of energy-switching helical bacteria." Nature Photonics 6(10): 680-686.

BP 13.5 Tue 10:45 H44

Subsurface Imaging of Cells Using Atomic Force Acoustic Microscopy at GHz Frequencies — •Matthias Büchsenschütz-Göbeler[1], Jan Rother[3], Andreas Janshoff[3], Walter Arnold[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

We describe a technique to image subsurface structures in living biological cells (e.g. Madin Darbin canine kidney cells, type II) using Atomic Force Acoustic Microscopy operating at 1 GHz. The cells are insonified with 1 GHz ultrasonic waves which are amplitude modulated at a fraction or multiple frequency of cantilever contact-resonance [1]. The transmitted signals are demodulated by the nonlinear tip-surface interaction, enabling one to image the inner structure of the cell based on their ultrasonic scattering power. The latter one is determined by the ultrasonic frequency, the acoustic mismatch between the elastic properties of the host material (cytoplasm) and the subsurface objects to be visualized (e.g. nucleus), by their geometry and by diffraction effects. Interference fringes can be seen in both the amplitude and phase images. Besides images, we will present an interpretation of the contrast mechanism for imaging. Financial support by the DFG SFB 937 is thankfully acknowledged.

[1] Imaging of Subsurface Structures Using Atomic Force Acoustic Microscopy at GHz Frequencies, S. Hu and C. Su, and W. Arnold, J. Applied Phys. 109, 084324 (2011)

BP 13.6 Tue 11:00 H44

Magnetic spin imaging at ambient conditions — Steffen Steinert[1], •Florestan Ziem[1], Andrea Zappe[1], Nicolas Götz[1], Liam Hall[2], Lloyd Hollenberg[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]School of Physics, University of Melbourne, Victoria 3010, Australia

A variety of magnetic imaging and sensing methods exist, including NMR, SQUIDs, atomic vapors and magnetic resonance force microscopy. While NMR is a standard technique for imaging in living organisms and the other techniques achieve sensitivities down to single spins, currently no technique combines few spin sensitivity, submicron spatial resolution and ambient operational conditions. Negatively charged nitrogen-vacancy centers (NVs) in diamond are promising candidates to fill this gap. Since the spin state of the atomic-sized defect can be optically polarized and read out, NV centers allow for high resolution magnetic sensing via Zeeman-shift, spin precession and relaxometry. We employ an ensemble of implanted NVs for wide-field magnetic sensing and imaging. Applications to microfluidic spin detection and magnetic spin imaging with diffraction limited resolution are presented. Several spin species are analyzed in regard to their possible application as magnetic sensing markers.

BP 13.7 Tue 11:15 H44

Motion induced oscillations of *Physarum polycephalum* detected by AlGaN-GaN High Electron Mobility Transistors — •Thomas Lippelt[1,2], Hartmut Witte[1], Marcus J. B. Hauser[2], and Alois Krost[1] — [1]Otto-von-Guericke-Universität Magdeburg, Inst. Exp. Phys., Abt. Halbleiterepitaxie — [2]Otto-von-Guericke-Universität Magdeburg, Inst. Exp. Phys., Abt. Biophysik

Due to the high sensitivity and biocompatibility of planar AlGaN/GaN High Electron Mobility Transistors (HEMTs) arrangements, such a device may be used as a biosensor in vast, living systems like amoebal cells, for sensing cellactivity. The scope of AlGaN/GaN HEMT structures for in situ detection of cell movement and growth of extended, living organisms like slime molds was studied in this contribution. As a object of investigation, we chose the *Physarum polycephalum*, a slime mold which represents one giant single cell with remarkable abilities to build network-like structures. While migrating over the HEMT sensing area, the slime mold was video monitored and the source-drain-impedance at 10 kHz has been recorded. By correlating the gray values of the video pictures and the source-drain-impedance it was found that the periodic cell movements affect the source-drain-impedance and cause oscillations with characteristic cycle periods from 100s to 140s.

BP 13.8 Tue 11:30 H44

Observing lipid diffusion in membranes with microsecond time and nanometer spatial resolution — •Susann Spindler[1], Chia-Lung Hsieh[2], Jens Ehrig[1], and Vahid Sandoghdar[1] — [1]MPI for the science of light, Erlangen, Germany — [2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan

Lipid membranes play an important role in biological cells not only by defining the boundaries of the cell and cell organelles, but also by taking an active part in membrane trafficking and signaling. Remarkably, while a great deal is known about lipid membranes, a large number of fundamental questions remains open. These are for example issues concerning the local nanoscopic heterogeneity of the membrane induced via lipid–lipid and lipid–protein interactions. While this nanoorganisation is believed to be crucial for the high functionality of the cell membrane, it is still far from being well understood. To address this issue, a high spatial and temporal resolution is needed.

In our laboratory, we have developed a powerful approach for single-particle-tracking based on interferometric scattering (iSCAT) microscopy, which meets these requirements. By attaching small gold nanoparticles of 20 nm diameter to lipid molecules and detecting their weak linear scattering signal by iSCAT, we are able to localize the position of the molecules with nanometer-accuracy within microseconds. This allows us to detect even very small deviations from free diffusion, opening the door to studying membrane dynamics with unprecedented clarity. We will present experimental data for a variety of systematic studies.

BP 13.9 Tue 11:45 H44

Quantifying Lipid and Protein Diffusion in Black Lipid Membranes — •Kerstin Weiss and Jörg Enderlein — Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany

Lipid diffusion is crucial in many biological processes. However, accurately determining diffusion coefficients in membranes remains difficult. We used dual-focus fluorescence correlation spectroscopy (2f-FCS) to measure lipid diffusion in black lipid membranes (BLMs), i.e. lipid bilayers spanned over a pore. To generate these bilayers a commercially available setup is employed. We first tested the effect of different ionic strengths in neutral and negatively charged bilayers. Moreover, we investigated the influence of mono- vs. divalent ions. While monovalent ions have no effect on lipid diffusion in both systems, addition of divalent ions severely decreased the lipid*s diffusion coefficient in negatively charged BLMs. Furthermore, the investigated the validity of the Saffman-Delbrück model which is used to describe protein diffusion in lipid membranes.

BP 14: Biomaterials and Biopolymers I (joint with CPP)

Time: Tuesday 9:30–13:00 Location: H34

Invited Talk BP 14.1 Tue 9:30 H34

Hierarchical Multi-Step Folding of Polymer Bilayers — Georgi Stoychev[1,2], Sebastien Turcaud[3], John Dunlop[3], and •Leonid Ionov[1] — [1]Leibniz Institute of Polymer Research Dresden, Hohestr. 6, 01069, Dresden, Germany — [2]Technische Universität Dresden, Physical Chemistry of Polymer Materials, 01062, Dresden, Germany — [3]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14424, Potsdam, Germany

We investigated the actuation of patterned bilayers placed on a substrate. We found that films display several kinds of actuation behavior such as wrinkling, bending and folding that result in a variety of shapes. Based on experiments and modeling, we argued that rectangular bilayers start to roll from the corners due to quicker diffusion of water. Rolling from long-side starts later and dominates at high aspect ratio[1].

It was also demonstrated that one can introduce hinges into the folded structure by proper design of the bilayers external shape without having to use site selective deposition of active polymers. Experimental observations lead us to derive four empirical rules backed up by theoretical understanding as well as simulations. We then demonstrated how those rules can be used to direct the folding of edge-activated polymer bilayers through a concrete example - the design of a 3D pyramid[2].

[1] Stoychev et al, "Hierarchical Multi-Step Folding of Polymer Bilayers", Adv.Func.Mat., published online Nov 26, 2012

[2] Stoychev et al, "Shape-Programmed Folding of Stimuli-Responsive Polymer Bilayers", ACS Nano, 2012, 6(5), 3925-3934

BP 14.2 Tue 10:00 H34

Mechanical properties of poly-L-lysine (PLL) / hyaluronic acid (HA) multilayer films measured by AFM — •Johannes Hellwig, Cagri Üzüm, and Regine von Klitzing — Stranski-Laboratorium, Institut für Chemie,TU Berlin, Strasse des 17. Juni 124, 10623 Berlin, Germany

In recent years smart biomaterials have become a highly developing field of interest for biomedical applications, e.g. drug delivery. The layer-by-layer (LbL) technique gives the opportunity to build up self assembled polyelectolyte multilayer films (PEM) with defined architecture, physical and chemical properties. PEM made of poly-L-lysine (PLL) and hyaluronic acid (HA) were produced by using the LbL technique. Potential applications of these PEMs require controlling of the adhesion behaviour by tuning their elastic/viscoelastic properties. In this study mechanical properties of LbL coated poly(L-lysine)/hyaluronan PLL/HA films were studied by scanning- and colloidal-probe atomic force microscopy as a function of indentation velocity, number of polymer deposition steps and temperature. Film growth was investigated by two independent AFM methods: scratch-and-scan and full-indentation[1]. Film thickness increases linearly with polymer deposition steps. The Young*s modulus ranges between 15 and 40 kPa and does not depend on the film thickness. Stress relaxation and creep compliance measurements indicate a viscoelastic film behaviour with multiple relaxation mechanisms.

[1] Üzüm, C.; Hellwig, J.; Madaboosi, N.; Volodkin, D.; v. Klitzing, R. Beilstein J. Nanotechnol. 2012, 3, 778*788.

BP 14.3 Tue 10:15 H34

Single-Virus Force Measurements on sialic acid — •Valentin Reiter[1], Sumati Bhatia[3], Manuel Gensler[1], Christian Sieben[2], Daniel Lauster[2], Andreas Herrmann[2], Rainer Haag[3], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt-Universität zu Berlin — [2]Department of Biology, Humboldt-Universität zu Berlin — [3]Department of Chemistry, Freie Universität Berlin

We study the multivalent effects in the binding and dissociation processes of sialic acid with the viral membrane protein hemagglutinin using scanning force microscopy (SFM) based single-virus force measurements (SVFM). Since an infectious disease has to start with the attachment of a virus to the cell membrane, this binding as well as its dissociation has to be carefully analyzed [1]. This is done by creating a mixed self assembled monolayer (MSAM) on gold from synthesized compounds, terminated by lipoic acid. The compounds are functionalized with sialic acid and disfunctionalized with hydroxide. Inactivated influenza viruses are attached to a silicon nitrate SFM cantilever via a polyethylene glycol spacer. With this setup SVFM is performed in aqueous solution. The ratio of functionalized to disfunctionalized molecules on the MSAM enables the control of the degree of multivalency of the binding and therefore the realization of mono-, bi-, and trivalent connections. On the other hand SVFM are performed at different loading rates to estimate specific binding parameters, such as the average rupture length and bond life time.

[1] C. Sieben et al., *PNAS*, **2012**, *109*, *34*, 13626-13631.

BP 14.4 Tue 10:30 H34

Response of major ampullate silk of Nephila pilipes to pressure and tensile stress as measured by FTIR spectroscopy — •Markus Anton[1], Wilhelm Kossack[1], Christof Gutsche[1], Roxana Figuli[2], Periklis Papadopoulos[3], and Friedrich Kremer[1] — [1]Universität Leipzig, Institut für Experimental Physik I, Linnéstraße 5, 04103 Leipzig, Germany — [2]Karlsruher Institut für Technologie, Institut für Technische Chemie und Polymerchemie, Engesserstraße 18, 76128 Karlsruhe, Germany — [3]Max Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Nanocrystals composed mainly of β-sheet polyalanine are reposonsible for the high toughness of major ampullate (dragline) spider silk. Fourier-Transform infrared (FTIR) spectroscopy is employed to study their response to (i) uniaxial stress and (ii) hydrostatic pressure. In the former a red shift and in the latter a blue shift of the vibration of polyalanine β-sheets at 965 cm^{-1} is observed. In both cases a linear dependence is evident, which bends off for hydrostatic pressure greater than 1.4 GPa and is fully reversible up to 7 GPa. The seamless connection of negative and positive pressure regimes corroborate quantitatively our structural model of spider silk [P. Papadopoulos et al., Eur. Phys. J. E 24 (2007) 193, P. Papadopouloset al., Colloid Polym. Sci. 287 (2009) 231, R. Ene et al., Soft Matter 5 (2009) 4568] as composed of *pre-stressed* alanine-rich nanocrystals embedded in a glycine-rich amorphous matrix. It is also confirmed that nanocrystals withstand high pressures without undergoing structural transition or deteriorating their mechanical properties.

BP 14.5 Tue 10:45 H34

Polarized confocal Raman microscopy and EBSD: A comparative study studying calcite crystalline regions within the tergite cuticle of terrestrial isopods. — •Christian Reisecker[1], Erika Griesshaber[2], Bastian Seidl[3], Andreas Ziegler[3], and Sabine Hild[1] — [1]Institute of Polymer Science, Johannes Kepler Universität Linz, Altenbergstr. 69, 4040 Linz, Austria — [2]Department of Earth and Environmental Sciences, LMU, Theresienstr. 41, 80333 München, Germany — [3]Facility for Electron Microscopy, University of Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Recently, isopods gained increasing amount of interest in terms of biomometics as they combine quite diverse properties within their tergite cuticle such as hardness in the outer parts of the cuticle and softness in the more inner part, where muscles will be attached. This is achieved via a strong hierarchical arrangement of organic-chitin-protein fibers, which are arranged in a twisted plywood structure and inorganic materials. The organic matrix is hardened by carbonates in crystalline (calcite) and non-crystalline modification (amorphous calcium carbonate, ACC). This study focusses on the outer, mainly crystalline parts within the tergite cuticle of isopods. Confocal Raman microscopy is a useful tool to study the chemical and structural composition of isopods, as it provides a spatial resolution below 300 nm. Polarized confocal Raman microscopy and EBSD will be utilized to determine different domains and layers of calcite crystals. It has been demonstrated that depending on the species, the calcite region consists of domains with different orientations concerning its bravais lattice.

BP 14.6 Tue 11:00 H34

Mineralization of calcium containing compounds at the liquid-liquid interface — •Steffen Bieder[1], Florian Wieland[2], Patrick Degen[3], Michael Paulus[1], Julia Nase[1], Andre Steffen[1], Bridget Murphy[4], Heinz Rehage[3], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, — [2]Helmholtz Zentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht — [3]Fakultät Chemie, Technische Uni-

versität, D-44221 Dortmund — [4]Institut für Experimentelle und Angewandte Physik, CAU, Leibnizstraße 19, D-24098 Kiel

Nature forms structures from inorganic and organic components for different purposes, e.g. protection or stabilization. Accordingly, organisms have developed the concept of biomineralization providing highly controlled growth processes under ambient conditions. For instance the formation of teeth, bones or shells demonstrates the high degree of perfection and control, which can not be reached by human technology until now. We studied the mineralization of calcium containing compounds at the liquid-liquid interface. A solution of water and calciumhydrogencarbonat is covered by toluene. We added different fatty acids in order to investigate their influence on the growing layer at the liquid-liquid interface. We observed the layer formation by grazing incidence diffraction (GID) and x-ray reflectivity (XRR). The extracted data show an formation of calcium soaps at the interface. GID data reveal that the forming crystallites are highly orientated with the 00l axis perpendicular to the sample surface. We acknowledge BMBF(05 K10 FK2) and (05K10PEC) for financial support.

15 min. break

BP 14.7 Tue 11:30 H34

Probing the electronic structure of Proline in aqueous solution by soft RIXS — •Frank Meyer[1], Andreas Benkert[1,2,8], Sankaranarayanan Nagarajan[3], Regan Wilks[4], Marcus Bär[4], Wanli Yang[5], Michael Zharnikov[3], Clemens Heske[2,6,7], Lothar Weinhardt[2,6,7], and Friedrich Reinert[1,8] — [1]Exp. Phys. VII, Universität Würzburg — [2]Inst. for Photon Science, KIT — [3]Angew. Phys. Chemie, Universität Heidelberg — [4]Solar Energy Research, HZB — [5]ALS, Lawrence Berkeley National Laboratory — [6]Dept. of Chemistry, University of Nevada, Las Vegas — [7]ANKA Synchrotron Radiation Facility, KIT — [8]Gemeinschaftslabor für Nanoanalytik, KIT

Amino acids are organic molecules that are highly relevant for many biological macro-molecules. Defining their function, the electronic structure of these molecules and, in particular, the interaction with biologically relevant solvents is of fundamental interest. In contrast to the majority of amino acids in which the functional groups (carboxyl, amino, side chain) are connected via one carbon atom, in proline the amino group and the side chain are connected in a heterocyclic compound, forming a pyrrolidine ring. We present resonant inelastic soft x-ray scattering (RIXS) maps of proline in aqueous solution at different pH values. Upon protonation and deprotonation, strong changes in the maps are observed. The results will be compared with RIXS data of solid state and gas phase proline, as well as other amino acids (i.e., glycine, cysteine). We find a distinctly different electronic structure than that observed for glycine and cysteine, as well as a significantly influence of the water environment.

BP 14.8 Tue 11:45 H34

Structure formation in homologous peptides: Ac-Ala$_6$-Lys(H$^+$) versus Ac-βAla$_6$-Lys(H$^+$) — •Franziska Schubert, Carsten Baldauf, Mariana Rossi, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

β-peptides are non-natural peptides composed of β-amino acid residues that feature one additional methylene group in the backbone compared to natural α-amino acids. Due to their larger flexibility, β-peptides are valuable for the design of new peptides with specific chemical or pharmacological properties. We here investigate the differences in structure formation between α- and β-peptides from first principles employing density-functional theory (DFT) with the PBE functional corrected for van der Waals interactions[1]. We focus this presentation on a comparison of Ac-βAla$_6$-Lys(H$^+$) and Ac-Ala$_6$-Lys(H$^+$) under *in vacuo* "clean-room" conditions and compare to experimental ion mobility spectrometry[2]. Our conformational search is based on replica exchange molecular dynamics. After generating a large pool of force field-based structures, we relax thousands of conformers with DFT. For the β-peptide, the finite-T vibrational free energy part is essential to recover a conformational hierarchy consistent with experiment. While Ac-Ala$_6$-Lys(H$^+$) is found to be α-helical at 300K, Ac-βAla$_6$-Lys(H$^+$) is seen to vary between 3_{10}, α, and π analog helices. Our simulations show that conformational entropy plays a critical role, and an *ab initio* quantitative assessment is a big challenge that we (and the field) must meet next. [1] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009); [2] S. Warnke, K. Pagel, G. von Helden, Fritz-Haber-Institut.

BP 14.9 Tue 12:00 H34

Structure and Dynamics of Myelin Basic Protein as a Model System for Intrinsically Disordered Proteins — •Andreas Stadler[1], Laura Stingaciu[2], Aurel Radulescu[3], Olaf Holderer[3], Clement Blanchet[4], Ralf Biehl[1], and Dieter Richter[1] — [1]Forschungszentrum Jülich, JCNS-1/ICS-1, 52425 Jülich, Germany — [2]Forschungszentrum Jülich, JCNS, Outstation at the Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [3]Forschungszentrum Jülich, JCNS, Outstation at FRM II, 85747 Garching, Germany — [4]EMBL, Hamburg Unit, EMBL c/o DESY, Notkestrasse 85, Hamburg 22607, Germany

Myelin basic protein (MBP) is a major component of the myelin sheath in the central nervous system. In aqueous solution MBP is primarily unstructured. From a biophysical point of view, the disordered protein can serve as a model system to study the physical properties of disordered or unfolded proteins.

Neutron and X-ray scattering experiments were performed on the protein in solution. Small angle scattering and neutron spin-echo spectroscopy allowed us to gain quantitative information on the structural and the dynamical properties of MBP. The results of these experiments will be presented and compared to different models of polymer theory.

BP 14.10 Tue 12:15 H34

Structure and disintegration of nanoparticles from clinically relevant polymers — •Margarita Dyakonova[1], Anna Bogomolova[2], Sergey Filippov[2], Aurel Radulescu[3], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Physik weicher Materie, Garching — [2]Institute of Macromolecular Chemistry, Prague, Czech Republic — [3]JCNS at FRM II, Garching

We investigate clinically relevant polymers based on N-(2-hydroxypropyl methacrylamide) (HPMA) which carry both a cancer drug, namely doxorubicin, and a hydrophobic targeting group, namely cholesterol derivatives. We focus on the dependence of the structure of the nanoparticles formed by these conjugates on the polymer architecture, the cholesterol content of cholesterol and the pH value [1]. Fluorescence correlation spectroscopy showed that the onset of nanoparticle formation depends on the cholesterol content. A step-like increase of the hydrodynamic radius with conjugate concentration indicates that the existing nanoparticles associate rather than to grow continuously. SANS revealed that even small amounts of cholesterol derivatives results in the formation of nanoparticles. At neutral pH values, these are ellipsoids, whereas under acidic conditions, cholesterol is released and forms large crystals. Time-resolved SANS during a stopped-flow experiment showed that, in dependence of the hydrophobicity of the cholesterol derivatives, a change in pH leads to changes of the conformation of the HPMA chains.

[1] S. Filippov, M. Dyakonova, C.M. Papadakis et al., *Biomacromolecules* **13**, 2594 (2012)

BP 14.11 Tue 12:30 H34

Reduction - oxidation photocycle dynamics of flavins in starch films — •Alfons Penzkofer — Fakultät für Physik, Universität Regensburg, Universitätsstrasse 31, D-93053 Regensburg, Germany

The blue-light photo-reduction and dark re-oxidation of the flavins riboflavin and lumiflavin in starch (α-amylose) films was studied by absorption and luminescence spectroscopy. Blue-light sample excitation caused an absorption, fluorescence, and phosphorescence decrease which recovered in the dark. The photo-reduction and dark re-oxidation cycle could be repeated. The efficiency of photo-reduction decreased with exposed excitation energy, and the speed of re-oxidation in the dark slowed down with time after excitation. The absorption did not fully recover. The fluorescence efficiency after long time of storage in the dark increased beyond the initial oxidized flavin fluorescence efficiency. Flavin photo-excitation is thought to cause a starch-flavin restructuring (static fluorescence quenching center formation) enabling enhanced photo-induced starch to flavin electron transfer with subsequent flavin reduction and starch oxidation (oxystarch formation). In the dark after light switch-off, thermal reversion of flavin reduction and starch oxidation occurred and fluorescence quenching decreased.

BP 14.12 Tue 12:45 H34

Study of phase transitions on DPPC bilayers deposited by PVD on top of low viscosity chitosan scaffolds of different thicknesses — •Maria J. Retamal, Carmen Gonzalez, Mauricio Sarabia, Marcelo Cisternas, and Ulrich G. Volkmann — Surface Lab, Fac. de Fisica, P. Universidad Catolica de Chile, Chile

The porous nature of chitosan and its non-solubility in water could be an efficient matrix able to absorb water molecules and their delivery to a system. Chitosan of low viscosity (CH) and 1,2 *dipalmitoyl-sn-3-phosphoglycerocholine (DPPC) over silicon wafer (SiO2/Si(100)) as substrate were used to conform an artificial membrane, silicon wafer/CH-DPPC. The deposition was made by Physical Vapor Deposition (PVD) and thickness was controlled in situ with Very High Resolution Ellipsometry (VHRE), achieving chitosan films with precise thicknesses between 10Å and 200Å, and a 60Å thin DPPC bilayer on top. We focus on the precise thickness control of the thin films, and the related formation of interstitial channels, that favor the prolonged humidification in the system and the discovery of the most suitable thickness of the chitosan scaffold for best artificial membrane formation and stability. The characterization of the artificial membrane was realized using VHRE, IE (Imaging Ellipsometry) and Atomic Force Microscopy (AFM), with the finality to determine the possible phase transition temperatures.

M.J. R. and C. G. acknowledges CONICYT and VRI Nr. 10/2010 (PUC), respectively. Work supported by FONDECYT project Nr. 1100882.

BP 15: DNA/RNA and related enzymes

Time: Tuesday 12:00–14:00 Location: H43

Topical Talk BP 15.1 Tue 12:00 H43

Protein diffusion on DNA — •Ralf Seidel — Institut für Molekulare Zellbiologie, Westfälische Wilhelms-Universität Münster, Germany — BIOTEC, Technische Universität Dresden, Germany

Diffusion is a major transport mechanism within living systems. Recently protein diffusion along elongated cellular structures (e.g. cytoskeletal filaments or DNA) that is often termed one-dimensional diffusion, has gained increasing interest. This is, because confinement of the diffusion path can enhance the success rate of localizing a target on the particular structure. Here we focus on a new aspect, namely that protein diffusion along DNA can be itself a central part of an enzymatic reaction. Using magnetic tweezers and fluorescence techniques we provide single-molecule observations of different enzymes on DNA: (i) a monomeric restriction enzyme that needs to turn itself on DNA to cut both strands of the helix, (ii) a restriction enzyme that uses energy from ATP hydrolysis to license fast diffusion originating from its target site and that finally triggers DNA degradation at a distant target and (iii) a helicase, i.e. an ATP-powered motor enzyme which unwinds duplex DNA, that uses diffusion on single stranded DNA to position itself in a correct orientation on its substrate. These examples suggest an important role of one-dimensional diffusion during fundamental biochemical reactions.

BP 15.2 Tue 12:30 H43

Intracellular Conformations of Human Telomeric Quadruplexes studied by Electron Paramagnetic Resonance Spectroscopy — •Malte Drescher — Fachbereich Chemie, Graduiertenschule Chemische Biologie und Zukunftskolleg, Universität Konstanz

Guanosine-rich nucleic acids fold into four-stranded structures called quadruplexes. In contrast to duplex structures, quadruplexes show a high degree of polymorphism with respect to topological features. The G-rich human telomeric repeats at the end of the chromosomes have generated much interest. As a result of their potential to switch between folded and unfolded state, the formation of quadruplex structures is suspected to play important roles in telomere maintenance and cell cycle control.

G-quadruplex topologies of the human telomeric sequence were investigated exploiting long-range distance measurements by electron paramagnetic resonance spectroscopy (EPR) in combination with site-directed spin labeling.

Using novel in-cell EPR we show for the first time that the human telomeric repeat in cellula forms a mixture of co-existing parallel and antiparallel quadruplex conformations.

BP 15.3 Tue 12:45 H43

A realistic potential for DNA-related biophysical processes — •Maria Fyta[1,2], Chia Wei Hsu[2], Greg Lakatos[2], Simone Melchionna[3,4], and Efthimios Kaxiras[2,4] — [1]Institut für Computerphysik, Universität Stuttgart, Germany — [2]Department of Physics, Harvard University, Cambridge MA 02138, U.S.A — [3]IPCF-CNR, Università La Sapienza, P.le A. Moro 2, 00185 Rome, Italy — [4]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, U.S.A.

Ab initio total-energy calculations based on density functional theory (DFT) are used to derive the coarse-grained interactions between DNA nucleotides. The interactions take into account base and sequence specificity, and are decomposed into physically distinct contributions that include hydrogen bonding, stacking interactions, backbone, and backbone-base interactions. The interaction energies of each contribution are calculated from DFT for a wide range of configurations. These interactions are then fitted by simple analytical expressions and can be used in a coarse-grained model for double-stranded DNA. Within this model each nucleotide is reduced into two sites, the base site and the sugar-phosphate site. Although this model is not derived from experimental data, it successfully reproduces the stable B-DNA structure and gives good predictions for the persistence length. It has already been used to model stretching experiments of B-DNA, as well as bubble formation within a thermalized DNA molecule. The potential may be used to realistically probe dynamics of DNA strands in various environments at the μs time scale and the μm length scale.

BP 15.4 Tue 13:00 H43

Deprotonation mechanism and the unfolding free energy landscape of a DNA i-motif — •Jens Smiatek[1] and Andreas Heuer[2] — [1]Institut für Computerphysik, Universität Stuttgart, Germany — [2]Institut für Physikalische Chemie, WWU Münster, Germany

We present the results of atomistic Molecular Dynamics simulations of a single-stranded protonated DNA i-motif. We are able to determine the full unfolding and deprotonation mechanism by using a Metadynamics approach. The release of protons which form the stabilizing hemiprotonated cytidine pairs can be identified as a two-step process which is obligatory for a partial unfolding of the i-motif into a hairpin structure. The shape of the free energy landscape indicates the native configuration as the global energetic minimum with a free energy barrier of roughly 9 kcal/mol which validates the significant stability of the i-motif in acidic solution. We further present a kinetic model for the unfolding process in good agreement to experimental results.

BP 15.5 Tue 13:15 H43

Identifying chromatin structure during DNA repair by super-resolution microscopy — •Judith Seel and Günther Dollinger — Universität der Bundeswehr München, Neubiberg, Germany

High LET irradiation of living cells using heavy ions generates a high amount of DNA DSB in close vicinity to each other. Various repair proteins and damage markers cluster to the damage sites, such as gamma-H2AX and 53BP1, forming so-called ionizing radiation induced foci of a gross size of about 1um. While structures of this size can be easily resolved using a conventional fluorescence microscope, its substructures cannot be resolved due to the diffraction limit of about 250nm in conventional fluorescence microscopy. For analyzing foci fine-structures systematically, Stimulation Emission Depletion Microscopy (STED) is utilized, which provides a lateral resolution of about 60nm fwhm.

With these improvements the microscopic images clearly indicate a fine-structure when 53BP1 is stained with two colors and the quantitative analysis proves its existence at a scale of a few hundert nm. Using the same methods with images where one color labels 53BP1 and the other gamma-H2AX, it can be shown that there is no total correlation between these two markers on a small scale.

Using these experimental and analytical methods it is possible to determine the way of clustering of one single DNA damage marker to DSB to clarify the structure of a DSB and the structure of chromatin architecture. Secondly, the comparison of two damage markers gives a deeper understanding of the interaction of repair markers and at the end maybe the possibility to decode the structure of DNA repair.

BP 15.6 Tue 13:30 H43

Entropy in DNA Double-Strand Break Detection and Signaling — •Yang Zhang, Christina Schindler, and Dieter W. Heermann — Institute for Theoretical Physics, Heidelberg Univer-

sity, Heidelberg, Germany

In biology, the term entropy is often understood as a measure of disorder - a restrictive interpretation that can even be misleading. Recently it has become clearer and clearer that entropy, contrary to conventional wisdom, can help to order and guide biological processes in living cells. DNA double-strand breaks (DSBs) are among the most dangerous lesions and efficient damage detection and repair is essential for organism viability. However, what remains unknown is the precise mechanism of targeting the site of damage within billions of intact nucleotides and a crowded nuclear environment, a process which is often referred to as recruitment or signaling. Here we show that the change in entropy associated with inflicting a DSB facilitates the recruitment of damage sensor proteins. By means of computational modeling we found that higher mobility and local chromatin structure accelerate protein association at DSB ends. We compared the effect of different chromatin architectures on protein dynamics and concentrations in the vicinity of DSBs, and related these results to experiments on repair in heterochromatin. Our results demonstrate how entropy contributes to a more efficient damage detection. In conclusion, we identify entropy as the physical basis for DNA double-strand break signaling.

BP 15.7 Tue 13:45 H43

Towards Darwinian Molecular Evolution in a Thermal Trap — Christof Mast[1], •Severin Schink[2], Ulrich Gerland[2], and Dieter Braun[1] — [1]Systems Biophysics, LMU Munich, Germany — [2]ASC for Theoretical Physics, LMU Munich, Germany

The formation of polymers such as RNA and their replication is essential for the emergence of life. According to the RNA-world hypothesis the first polymerases were basic RNA strands of several hundred bases. Even with the help of surface catalysis and high monomer concentrations no polymerization of RNA longer than 20 bases could be demonstrated using prebiotic chemistry. Replication reactions are avoided by template inhibition and dilution. Thermal traps can overcome both problems: Temperature gradients in porous rock locally enhance the polymer concentration exponentially better for longer polymers. Since the mean polymer length depends on its local concentration, polymerization and trapping are mutually self-enhanced leading to a hyper-exponential escalation of polymer length. The theory is experimentally confirmed with sticky ended DNA. An extrapolation to the RNA world shows that a short 5 cm crack is likely to generate 100mers of RNA with micromolar concentrations even under unfavorable conditions. We experimentally show that thermals traps can drive exponential replication reactions: Convective flow drives a PCR while concurrent thermophoresis accumulates the replicated 143bp DNA and prevents the diffusion into the bulk solution. The time constant for accumulation is 92s while DNA is doubled every 50s.

BP 16: Evolutionary Game Theory (joint with SOE and DY)

Time: Tuesday 15:00–16:00 Location: H37

BP 16.1 Tue 15:00 H37

How selection pressure changes the nature of social dilemmas in structured populations — •Flavio Pinheiro[1,2], Francisco Santos[1,3], and Jorge Pacheco[1,4] — [1]ATP-Group CMAF at Universidade de Lisboa, Lisbon, Portugal — [2]Centro de Física at Universidade do Minho, Braga, Portugal — [3]Departamento de Engenharia Informática & INESC-ID, IST-UTL, Lisboa Portugal — [4]Departamento de Matemática e Aplicações at Universidade do Minho, Braga, Portugal

When members of a population engage in dyadic interactions reflecting a prisoner's dilemma game, the evolutionary dynamics depends crucially on the population structure, described by means of graphs and networks. Here, we investigate how selection pressure contributes to change the fate of the population. We find that homogeneous networks, in which individuals share a similar number of neighbors, are very sensitive to selection pressure, whereas strongly heterogeneous networks are more resilient to natural selection, dictating an overall robust evolutionary dynamics of coordination. Between these extremes, a whole plethora of behaviors is predicted, showing how selection pressure can change the nature of dilemmas populations effectively face. We further show how the present results for homogeneous networks bridge the existing gap between analytic predictions obtained in the framework of the pair-approximation from very weak selection and simulation results obtained from strong selection.

BP 16.2 Tue 15:15 H37

How 'first carrot, then stick' incentives promote cooperation — •Tatsuya Sasaki[1,2], Xiaojie Chen[1], Åke Brännström[3,1], and Ulf Dieckmann[1] — [1]International Institute for Applied Systems Analysis, Laxenburg, Austria — [2]University of Vienna, Vienna, Austria — [3]University of Umeå, Umeå, Sweden

Social institutions often use rewards and penalties to promote cooperation. As providing such incentives tends to be costly, it is important to find efficient strategies for gauging positive and negative incentives as a situation demands. Most game-theoretical studies of cooperation have, however, modeled rewarding and punishing in isolation and by focusing on peer sanctioning, through which each player separately decides whether or not to sanction a co-player.

Here, we study how a sanctioning policy we call 'first carrot, then stick' affects the evolution of cooperation in public good games. Assuming the existence of institutions that can provide incentives on a limited budget, we examine an adaptive sanctioning policy that switches the incentive from rewarding to punishing when defectors decrease below a certain frequency. We find that in well-mixed populations this policy is more efficient in promoting and maintaining full cooperation than either rewards or penalties alone. We also demonstrate that this finding extends to spatially structured populations. Such an institutional hybrid incentive with adaptive feedback is a simple yet unifying solution for encouraging cooperative behaviors.

BP 16.3 Tue 15:30 H37

Learning, Evolution and Population Dynamics — Juergen Jost and •Wei Li — MPI for Math. in the Sci.

We study an iterated game, in which players from opposite populations are randomly paired, for the investigation of the interplay between individual optimization and population effects and for the comparison of different strategies and learning schemes. Players can rely on the information from previous encounters. A population adapts by selection, and/or the members of the population could learn individually, e.g., by reinforcement learning, or socially, via imitation.

The situation each player faces is changing, as coevolution exerts a high pressure on any learning strategy. Thus, the game between the populations is about quickly finding and converging to a favorable equilibrium. Within the population, the contest is about getting higher pay-offs.

The first aspect favors simple evolutionary schemes or learning strategies over more complex ones. The second aspect relates to the most effective use of the information from previous rounds or available within some social network inside the population.

We find an improved reinforcement learning that outperforms most evolutionary strategies, as well as the standard reinforcement learning with optimal parameters. The best imitating strategy here is payoff-biased. Imitating behavior can spread within a mixed population who can defeat a pure population with solely individual learners, independently of the precise learning scheme employed.

BP 16.4 Tue 15:45 H37

Banish or vanish? The evolution of cooperation by social exclusion — •Tatsuya Sasaki[1,2] and Satoshi Uchida[3] — [1]International Institute for Applied Systems Analysis, Laxenburg, Austria — [2]University of Vienna, Vienna, Austria — [3]Rinri Institute, Tokyo, Japan

Fines and exclusion are ubiquitous, yet very different ways of punishing freeriders. In the former, punishers are allowed to fine freeriders at a cost to themselves. It is clearly difficult for only fines to promote cooperation due to this punisher's cost. Less clear is the latter, in which punishers are allowed to exclude freeriders from the common good at a cost to themselves. When does exclusion solve the commons dilemma?

We investigate the replicator dynamics in standard public good games with costly exclusion. Costly exclusion reduces the group size, but not necessarily the group benefit, and thus, the punisher's net payoff may increase through excluding freeriders. We demonstrate how ex-

clusion of freeriders can establish a coercion-based regime. Our results do not require a genetic relationship, repeated interaction, reputation, or group selection. Instead, only a limited number of freeriders are required to prevent the second-order freeriders from eroding the social immune system.

BP 17: Biomaterials and Biopolymers II (joint with CPP)

Time: Wednesday 9:30–12:45 Location: H43

Topical Talk BP 17.1 Wed 9:30 H43

Processing of recombinant proteins for biomaterials applications: about spider silk and more — •Thomas Scheibel — Universität Bayreuth, Lehrstuhl Biomaterialien, 95440 Bayreuth, Germany

Proteins reflect one fascinating class of natural polymers with huge potential for technical as well as biomedical applications. One well-known example is spider silk, a protein fiber with excellent mechanical properties such as strength and toughness. During 400 million years of evolution spiders became outstanding silk producers. Most spider silks are used for building the web, which reflects an optimized trap for flying prey. We have developed biotechnological methods using bacteria as production hosts which produce structural proteins mimicking the natural ones. Besides the recombinant protein fabrication, we analyzed the natural assembly processes and we have developed spinning techniques to produce protein threads closely resembling natural silk fibers. In addition to fibers, we employ silk proteins in other application forms such as hydrogels, particles or films with tailored properties, which can be employed especially for biomaterials applications.

BP 17.2 Wed 10:00 H43

Nano-confined protein anchors, structured by STED lithography, probed by dSTORM. — •Richard Wollhofen[1], Moritz Wiesbauer[1,2], Kurt Schilcher[2], Jaroslaw Jacak[1,2], and Thomas A. Klar[1] — [1]Johannes Kepler University, Linz, Austria — [2]Upper Austria University of Applied Sciences, Linz, Austria

The ability to place individual proteins onto nano-confined structures plays a constantly growing role in bioscience, from basic studies in biology to development of nanosensors. One of the possibilities to generate sub-micrometer sized structures is direct laser writing (DLW) lithography. The resolution of DLW can be enhanced by stimulated emission depletion (STED) for assembly of polymeric structures down to several tens of nanometers [1]. Using a pulsed 780nm laser for two-photon DLW and a 532nm laser for STED, we are able to obtain structure sizes of down to 55nm and manufacture two clearly separated lines with 120nm distance [2]. The structures show good biocompatibility and allow an easy biofunctionalization with proteins down to the single protein level. We use direct stochastic optical reconstruction microscopy (dSTORM), which enables determination of protein density at a nanoscale level [3]. Combining STED lithography with dSTORM allows us to produce and characterize biocompatible structures, applicable to many biological assays. [1]J. Fischer et al.,Adv.Mat.,Vol.22,Nr.32,pp.3578-3582(2010); [2]R.Wollhofen et al.,submitted; [3]S. van de Linde et al.,Photochem.&Photobiol.Sc.,Vol.8,Nr.4,pp.465-469(2009);

BP 17.3 Wed 10:15 H43

Influence of direct laser written three-dimensional topographies on osteoblast-like cells — •Judith K. Hohmann[1], Erik H. Waller[1], Rainer Wittig[2], Rudolf Steiner[2], and Georg von Freymann[1] — [1]Physics Department and Research Center OPTIMAS, University of Kaiserslautern — [2]Institute for Laser Technologies in Medicine and Metrology (ILM) at the University of Ulm

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 [1]. 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. In general, results generated in such two-dimensional systems can hardly be transferred to natural, three-dimensional conditions.

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. We aim at understanding the relation between various three-dimensional structures and viability parameters of osteoblastic cells. To observe cellular behavior, SaOs-2 osteosarcoma cells are seeded onto the structures in order to test proliferation, morphology, adhesion and differentiation via fluorescence and staining techniques. These results might lead to novel dental implant surfaces which promote osseointegration. [1]Nikkhah et al. Biomaterials 33 (2012) 5230-5246

BP 17.4 Wed 10:30 H43

Biocompatibility of Fe-Pd ferromagnetic shape memory alloys - influence of surface roughness and protein coatings — •Uta Allenstein[1,2,3], Yanhong Ma[2], Ariyan Arabi-Hashemi[2], Stefan G. Mayr[2,3,4], and Mareike Zink[1] — [1]Division of Soft Matter Physics, Institute for Experimental Physics I, University of Leipzig — [2]Leibniz-Institute for Surface Modifications (IOM) — [3]Translational Center for Regenerative Medicine (TRM), University of Leipzig — [4]Faculty of Physics and Earth Sciences, University of Leipzig

Recent decades have seen a huge turn in implantology and biomaterial development towards regenerative medicine. The approach in orthopedic surgery is no longer to just replace damaged tissue by a passive implant that evokes the least possible interference with biological tissue, but rather to provide active stimulation and actuation. Fe-Pd ferromagnetic shape memory alloys are a promising new class of smart materials with a unique set of properties ideal for biomedical applications, including superelasticity, magnetically switchable strains and biocompatibility. In this study the latter was shown by in vitro experiments with NIH 3T3 fibroblasts, MCF 10A epithelial cells and HOB osteoblasts on vapor-deposited single crystalline $Fe_{70}Pd_{30}$ thin films and roughness graded polycrystalline splat-quenched samples. Proliferation, adhesion and morphology were assessed on substrates of different surface roughness and different adhesive coatings, such as fibronectin, laminin and poly-L-lysine, as well as RGD peptides.

BP 17.5 Wed 10:45 H43

Sorption of proteins to charged microgels: characterizing binding isotherms and driving forces — •Cemil Yigit, Nicole Welsch, Matthias Ballauff, and Joachim Dzubiella — Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany

We present a set of Langmuir binding models in which electrostatic cooperativity effects to protein sorption is incorporated in the spirit of Guoy-Chapman-Stern models, where the global substrate (microgel) charge state is modified by bound reactants (charged proteins). Application of this approach to lysozyme sorption to oppositely charged core-shell microgels allows us to extract the intrinsic, binding affinity of the protein to the gel, which is salt-concentration independent and mostly hydrophobic in nature. The total binding affinity is found to be mainly electrostatic in nature, changes many orders of magnitude during the sorption process, and is significantly influenced by osmotic deswelling effects. The intrinsic binding affinity is determined to be about 7 kT for our system. We additionally show that Langmuir binding models and those based on excluded-volume interactions are formally equivalent for low to moderate protein packing, if the nature of the bound state is consistently defined. Having appreciated this, a more quantitative interpretation of binding isotherms in terms of separate physical interactions is possible in future for a wide variety of experimental approaches.

BP 17.6 Wed 11:00 H43

Diffusion and Adsorption of Proteins in Mesoporous Environments — •Sebastian Mörz[1] and Patrick Huber[2] — [1]Experimental Physics, Saarland University — [2]Materials Physics and Technology, Hamburg University of Technology

In the recent years, several studies discussed the encapsulation of biomolecules in mesopourous materials and its potential applications

in e.g. protein chromatography or as novel means of controlled drug release. Both the diffusion of biomolecules under such confinement and the interaction with the surface of the host material are crucial to these applications.

In this study, we examine the adsorption of bovine heart cytochrome c onto the pore surface of the porous silica material SBA-15. Comparison between the folded and unfolded state of this protein allows us to separate the contributions from the different interaction mechanisms involved i.e. coulombic and hydrophobic interaction. Furthermore, we attempt a qualitative validation of the Stokes-Einstein equation for the diffusion of proteins in a porous anodized aluminum oxide membrane and its applicability for protein separation.

15 min break

BP 17.7 Wed 11:30 H43

FACS-sorting of particles to reduce the data variance in Optical Tweezers assisted Dynamic Force Spectroscopy measurements — •Tim Stangner[1], David Singer[2], Carolin Wagner[1], Christof Gutsche[1], Olaf Ueberschär[1], Ralf Hoffmann[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Institut für Experimentelle Physik I, Linnéstraße 5, 04103 Leipzig, Deutschland — [2]Biotechnologisch-Biomedizinisches Zentrum Leipzig, Fakultät für Chemie und Mineralogie, Deutscher Platz 5, 04103 Leipzig, Deutschland

By combining Optical Tweezers assisted dynamic force spectroscopy experiments with fluorescence activated cell sorting (FACS), we demonstrate a new approach to reduce the data variance in measuring receptor-ligand-interactions on a single molecule level by ensuring similar coating densities. Therefore, the carboxyfluorescein-labeled monophosphorylated peptide tau226-240[pThr231] is anchored on melamine resin beads and these beads are sorted by FACS to achieve a homogeneous surface coverage. To quantify the impact of the fluorescence dye on the bond parameters between the phosphorylated peptide and the corresponding phosphorylation specific anti-human tau monoclonal antibody HPT-104, we perform dynamic force spectroscopy and compare the results to data using unsorted beads covered with the non-fluorescence peptide analogue. Finally, we demonstrate that the data variance of the relative binding frequency is significantly decreased by a factor of 3.4 using presorted colloids with a homogeneous ligand coating compared to unsorted ones.

BP 17.8 Wed 11:45 H43

Thermal vibrations reduce the efficacy of sacrificial bonds — •Soran Nabavi[1], Matthew J. Harrington[2], Peter Fratzl[2], Oskar Paris[1], and Markus A. Hartmann[1] — [1]Institute of Physics, Montanuniversitaet Leoben, Leoben, Austria — [2]Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

Mussel byssal threads are a fascinating biological material combining high stiffness, toughness and extensibility. Experimental studies suggest that these outstanding properties are achieved by using so called sacrificial bonds (SBs) which are weaker than the covalent bonds holding the structure together and that can form and open reversibly [1]. The SBs break before the covalent bond rupture, providing hidden length and allowing for efficient energy dissipation.

In this study computer simulations are used to investigate the effect of SBs on the mechanical properties of a single polymeric chain. Special emphasis was put on the interplay of covalent and sacrificial bonds and the effect of thermal vibrations that have been largely overlooked in the description of SBs so far. In a simple setting with only one SB it is found that molecular chain fluctuations reduce the efficacy of SBs. Even for SBs with rather high binding energies of ˜1 eV backbone fluctuations lead to a rupture of SBs before external loading sets in. Thus, the theoretical strength of SBs is reduced more than a factor of two. This effect increases with increasing polymeric chain length and with increasing temperature.

[1] M. J. Harrington et al., J. Struct. Biol. 167, 47 (2009)

BP 17.9 Wed 12:00 H43

Benchmarking the water-peptide interaction — •Sucismita Chutia, Mariana Rossi, and Volker Blum — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

The interaction between water molecules and the hydration sites of peptides is critical for any quantitative modeling of solvated peptides. We address this interaction for the successive hydration of two peptides for which accurate experimental reference data exist: Ac-Ala_5-$LysH^+$ (non-helical) and Ac-Ala_8-$LysH^+$ (helical). In particular, finite-temperature Gibbs reference water binding energies ΔG_0 and equilibrium constants are known [1,2]. However, earlier force-field predicted preferred water binding sites do not agree with one another. We present an exhaustive first-principles study (density-functional theory based on the van der Waals corrected PBE functional) that demonstrates [3]: (i) There is a close competition between possible hydration sites (protonated carboxyl group or ammonium group). The preferred first hydration site breaks an intramolecular bond of the ammonium group in the unsolvated molecule. (ii) Calculated ΔG_0(T) are in remarkable agreement with experimental data. Lowest-energy H_2O H-bond networks are predicted for up to five H_2O molecules, and the connection to the solvated state is explored by ab initio molecular dynamics with up to 152 H_2O molecules. [1] Liu, Wyttenbach, Bowers, IJMS. *236*, 81 (2004) [2] Kohtani, Jarrold, JACS. *126*, 8454 (2004) [3] Chutia, Rossi, Blum, JPCB DOI: 10.1021/jp3098268

BP 17.10 Wed 12:15 H43

Biomolecular translocation through nanopores: from statistics to real DNA conformations — •Maria Fyta[1], Simone Melchionna[2], Sauro Succi[3], and Efthimios Kaxiras[4] — [1]Institut für Computerphysik, Universität Stuttgart, Germany — [2]IPCF-CNR, Università La Sapienza, P.le A. Moro 2, 00185 Rome, Italy — [3]IAC-CNR, Via dei Taurini 19, 00185 Rome Italy — [4]Department of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge MA 02138, U.S.A

We apply a multiscale computational scheme to model a biomolecule translocating through a narrow pore, an intensively studied subject due to its variety of applications such as ultra-fast DNA sequencing. The model uses a mesoscopic lattice Boltzmann method to treat the solvent and a Molecular Dynamics scheme to deal with the biomolecule. Our first results involve an anonymous polymer translocating in pure water. We have obtained important insight into the statistics and dynamics of the process. The translocation time exponent compares well with the experimental values, while we were able to monitor multiconformational translocation. As a next step, we include electrokinetic effects, i.e. ions, as well as a realistic quantum-mechanically derived potential for double stranded DNA. We are now able to reveal in more detail the structural conformations of the DNA molecule as well as the ion distribution within the pore. The results also provide a qualitative and quantitative understanding of the ionic conductance and DNA blockade as compared to the experiments. Our conclusions also involve the effect of the pore geometry in the DNA translocation process.

BP 17.11 Wed 12:30 H43

Driving forces in corneocyte expansion: a geometric perspective — •Myfanwy Evans[1] and Roland Roth[2] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Deutschland — [2]Theoretische Physik, Universität Tübingen, Deutschland

The arrangement of keratin in corneocytes, the dead cells in the outer layer of mammalian skin, are likely a highly ordered packing of helical filaments. This specific geometric arrangement allows the exotic physical property of cell expansion on prolonged exposure to water to occur in a mechanically stable and reversible regime. We examine the solvation free energy of a water-like solvent filling the volume of the corneocytes around the hydrophilic keratin fibres by the morphometric approach to energy landscapes. We find that the energy minimisation drives the system to absorb water and expand where water is available. During this expansion, the elastic energy in the keratin intermediate filaments increases, and the balance of the two forces forms a natural limit for the expansion process and the system maintain full reversibility.

BP 18: Membranes and Vesicles I

Time: Wednesday 9:30–12:15 Location: H44

Invited Talk BP 18.1 Wed 9:30 H44

Out-of-equilibrium membrane physics and cellular organelles. — •Pierre Sens — CNRS-ESPCI, Paris, France

Most molecules secreted or internalized by Eukaryotic cells follow well defined routes, the secretory and endocytic pathways, along which they are exposed to a succession of biochemical environments by sequentially visiting different membrane-bound organelles. Molecules internalized by endocytosis move from early to late endosomes before being sorted and carried to their final destination. Molecules synthesized in the endoplasmic reticulum go through the Golgi apparatus, itself divided into cis, medial and trans compartments (called cisternae), where they undergo post-transcriptional maturation and sorting. One fundamental issue underlying the organization and regulation of intracellular transport is whether progression along the transport pathways occurs by exchange between organelles of fixed biochemical identities (via the budding and scission of carrier vesicles), or by the biochemical maturation of the organelles themselves.

In this talk, I will present some aspects of the Physics of out-of-equilibrium membrane system, and discuss their relevance to intracellular transport. I will particularly focus on the dynamical coupling between biochemical maturation and phase separation of membrane components, and its possible relevance for the generation and maintenance of the Golgi apparatus.

BP 18.2 Wed 10:00 H44

Effect of thermal noise on vesicles and capsules in linear flow — •David Abreu and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Fluid vesicles and elastic capsules are micrometer-sized objects, which implies that they are subject to the influence of thermal fluctuations. In particular, their behaviour in linear flow might be affected by these fluctuations. However, most theoretical models and simulations neglect thermal noise, although it plays an important role in experiments [1].

First, we add thermal noise to reduced models of undeformable vesicles and capsules in shear flow and show that thermal effects are relevant under realistic conditions [2]. We analyze the steady states for the different dynamical regimes as well as the vicinity of dynamical transitions (i.e., tank-treading to tumbling) where intermittent behaviour due to noise always occurs.

For deformable vesicles in general flow [3], we show that thermal fluctuations have to be taken into account in order to correctly explain the trembling motion observed experimentally [1]. We recover the experimental phase diagram and analyze the statistical properties of the three steady states (tank-treading, tumbling and trembling), showing that thermal noise is strongly amplified during trembling.

[1] N. J. Zabusky et al., Phys. Fluids 23, 041905 (2011); M. Levant and V. Steinberg, submitted (2012).

[2] D. Abreu and U. Seifert, Phys. Rev. E 86, 010902(R) (2012).

[3] D. Abreu and U. Seifert, in preparation.

BP 18.3 Wed 10:15 H44

Quantitative understanding of the nonspecific vesicle-substrate adhesion — •Daniel Schmidt[1], Udo Seifert[1], and Ana-Sunčana Smith[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart — [2]Institut für Theoretische Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg

Phospholipid membranes in cellular and biomimetic systems exhibit significant thermal fluctuations. These fluctuations play an important role in the regulatory mechanisms of the cell recognition process, when a cell binds to another cell membrane or, as in biomimetic systems, to a rigid substrate. The presence of such a substrate is manifested by the emergence of a non-specific potential, the strength of which is coupled to the membrane tension. The latter in turn affects the fluctuations in a fashion that is not fully understood.

Here we develop a procedure for the accurate determination of the membrane tension and the strength of the non-specific potential from experimental data, independent of the choice of the measurable - the membrane shape, the spatial or the temporal correlation functions. We achieve this goal after overcoming the limitations of the typically used, harmonic approximation of the potential. Additionally, we extract the true fluctuations from the apparent ones, which are modified due to the finite temporal and spatial resolution in microscopy. As a result, we obtain the first coherent view of the behavior of the membrane in a vicinity of a substrate, in a system that is of a finite size and away from the unbinding transition.

BP 18.4 Wed 10:30 H44

Curvature as a Mechanism for Biomolecule Localisation in Bacterial Cells — •Lars D. Renner[1,2], Prahathess Eswaramoorthy[3], Kumaran S. Ramamurthi[3], Douglas B. Weibel[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [2]University of Wisconsin-Madison, Madison, WI, USA — [3]National Cancer Institute, Bethesda, MD, USA

One of the central questions in cell biology is how the temporal and spatial organization of the cell machinery within the cell is established, maintained, and replicated. In Eubacteria, an understanding of the cellular organization of proteins is just beginning to take shape. Recent data suggests that there are geometric cues for the localization of proteins and lipids in bacteria. We found that microdomains of cardiolipin (CL) preferentially localize to regions of large, negative curvature. We use a top-down approach that combines in vivo and in vitro experiments with E. coli and B. subtilis cells. We find that a critical difference in the radius of curvature ΔC (curvature difference between cell poles and midcell) of approx. 0.5 μm^{-1} is required to drive the polar localization of MinD and DivIVA. Our data provides support for curvature as a general mechanism for regulating the spatial organization in bacterial membranes. This research expands our understanding of Eubacterial cell biology and provides insight into the spatial and temporal dynamics of membranes and their role in cell biology.

BP 18.5 Wed 10:45 H44

Shape determines membrane protein cluster formation — Diana Morozova, Matthias Weiss, and •Gernot Guigas — Experimental Physics I, University of Bayreuth

About 30% of all protein species in a cell are membrane proteins. They take part in a multitude of vital cellular processes, e.g. signal and mass transfer at the plasma membrane. In many cases, membrane proteins need to cluster to perform their specific duty. Using mesoscopic simulations, we have studied the influence of protein shape on the clustering ability. We show via the potential of mean force that lipid-mediated interactions between transmembrane proteins depend on two key parameters [1]: the shape of the proteins' hydrophobic domain and their hydrophobic mismatch. Protein interactions can be attractive or repulsive, depending on the characteristic bilayer perturbations induced by the proteins. These findings are compared to results on peripheral membrane proteins that reside only in one leaflet of the membrane [2]. Here, we observe various higher-order structures depending on the size and penetration depth of the protein's hydrophobic moiety. Surprisingly, even clustering across opposing leaflets of a bilayer is observed.

[1] D. Morozova, M. Weiss, and G. Guigas, Soft Matt. 8, 11905 (2012). [2] D. Morozova, G. Guigas, and M. Weiss, PLOS Comp. Biol. 7, e1002067 (2011).

15 min break

BP 18.6 Wed 11:15 H44

Specific binding of chloride ions to lipid vesicles and implications at molecular scale — •Volker Knecht[1] and Benjamin Klasczyk[2] — [1]Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, Hermann-Herder Strasse 3, D-79104 Freiburg — [2]MELAG Medical Technology, D-10829 Berlin

Biological membranes comprised of lipids and proteins are in contact with electrolytes like aqueous NaCl solutions. Based on molecular dynamics (MD) simulations it is widely thought that Na^+ ions specifically bind to POPC bilayers while Cl^- ions merely form a diffuse layer of counterions screening the positive membrane charge due to the Na^+ ions. I will present a comparison of recent data from electrophoresis and isothermal calorimetry experiments indicating that in fact both ion species show very similar affinities. Force field issues with the MD

studies are highlighted by our finding that a widely used simulation setup showing asymmetric affinities of Na^+ and Cl^- ions for POPC bilayers overestimates the effect of NaCl on the electrophoretic mobility of a POPC membrane by an order of magnitude. Implications for previous simulation results on the effect of NaCl on the structure of the membrane and the interfacial water are discussed. Our results suggest that a range of published simulation results on the interaction of NaCl with PC bilayers have to be reconsidered and revised.

BP 18.7 Wed 11:30 H44

Interbilayer repulsion force from coarse-grained simulations — •Yuliya Smirnova[1], Volker Knecht[2], and Marcus Müller[1] — [1]Georg August University, Institute for Theoretical Physics, Göttingen, Germany — [2]University of Freiburg, Institute of Physics, Freiburg, Germany

Using the coarse-grained MARTINI model of POPC lipids and water [1] we study interactions between bilayer membranes with and without external forces applied to the system. Upon dehydration the bilayer structure changes differently: without external forces, the membrane thickness increases; with an external force acting on the center of mass of the bilayers, however, membranes laterally stretch. We find that in both cases the interbilayer forces decay exponentially with slightly different decay lengths and substantially different pre-exponential coefficients. We propose a way to estimate hydration repulsion between lipid bilayers from both simulations and our results for the disjoining pressure are in good agreement with experimental results.

[1] Marrink S.J.; Risselada H.J.; Yefimov S.; Tieleman D.P.; de Vries A.H. J. Chem. Phys. B, 2007, 111, p 7812.

BP 18.8 Wed 11:45 H44

Phase separation in a Lipid/Cholesterol System: Coarse-grained and United-atom Simulations — •Davit Hakobyan and Andreas Heuer — WWU Münster, Institut für Physikalische Chemie, Münster, Germany

The separation of liquid-ordered and liquid-disordered phases of lipids in membranes is a subject of continuous experimental as well as theoretical investigations.

Microscale coarse-grained (CG) and united-atom (UA) simulations are performed to investigate the phase separation of a membrane bilayer for the ternary system of saturated 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) and unsaturated 1,2-dilinoleoyl-sn-glycero-3-phosphocholine (DUPC) and cholesterol (CHOL). The results of 9 microsecond UA simulation demonstrate the onset of phase separation and are compared with the results of the corresponding CG system. While sharing the structural features of phase separation in the CG model, the onset of de-mixing for the UA model is nearly two orders of magnitude slower. This factor can be rationalized by the different short-time diffusion constants.

Various system properties such as order parameters, lipid - CHOL and CHOL - CHOL interactions are compared between the UA and the CG models. From the structural perspective the phase separation process appears to be rather similar for both models, which illustrates once more the power of using CG approaches. The results are further extended by analysis of different unsaturated lipids, different CHOL concentrations as well as different UA force fields.

BP 18.9 Wed 12:00 H44

Compatible solutes and their effects on DPPC lipid bilayers: a computer simulation study — •Jens Smiatek[1], Rakesh Kumar Harishchandra[3], Hans-Joachim Galla[3], and Andreas Heuer[2] — [1]Institut für Computerphysik, Universität Stuttgart, Germany — [2]Institut für Physikalische Chemie, WWU Münster, Germany — [3]Institut für Biochemie, WWU Münster, Germany

The influence of compatible solutes on the properties of DPPC lipid bilayers is studied by semi-isotropic constant pressure (NPT) Molecular Dynamics simulations. Our findings indicate an increase of the surface pressure and the solvent accessible surface area in presence of higher hydroxyectoine concentrations. By free energy calculations of a single DPPC molecule in presence of hydroxyectoine, we are able to validate a modified free solvation energy. As a consequence of this effect, we conclude that the underlying reason for the observed increase of the surface pressure is given by a better solubility of the DPPC lipids. These results are also supported by regarding the ratio of the hydrophilic to the hydrophobic solvent accessible surface area.

BP 19: Focus Session: Dynamics of Adaptive Networks (joint with SOE and DY)

Adaptive Networks attracted recent interest through their dynamical properties that emerge from the interaction of two classes of processes (which may include stochasticity): (i) Growth and restructuring of the network topology itself, and (ii) Coupled dynamical systems defined on the network nodes. In this session, an introduction and overview into adaptive networks and their analytical and numerical investigation is complemented by their recent application to socio-economic, biological and epidemologic systems. (Session compiled by Eckehard Schöll, TU Berlin and Jens Christian Claussen, U Lübeck.)

Time: Wednesday 9:30–12:30 Location: H37

Topical Talk BP 19.1 Wed 9:30 H37

Adaptive Networks: Of social interactions and mathematical tools — •Anne-Ly Do — Max-Planck-Institut für Physik komplexer Systeme, Dresden

Adaptive networks are characterized by the co-evolution of local and topological degrees of freedom. Prime examples are networks of social interactions: Individuals are altered and shaped through interaction with others. On the other hand, they can often decide with whom to interact. Adaptive network models of social systems have attracted keen interest as they promise to provide the key to a number of prominently discussed phenomena such as fragmentation of groups into like-minded subgroups, evolution or break-down of social structures promoting cooperation, and emergence of fairness and leadership. In this talk, I review recent studies that link emergent phenomena in social systems to adaptive feedback in the respective interaction nets. Moreover, I discuss the analytical techniques used, thus aiming to outline both, findings and tools.

BP 19.2 Wed 10:00 H37

Controlling cluster synchronization by adaptive network topology — •Judith Lehnert[1], Anton Selivanov[2], Alexander Fradkov[2,3], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik,TU-Berlin, Hardenbergstr 36, 10623 Berlin, Germany, — [2]SPb State University, Universitetskii pr.28, St.Petersburg, 198504 Russia — [3]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 on 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. Our method is robust towards different initial conditions. Furthermore, it is not necessary to adapt the network as a whole but it is sufficient to apply the method to a subset of the links to control the dynamics of all nodes. Finally, we discuss the topological characteristics of the network after successful control.

BP 19.3 Wed 10:15 H37

Resilience of collective dynamics in fluctuating network environments — •Alexander Grimm — ETH Zürich, Chair of Systems Design, Switzerland

Do totalitarian networks perform better than democratic networks? What is the most appropriate hierarchy level for networks embedded in volatile environments? We use agent-based models to discover the effect of hierarchy on performance in networks located in highly fluctu-

ating environments. We investigate the emergence of collective dynamics of many units embedded in complex network environments which change boundary conditions constantly. The agents have to adopt their behavior due to these constantly changing conditions. Although the individual node properties do not change, the network shows permanently changing structure with enormously differing properties. The fluctuating environments come into force via three different dynamics which happen on different time scales in adiabatic approximations. We show that a synchronization process is a good approach to model information transfer. The information transfer in the model interlinks the three dynamics. First, the link formation process is the most fundamental process. It is driven by centrality. Second, the a synchronization process describes the information transfer among the nodes. And third, an endogenized node churn removes those nodes which deviate from the networks' common culture. In differing hierarchy values we find a phase transition in centrality. Hysteresis effects and trade-off properties make it possible to determine the most appropriate topology of the network, given its operation area.

BP 19.4 Wed 10:30 H37

Absence of epidemic thresholds in a growing adaptive network — •Güven Demirel[1] and Thilo Gross[2] — [1]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [2]University of Bristol, Bristol, United Kingdom

In epidemics on network, a central role is played by the degree distribution, i.e. the distribution of the number of neighbors of nodes. In particular in scale-free networks, where the variance of the degree distribution diverges, no epidemic thresholds exist, such that even diseases with arbitrary low infectiousness can percolate. By contrast, in networks where the variance of the degree distribution is finite, diseases generally need to surpass a threshold infectiousness to persist. In the real world the degree distribution is not independent of epidemics, but is shaped through disease induced behavioral changes and mortality in a complex interplay. Here, we consider the growth of a network from which nodes are simultaneously removed due to disease-induced mortality. We show analytically and numerically that in this system no epidemic thresholds exists, although the interplay between network growth and epidemic spreading leads to networks in which the degree distribution has a finite variance.

BP 19.5 Wed 10:45 H37

Hierarchical transport structures in the network of *Physarum polycephalum* — •Werner Baumgarten and Marcus J. B. Hauser — Abteilung Biophysik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

The plasmodium of the slime mould *Physarum polycephalum* consists of a single multinucleate giant amoeboid cell that forms a characteristic two-dimensional vein network. Through the entire tubular network protoplasm is transported periodically back and fro. During evolution this transportation network is optimized for efficiency [1].

The vein network of *P. polycephalum* is considered a weighted undirected graph, with veins as edges and branching points as nodes, the weight is given by the local drag of each vein [2]. A graph analysis is performed on the network of *P. polycephalum* based on the conjecture of laminar flow in the veins. Experiments to quantify the structure were carried out on multiple scales. We demonstrate that the network posses a self-similar hierarchic structure which consists of nested loops of veins of decreasing transport efficiency. These results are used to describe the network evolution.

[1] A. Tero, S. Takagi, T. Saigusa, K. Ito, D. P. Bebber, M. Fricker, K. Yumiki, R. Kobayashi, T. Nakagaki, 2010, Science, 327, 439

[2] W.Baumgarten, T. Ueda, M.J.B. Hauser, Phys. Rev. E 2010, 82, 046113

BP 19.6 Wed 11:00 H37

Natural emergence of clusters and bursts in network evolution — •James Bagrow and Dirk Brockmann — Northwestern University

Network models with preferential attachment, where new nodes are injected into the network and form links with existing nodes proportional to their current connectivity, have been well studied for some time. Extensions have been introduced where nodes attach proportional to arbitrary fitness functions. However, in these models attaching to a node increases the ability of that node to gain more links in the future. We study network growth where nodes attach proportional to the clustering coefficients, or local densities of triangles, of existing nodes. Attaching to a node typically lowers its clustering coefficient, in contrast to preferential attachment or rich-get-richer models. This simple modification naturally leads to a variety of rich phenomena, including aging, non-poissonian bursty dynamics, and community formation. This shows that complex network structure can be modeled without artificially imposing multiple dynamical mechanisms.

BP 19.7 Wed 11:15 H37

Evolution of Cooperation on Stochastic Dynamical Networks — •Bin Wu and Arne Traulsen — Research Group for Evolutionary Theory, Max-Planck-Institute for Evolutionary Biology, Plön, Germany

Cooperative behavior that increases the fitness of others at a cost to oneself can be promoted by natural selection only in the presence of an additional mechanism. One such mechanism is based on population structure, which can lead to clustering of cooperating agents. Recently, the focus has turned to complex dynamical population structures such as social networks, where the nodes represent individuals and links represent social relationships. We investigate how the dynamics of a social network can change the level of cooperation in the network. Individuals either update their strategies by imitating their partners or adjust their social ties. For the dynamics of the network structure, a random link is selected and breaks with a probability determined by the adjacent individuals. Once it is broken, a new one is established. This linking dynamics can be conveniently characterized by a Markov chain in the configuration space of an ever-changing network of interacting agents. Our model can be analytically solved provided the dynamics of links proceeds much faster than the dynamics of strategies. This leads to a simple rule for the evolution of cooperation: The more fragile links between cooperating players and non-cooperating players are (or the more robust links between cooperators are), the more likely cooperation prevails. Our approach may pave the way for analytically investigating coevolution of strategy and structure.

Topical Talk BP 19.8 Wed 11:30 H37

Bio-molecular Networks: Structure, Function, Evolution — •Michael Lässig — Institut für theoretische Physik, Universität zu Köln

In biological systems, networks exist at multiple levels. One is structure: components of a system are linked because they are close in space. An example is the adjacency of amino acids in a protein. Another level is function: components are linked because they do something together, such as the genes in a regulatory or metabolic network. In this talk, I discuss how structure and function networks shape the evolutionary dynamics of organisms and species - and conversely, how evolutionary observations can uncover underlying functional networks. I use two examples: the evolutionary properties of gene regulatory networks and the evolution of the human influenza virus.

Topical Talk BP 19.9 Wed 12:00 H37

Adaptive networks and critical dynamics — •Stefan Bornholdt — Institut für Theoretische Physik, Universität Bremen

Dynamical networks have been studied from the perspective of statistical physics, motivated by questions of information processing in neural networks and genetic networks. In both applications, hypotheses have been discussed that relate optimality of information processing to dynamical criticality in the networks. Consequently, toy models for adaptive networks have been constructed that robustly establish criticality in the network. Here I review a particularly simple model class based on models from physics and discuss its application to the phenomenon of criticality in biological neural networks.

[1] M. Rybarsch and S. Bornholdt, Self-organized criticality in neural network models, in: "Criticality in Neural Systems", Niebur E, Plenz D, Schuster HG (eds.) 2013 (in press); arXiv:1212.3106.

[2] M. Rybarsch and S. Bornholdt, Binary threshold networks as a natural null model for biological networks, Phys. Rev. E 86 (2012) 026114.

[3] M. Rybarsch and S. Bornholdt, Self-organization to criticality in neural networks: A minimal model with binary threshold nodes, arXiv:1206.0166.

BP 20: Statistical Physics in Biological Systems II (joint with DY)

Time: Wednesday 15:00–17:30 Location: H43

Topical Talk BP 20.1 Wed 15:00 H43

Challenges of Neurophysics — •Theo Geisel — Max Planck Institute for Dynamics and Self-Organization & Bernstein Center for Computational Neuroscience, Universität Göttingen

As you are reading these lines, millions of neurons are activated in your brain and communicate by sending short pulses to each other. It is a major aim of neurophysics to understand the collective dynamics of large biological neural networks and to determine how they carry out complex computations. Recent progress of experimental techniques allows monitoring the activity of large numbers of cells in parallel and with single cell resolution even in freely moving animals. These techniques together with targeted optogenetic stimulation promise to considerably advance our insight into the function of collective neuronal dynamics in the near future.

On the other hand, these networks exhibit features that let them elude standard theoretical treatment: E.g. the units of the network interact asymmetrically and at discrete times only, i.e. not continuously as in conventional many-body theory in physics. There are significant interaction delays, which formally make the systems infinite-dimensional. Complex connectivities give rise to novel multi-operator problems, for which new methods based on graph theory are devised to reach rigorous analytic results. The talk reviews challenges and recent progress in characterizing the dynamics and function of these networks.

BP 20.2 Wed 15:30 H43

Retinal light collectors enhance underwater vision — •Moritz Kreysing[1], Kristian Franze[2], Mike Francke[3], Andreas Reichenbach[3], and Jochen Guck[4] — [1]Systems Biophysics, Department of Physics, LMU München, Germany — [2]Department of Physiology, Development and Neuroscience, Cambridge University, UK — [3]Paul Flechsig Institute, University of Leipzig, Germany — [4]Biotechnology Center, TU Dresden, Germany

Vision at low light intensities relies on photoreceptors being able to detect individual photons. As an accepted rule, the light sensitive portions of vertebrate rods and cones, namely outer segments, increase in volume the darker the animals' habitat gets, in order to enhance the probability to capture incident photons. Consequently, the biggest outer segments are found in fish living in the deep sea. A peculiar exception to this rule are the eyes of some deep sea fish, as well as fish living in highly turbid rivers. In their retinas relatively short outer segments are bundled into spatially isolated groups, clearly not meant to maximize the probability of photon absorption. Based on a detailed morphological and optical study of multilayer light-collectors surrounding these segments [1], we argue that under extreme conditions in which quantum noise, i.e. the rate of spontaneous photo-pigment activation, becomes comparable to the rate of photon arrival, visual sensitivity cannot be achieved by large outer segments anymore. Instead the retinal focusing of light on very small receptors is the only way to lower the visual threshold further, or to see at near IR wavelengths. Reference: 1. M. Kreysing et al., Science 336(6089):1700-1703 (2012).

BP 20.3 Wed 15:45 H43

Monte Carlo simulation of the patterns of histone acetylation in response to MS-275 — •Davoud Pouladsaz[1] and Azadeh Ebrahimi[2] — [1]Department of Biological Physics, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Neuropathology, Faculty of Medicine, University of Tübingen, Tübingen, Germany

Abnormal activities of histone decaetylases (HDACs) are considered to be associated with various neurological disorders, from oncogenesis, to neurodegenerative and psychiatric disorders. In this scheme, HDACs are potential targets for therapeutic development. HDAC inhibition has been reported in several studies to improve cognitive function and increase neural longevity. A novel HDAC inhibitor is MS-275, a benzamide derivative with in vivo antitumor activity and selectivity against HDAC1 and HDAC3. We perform computer simulations based on Monte Carlo method in order to describe the patterns of histone acetylation in the brain in response to MS-275. According to previous experimental results, MS-275 is a potent brain region-selective HDAC inhibitor. We theoretically produce similar acetylation profiles associated with the measurements in different regions of the brain, and calculate the changes in the acetylation by means of stochastic processes representing the inhibition of HDACs. The theoretical results show significant correlation to experimental measurements.

BP 20.4 Wed 16:00 H43

NAD(P)H Dynamics in Yeast Populations — •André Weber[1,2], Yury Prokazov[2], Werner Zuschratter[2], and Marcus J B Hauser[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Leibniz-Institut für Neurobiologie Magdeburg, Germany

NAD(P)H is the most important electron carrier in living cells and therefore it plays a key-role in numerous cellular processes. It is directly involved in glycolysis and Krebs cycle and its autofluorescence acts as an indicator for metabolic dynamics and enzyme activity in cells. The amount of NAD(P)H is reflected by its emitted light intensity. Furthermore, it is possible to discriminate between free and protein-bound NAD(P)H through fluorescence lifetimes. Using single photon counting fluorescence microscopy, we study glycolytic oscillations and metabolic changes in yeast cell populations via NAD(P)H imaging.

Yeast cells show synchronised glycolytic oscillations for high population densities which can be detected as global oscillations. These global oscillations become quiescent, when the population density drops below a critical value. Our results show that individual cells remain oscillatory even at very low cell densities (e.g. 1×10^5 cells/ml). The transition from global oscillations to a quiescent population signal is caused by the desynchronisation of the oscillations of individual cells. This is characteristic for a Kuramoto transition to incoherence. Spatially resolved measurements at low cell densities uncover that even cells that adhere to their neighbours oscillate with their own, independent frequencies and phases.

BP 20.5 Wed 16:15 H43

Description of polarity reorientation in the wing of the fruit fly by liquid crystal hydrodynamics — •Matthias Merkel[1], Andreas Sagenr[2], Raphael Etournay[2], Suzanne Eaton[2], and Frank Jülicher[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany

Epithelia are two-dimensional sheets of cells, which often exhibit large-scale patterns of planar cell polarity (PCP) in the tissue plane. Within a single cell, PCP is reflected in an anisotropic distribution of a class of proteins, called PCP proteins. We study PCP in the wing epithelium of the fruit fly. During development of the fly, two processes are observed: cell polarity reorients on large scales and a complex flow field reshapes the wing. This flow field includes a stereotypical pattern of tissue shear. We quantify polarity patterns in wild type and mutant wings. To interpret these patterns, we discuss a simple hydrodynamic model for polarity reorientation from liquid crystals theory. Our model consists of local polarity interactions and a coupling of polarity to tissue shear and tissue rotation. We find, that we can fit stationary states of our hydrodynamic description to the polarity patterns of the adult wings. These fits suggest that the sign of the coupling of polarity to tissue shear depends on the local expression of a PCP protein. We underpin our findings by numerical solutions of the polarity dynamics.

BP 20.6 Wed 16:30 H43

Optimization of shape for cargo transport with bead-spring microswimmers — •Jayant Pande and Ana-Sunčana Smith — Cluster of Excellence: EAM, and Institute for Theoretical Physics, Friedrich Alexander University Erlangen-Nürnberg, Germany

Microswimmers are entities that are capable of swimming in fluids at very low Reynolds numbers. A simple model of a microswimmer was introduced by Najafi and Golestanian, and consists of three spheres connected in series by two arms. This model could be used as a basis for constructing cargo-carrying micromachines, with the cargo making up the spheres in the swimmer. To determine whether other shapes for the bodies lead to more efficient swimming, we augment this model by replacing the spheres by general ellipsoids of revolution and including springs between these ellipsoids. The velocities of such three-ellipsoid swimmers acting under the influence of sinusoidal driving forces are calculated, assuming that either the deformations of the arms or the

driving forces are known. Comparing the velocities of different swimmers for a given cargo volume leads to a determination of the optimum body shapes and mechanism of propagation. We observe that a rich behaviour for the velocity curve is obtained, depending on the relative magnitudes of the spring constant and the fluid viscosity. The theoretical calculations are supported by simulations using a framework combining "waLBerla", a lattice-Boltzmann method based fluid solver, and "pe", a rigid body physics engine. The simulation results are found to agree well with the calculated values.

BP 20.7 Wed 16:45 H43

On the collective motion of Chlamidomonas cells — •Johannes Greber[1], Salima Rafai[2], Philippe Peyla[2], and Walter Zimmermann[1] — [1]Universität Bayreuth, D-95447 Bayreuth, Germany — [2]Universite Joseph Fourier, F-38402 Grenoble, France

Swimming Chlamydomonas cells have a n eyespot registrating light comming from a light source far away enabling the cell to orient its direction of motion towards the light. This motion is called phototaxis.

During the propelling process, each cell generates a flow field with an atracting part in the direction of motion and a repelling part perpendicular to this direction. Due to this flow field a stable collectiv motion of a cloud of cells is impossible as long as no direction of motion is prefered by the cells.

We present experimental results and a theoretical analysis based on a model called "Puller" on the collectiv motion of Chlamydomonas cells.

BP 20.8 Wed 17:00 H43

Elastic coupling effects in cooperative transport by molecular motors — •Florian Berger, Corina Keller, Stefan Klumpp, and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Theory & Biosystems, 14424 Potsdam, Germany

Intracellular transport of cargos is achieved by the cooperative action of molecular motors, which pull the cargo along cytoskeletal filaments. To study this mechanism systematically in vitro, engineered constructs coupling a defined number of molecular motors have recently been introduced. These motors are elastically coupled via their common cargo, which may influence the motors' velocity and/or enhances their unbinding from the filament. Starting from the single molecule properties, we introduce a theoretical framework for cooperative transport which is consistent with recent experiments and provides novel testable predictions about the behavior of elastically coupled kinesin, dynein and myosin motors. Such an approach relates the single motor properties directly to the cooperative dynamics. As an example, we show that the overall cargo run length can either increase or decrease as a function of the single motor velocity depending on the single motor unbinding mechanism.

BP 20.9 Wed 17:15 H43

Teams of molecular spiders: Cooperative effects enhance the transport properties — •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

Molecular spiders are synthetic molecular motors based on DNA nanotechnology. While natural molecular motors have evolved towards very high efficiency, it remains a major challenge to develop efficient designs for man-made molecular motors. Inspired by biological motor proteins like kinesin and myosin, molecular spiders comprise a body and several legs. The legs walk on a lattice that is coated with substrate which can be cleaved catalytically. We propose a novel molecular spider design in which n spiders form a team. Our theoretical considerations show that coupling several spiders together alters the dynamics of the resulting team significantly. Although spiders operate at a scale where diffusion is dominant, spider teams can be tuned to behave nearly ballistic, which results in fast and predictable motion. Based on the separation of time scales of substrate and product dwell times, we develop a theory which utilises equivalence classes to coarse-grain the microstate space. In addition, we calculate diffusion coefficients of the spider teams, employing a mapping of an n-spider team on an n-dimensional random walker on a confined lattice. We validate these results with Monte Carlo simulations and predict optimal parameters of the molecular spider team architecture which makes their motion most directed and maximally predictable.

BP 21: Membranes and Vesicles II

Time: Wednesday 15:00–16:30 Location: H46

Invited Talk BP 21.1 Wed 15:00 H46

Mimicking cellular membranes: lessons from reconstitution — •Eva Schmid — Department of Bioengineering, UC Berkeley, USA

Cellular membranes are much more than passive barriers that encapsulate biochemical reactions - they are actively involved in driving complex biological processes and play a critical role in the communication between cells and their surroundings. Biological membranes exhibit a meticulously controlled asymmetric distribution of phospholipids, and are populated by a surprisingly high density of proteins. It is now understood that proteins and lipids do not randomly diffuse in plane as a two-dimensional fluid but are laterally organized. However, it is not yet clear how this organization comes about and what physical consequences it has on different membrane processes such curvature generation, membrane fusion or the formation of membrane interfaces. Efforts to understand biological membranes are often held back by the interconnected complexity of biochemical reactions in the cell. An emerging complementary approach to traditional biological research is to build cellular features component-by-component from the bottom up, thereby isolating the pathway of interest.

This talk will describe recent in vitro reconstitution experiments using purified lipids and proteins that suggest how physical boundary conditions can be essential and sufficient regulators of membrane organization.

BP 21.2 Wed 15:30 H46

Optothermal manipulation of lipid membranes — •Patrick Urban, Silke Kirchner, Theobald Lohmüller, and Jochen Feldmann — Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Amalienstrasse 54, 80779 München, Germany

Light absorbed by gold nanoparticles is very efficiently transformed into heat. Such particles can thus be used as small and localized heat sources that can be switched on and off by a short light pulse.

In our work, we take advantage of this property to investigate the physical consequences of heating on lipid membranes and thermosensitive trans-membrane proteins.

Giant unilamellar vesicles (GUVs) made of diphytanoylphosphatidylcholine (DPhPC) are prepared by electroformation and functionalized with 80 nm Au-nanoparticles. The particles are heated with a short laser pulse at the particle resonance frequency. The amount of heat can be controlled by the laser power and the pulse duration. The consequences of localized heating on the membrane properties are investigated by planar patch-clamp and fluorescence methods. Besides membrane studies, we aim to extend our approach to investigations of thermosensitive transmembrane proteins that are incorporated in the phospholipid bilayer.

BP 21.3 Wed 15:45 H46

Bilayer undulation dynamics in unilamellar phospholipid vesicles: Influence of temperature, cholesterol and trehalose — •Beate-Annette Brüning[1], Sylvain Prévost[1,2], Ralf Stehle[1], Roland Steitz[1], Peter Falus[3], Bela Farago[3], and Thomas Hellweg[4] — [1]Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [2]Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany — [3]Institut Laue-Langevin, B. P. 156, 38042 Grenoble Cedex 9, France — [4]Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

We report a combined dynamic light scattering (DLS) and neutron spin-echo (NSE) study on lipid vesicles composed of 1,2-dimyristoyl-sn-glycero-3-phosphatidylcholine (DMPC), respectively under the influence of temperature and the membrane additives cholesterol and trehalose. We study bilayer undulation and bulk diffusion dynamics using neutron spin-echo spectroscopy, on two distinct time scales, namely around 25 ns and 100 ns. Finally, we calculate the respective bilayer bending rigidities κ for all types of lipid vesicles. We observe a

bilayer softening around the main phase transition temperature T_m of the single lipid model system, and a bilayer stiffening the more cholesterol is added, whereas the insertion of trehalose hardly changes the bilayer undulations and membrane rigidity κ [1]. We explain our findings on the basis of a free volume available to lipid molecules in the membrane plane, which encounters the most pronounced changes in the acyl chain regime. [1] B. Brüning, S. Prévost, R. Stehle, R. Steitz, P. Falus, B. Farago, T. Hellweg, submitted.

BP 21.4 Wed 16:00 H46

Non-Equilibrium Dynamics in Lipid Multilayers - Time Resolved X-Ray Diffraction at In-House and Synchrotron Sources — •Tobias Reusch[1], Markus Osterhoff[1], Christina Bömer[1], Florian Schülein[2], Andre Beerlink[3], Dong-Du Mai[1], Achim Wixforth[2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Georg-August Universität Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik, Universität Augsburg, Germany — [3]Deutsches Elektronen Synchrotron, Hamburg, Germany

Collective excitations in biological membranes are of major importance for the understanding of numerous processes in living organisms. Studies of equilibrium properties revealed a rich spectrum of dynamics from the ps to the μs time scale. Out-of-equilibrium dynamics as driven by external forces, i.e. due to active membrane proteins, have remained largely unexplored.
We report on time resolved X-ray scattering experiments at in-house fs $Cu-K_\alpha$ and synchrotron (ID09B/ESRF, P08/PETRAIII) sources, using optical and surface acoustic wave (SAW) excitation mechanisms. Importantly, we were able to record specular and diffuse scattering at a signal level compatible with a full lineshape analysis. For SAW stimulated lipid bilayers the first time resolved electron density profile could be reconstructed at molecular resolution. A clear out of equilibrium behaviour can be observed for Texas-Red labeled lipid multilayers in case of short pulse optical excitation. These results are compared to theoretical predictions for non-equlibrium phenomena, possible implications for fluorescent microscopy experiments are discussed.

BP 21.5 Wed 16:15 H46

Physical vapor deposition (PVD) of 1,2-dipalmitoyl-sn-3-phosphoglycerocholine (DPPC) and membrane formation on SiO2/Si(100) substrate — •Ulrich G. Volkmann[1], María J. Retamal[1], Carmen González[1], Mauricio Sarabia[1], Marcelo Cisternas[1], Michael Kappl[2], and Tomás Corrales[2] — [1]Surface Lab, Facultad de Fisica, Pontificia Universidad Catolica de Chile, Chile — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Phospholipids have been currently of great interest in nanotechnology and applied sciences. One of the most widely used and interesting phospholipids is the surfactant 1,2-dipalmitoyl-sn-3-phosphoglycerocholine (DPPC). Different techniques have been developed in order to assure the complete formation of bilayers or multilayers and particularly to improve thickness accuracy. Between the most popular are spin-coating, dip-coating and Langmuir-Blodgett. In this work we explore the possibility to achieve controlled deposition of a DPPC bio-membrane, combining physical vapor deposition (PVD) on SiO2/Si(100) substrates under high vacuum conditions with high resolution Ellipsometry for very precise thickness control. The well known phase transitions of DPPC layers were analyzed during temperature cycles with Imaging Ellipsometry, AFM and Raman. Previous to and after the application of temperature cycles the film was inspected with SEM. We suggest a method for prolonged membrane humidification by deposition of an ultra thin porous poliglusam interlayer.

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BP 22: Biomechanics (joint focus session with jDPG)

This sessions discusses recent advances in our understanding of the mechanics of cellular systems with the concepts and methods from physics, both from the theoretical and from the experimental points of view. (Organizers Jochen Schneider for jDPG and Ulrich Schwarz for BP)

Time: Wednesday 15:00–16:45 Location: H6

Invited Talk BP 22.1 Wed 15:00 H6

Active Mechanical Processes in Cells and Tissues — •Frank Jülicher — Max Planck Institute for the Physics of Complex Systems, Nöthnitzerstrasse 38, 01187 Dresden

Living cells are extraordinarily dynamic and have the ability to generate movements and forces. This is particularly striking in the case of swimming microorganisms or the process of cell division. A key example for force generating processes in cells is the operation of molecular motors that interact with filaments of the cytoskeleton. In the cell, cytoskeletal networks form gel-like materials with unconventional active material properties that are the consequence of force generating processes. Active cellular processes have also interesting effects on larger scales. Tissues are collections of many cells which can also be considered as active media. Active processes in tissues result e.g. from cellular dynamics, cellular force generation and cell division. These processes introduce mechanical stresses and permit active rearrangements and flows in tissues. In recent years it has become increasingly clear that cells and tissues can also respond to mechanical conditions. Furthermore, there is evidence that mechanical feedbacks may be important in pattern formation processes by which complex organisms form in a developmental process from a single fertilized egg cell. Theoretical approaches are important to characterize the principles which govern the behaviors of active biomaterials and the formation of patterns. Furthermore, theoretical descriptions of cell dynamics and multicellular systems provide a key tool to understand complex dynamics observed in quantitative experiments in vitro and in vivo.

Invited Talk BP 22.2 Wed 15:30 H6

Cell mechanics: An experimental biophysicist's perspective — •Jochen Guck — Biotechnology Center, Technische Universität Dresden, Germany

The mechanical properties of cells are increasingly being investigated and it is well worth taking a closer look why. From a physics point of view, they prescribe the response to external forces and define the limits of a cell's interaction with its three-dimensional physical environment. Largely determined by the cytoskeleton, an internal polymer network regulated by intricate biochemical processes, cell mechanics also has an important biological component. The cytoskeleton is central to many biological functions, evolves during the normal differentiation of cells, and is characteristically altered in many diseases, including cancer. In this presentation I will review this link between physical description and biological function, describe some of the methods to measure cell mechanics and try to communicate the fascination of this topic from a personal point of view.

BP 22.3 Wed 16:00 H6

Flagellar synchronization independent of hydrodynamic interactions — •Benjamin Friedrich and Frank Jülicher — Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

Inspired by the coordinated beating of the flagellar pair of the green algae *Chlamydomonas*, we study theoretically a simple, mirror-symmetric swimmer, which propels itself at low Reynolds number by a revolving motion of a pair of spheres [1]. We show that perfect synchronization between these two driven spheres can result from the motion of the swimmer, which feeds back on the two spheres by local hydrodynamic friction forces. Hydrodynamic interactions, though crucial for net propulsion, contribute little to synchronization for this free moving swimmer. The swimmer design for optimal synchronization reflects a trade-off between the swimmer's ability to move and the premise of broken symmetries required for synchronization. This simple swimmer exemplifies a novel paradigm for hydrodynamic synchronization that could explain flagellar synchronization in *Chlamydomonas*.

[1] B.M. Friedrich, F. Jülicher: Phys. Rev. Lett. **109**, 138102(2012).

BP 22.4 Wed 16:15 H6

The muscle's force-velocity relation derived from a basic principle — •Michael Günther[1,2,3], Daniel Haeufle[1,2], and

Syn Schmitt[1,2] — [1]Universität Stuttgart, Institut für Sport- und Bewegungswissenschaft, Germany — [2]Stuttgart Research Centre for Simulation Technology (SimTech), Germany — [3]Friedrich-Schiller-Universität, Institut für Sportwissenschaft, Germany

In 1938, A.V. Hill extracted from heat and force measurements on frog muscles that the muscle's concentric force-velocity relation is a hyperbola. In 1957, A.F. Huxley published a model that could approximate the Hill relation from assuming eight microscopic parameters describing partly cross-bridge geometry and partly transition rates for cross-bridge attachment and detachment. Other Huxley-type models, using an increasing number of parameters, have been developed since then. In this presentation, we outline a very reduced set of assumptions that is sufficient to derive the Hill relation from the force equilibrium within a simple macroscopic arrangement of mechanical elements and very few further assumptions about the properties of these elements, all based on physiology. With just three elements, incorporating one force-dependent damper, just four mechanical parameters are needed to find a hyperbolic force-velocity relation. A most recent version of our model including a second damping element can even well explain the heat rate-velocity relation, assuming six parameters. From our model, it can be concluded that it might be erroneous to presume that using the isotonic condition guarantees a direct experimental determination of the properties of the active muscle part.

BP 22.5 Wed 16:30 H6

Dynamics of regenerating tissues under mechanical stress — •Claus Fütterer[1,2], Julia Fischer[1], Kao-Nung Lin[1], and Michael Krahe[1] — [1]Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik I, Universität Leipzig, 04103 Leipzig, Germany — [2]ranslationszentrum für Regenerative Medizin (TRM), Universität Leipzig

Hydra vulgaris tissue fragments regenerate and provide an ideal system to study the relation of single cell mechanics to tissue mechanics. We studied tissue toroids with about 1500 cells and studied the overall force fluctuations as well as single cell behaviour. We also applied continuous stress as well as stress pulses to the tissue and investigated the active and passive relaxation and contraction dynamics. We relate the mechanical measurements to the alpha and beta actin structures which form well organized supra-cellular structures responsible for the orchestration of the regeneration process.

BP 23: Networks, From Topology to Dynamics (joint with SOE and DY)

Time: Wednesday 15:45–17:00 Location: H37

BP 23.1 Wed 15:45 H37

Eigenvector centrality as a measure of influence in dynamics on networks — •Konstantin Klemm[1], M. Angeles Serrano[2], Victor M. Eguiluz[3], Maxi San Miguel[3], and Fakhteh Ghanbarnejad[4] — [1]Bioinformatics, Institute for Computer Science, Leipzig University, Germany — [2]Fisica Fonamental, University of Barcelona, Spain — [3]Institute for Cross-Disciplinary Physics and Complex Systems, Palma de Mallorca, Spain — [4]MPI for Physics of Complex Systems, Dresden, Germany

Definitions of centrality aim at quantifying the importance of a node in a given graph. Among many others, the degree, the betweenness and the closeness are examples of frequently used measures of centrality. Here we ask which notion of centrality is best suited for predicting the influence a node has on dynamics. The concept of dynamical influence is made rigorous for a class of dynamical rules that asymptotically lead the system to a stationary state $y(\infty)$ from any initial condition $y(0)$. Then the influence of node v is the dependence of the asymptotic state on the initial condition $y_v(0)$ at node v. We find that the principal eigenvector of the coupling matrix is an accurate predictor of influence for various kinds of dynamics [1,2], including critical epidemic and Ising models, Boolean networks, the voter model as well as Kuramoto and Rössler oscillators.

[1] Klemm et al., Scientific Reports 2, 292 (2012).
[2] Ghanbarnejad and Klemm, EPL 99:58006 (2012).

BP 23.2 Wed 16:00 H37

A macroscopic view on temporal networks — •Hartmut Lentz[1,2], Thomas Selhorst[1], and Igor M Sokolov[2] — [1]Friedrich-Loeffler-Institute, Federal Research Institute for Animal Health, 16868 Wusterhausen, Germany — [2]Humboldt-University of Berlin, 12489 Berlin, Germany

The concept of accessibility graphs can be extended to temporal networks. An accessibility graph (transitive closure) of a network contains a link, wherever there is a path of arbitrary length between node pairs. Building an accessibility graph by consecutively adding paths of growing length ("unfolding") yields information about the distribution of shortest path durations and reveals characteristic time-scales in temporal networks. Accessibility contributes a key element for a theoretical framework for the macroscopic analysis of temporal networks, because it maps the whole causal path structure of the system onto a single mathematical object. In addition, we define a causal fidelity, measuring the goodness of the static representation of a temporal network. The methods provided here can be implemented efficiently and their capability is demonstrated in applications, as shown by our discussion of three temporal network data sets, namely social contacts, livestock trade and sexual contacts.

Reference: Unfolding accessibility provides a macroscopic approach to temporal networks, arXiv:1210.2283.

BP 23.3 Wed 16:15 H37

Clustering coefficient of temporal networks — •Vitaly Belik[1,2], Igor M Sokolov[3], and Hartmut Lentz[3,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]Humboldt-University of Berlin — [4]Friedrich-Loeffler-Institute, Wusterhausen

The science of complex networks has experienced a tremendous development in recent years. Most of the research was devoted to static networks where interactions between nodes are aggregated over time. However with increasing availability of empirical data of high temporal resolution, the dynamics of networks becomes the focus of research. In the present study we generalize the concept of clustering coefficient to temporal networks allowing for arbitrary durations of triangles fulfilling the requirement of causality. In contrast to many algorithmic approaches, we build up on the current advances in the mesoscopic description of temporal networks [1]. We apply our approach to various empirical datasets, in particular a conference contact network and a mobile phone dataset, as well as to their randomized counterparts.

[1] Unfolding accessibility provides a macroscopic approach to temporal networks, H Lentz, T Selhorst, I M Sokolov, arXiv:1210.2283

BP 23.4 Wed 16:30 H37

Devil's Staircases, Crackling Noise and Phase Transitions in Percolation — •Jan Nagler — Max Planck Inst. f. Dyn. & Self-Organization

We identify and study certain phenomena in percolation that can subvert predictability and controllability in networked systems. We establish devil's staircase phase transitions, non-self-averaging, and power-law fluctuations in percolation. We provide exact conditions for percolation that exhibits multiple discontinuous jumps in the order parameter where the position and magnitude of the jumps are randomly distributed - characteristic of crackling noise. The framework is linked to fragmentation processes, where groups or particles repeatedly split up, to susceptible-infected type dynamics, and also to effects in ferromagnetic materials.

BP 23.5 Wed 16:45 H37

Resilience to Leaking - Dynamic Systems Modeling of Information Security — •Kay Hamacher — Department of Computer Science, Department of Physics & Department of Biology, Technische Universitaet Darmstadt, Germany

Leaking of confidential material is a major threat to information security. This insight become popular wisdom since Wikileaks, which hopes to attack 'unjust' systems or 'conspiracies'.

Eventually, such threats to information security rely on a biologistic argument on the benefits and drawbacks that uncontrolled leaking might pose for 'just' and 'unjust' entities. Such biological metaphors are almost exclusively based on the economic advantage of participants.

Here, I introduce a mathematical model of the complex systems dynamics implied by leaking. The complex interactions of adversaries are modeled by coupled logistic equations including network effects of econo-communication networks.

Situations might arise where leaking can strengthen the 'conspiracy'. The only impact leaking can have on an organization originates in the exploitation of leaks by a competing entity. We conclude that leaks can be used as a 'tactical mean' in direct adversary relations, but do not necessarily increase public benefit.

Within the model exploiting the competition between entities seems to be a more promising approach to control malicious organizations: divide-et-impera policies triumph here.

[1] K. Hamacher, "Resilience to Leaking - Dynamic Systems Modeling of Information Security", PLoS One, 2012, accepted

BP 24: Posters: Physics of Cells

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

BP 24.1 Wed 17:30 Poster C

Induced changes in spatio-temporal oscillations of the cell thickness in response to conflicting stimuli — •Mario Breitkopf and Marcus J. B. Hauser — Abteilung Biophysik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Plasmodia of the unicellular slime mould *Physarum polycephalum* form a vascular network where protplasma is pumped to and fro through the cell. The pumping is associated with differences in the thickness of the veins (and hence the thickness of the cell). To ensure effective pumping, certain domains of the cell oscillate in phase. The spatial coherence of these thickness oscillations can be affected by external stimuli, which allows this slime mould to make decisions.

Here we study the self-organized, spatiotemporal pattern of cell thickness oscillations that arise when the cell is exposed to two conflicting stimuli. This is realized by presenting the cell a mixture of a chemoattractant and a chemorepellant. We analyze the changes in thickness oscillations in order to unravel whether changes in the signal transduction pathways also translate into the macroscopic patterns of cell thickness oscillations.

BP 24.2 Wed 17:30 Poster C

Causes of retrograde flow in fish keratocytes — •Thomas Fuhs[1,2], Michael Goegler[1], Claudia A. Brunner[1], Charles W. Wolgemuth[3], and Josef A. Kaes[1] — [1]Division of Soft Matter Physics, Department of Physics, University of Leipzig, Leipzig, Germany — [2]Paul Flechsig Institute of Brain Research, University of Leipzig, Leipzig, Germany — [3]Departments of Physics of Molecular and Cellular Biology, University of Arizona, Tucson, AZ, United States of America

Confronting motile cells with obstacles doubling as force sensors we tested the limits of the driving actin-and-myosin-machinery. We could directly measure the force necessary to stop actin polymerization as well as the force present in the retrograde actin flow. Combined with detailed measurements of the retrograde flow velocity and specific manipulation of actin and myosin we found that actin polymerization and myosin contractility are not enough to explain the cells behavior. We show that ever-present depolymerization forces, a direct entropic consequence of actin filament recycling, are sufficient to fill this gap, even under heavy loads.

BP 24.3 Wed 17:30 Poster C

Spatio-temporal dynamics of plasmodial migration of the slime mould *Physarum polycephalum* — •Beatrice Rodiek[1], Tetsuo Ueda[2], and Marcus J. B. Hauser[1] — [1]Abteilung Biophysik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany — [2]Research Institute of Electronic Science, Hokkaido University, Sapporo, Japan

Spatio-temporal self-organization of large amoeboid plasmodial cells of the slime mould *Physarum polycephalum* was studied in relation to cell locomotion. During locomotion, the slime mould shows rhythmic contraction and expansion waves. We observe distinct patterns in wild-type strain and in one behavioural mutant. The pseudopodium extended either in a periodic back-and-forth manner or in a forward-stop fashion. Correspondingly, the propagation of the contraction waves either reached the vicinity of the front or left a stationary, non-oscillatory region near the front. Thus, the genetic differences in the cells of the same species may translate into different physical patterns of locomotion.

BP 24.4 Wed 17:30 Poster C

Investigation of the protoplasmic flow in veins of *Physarum polycephalum* — Sebastian Weise and •Marcus J. B. Hauser — Abteilung Biophysik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

The plasmodium of the *Physarum polycephalum* forms a characteristic, extended vascular network, which is used to transport the protoplasm through the giant cell. The transport is driven by peristaltic pumping and it reverses its direction periodically. The flow in the veins of *P. polycephalum* is always laminar, however, it is known that protoplasmic particles are effectively and rapidly distributed within the cell. To elucidate how an effective transport can be achieved in a system with laminar flow, we performed particle tracking velocimetry experiments. The flow of inserted particles is analyzed, and the role of vascular ramifications is addressed.

BP 24.5 Wed 17:30 Poster C

Collective cell migration in tumor colonies — •Janina Lange[1], Claus Metzner[1], Julian Steinwachs[1], Patrick Krauss[1], Pamela Strissel[2], and Ben Fabry[1] — [1]University of Erlangen-Nuremberg, Department of Physics, Biophysics Group — [2]University of Erlangen-Nuremberg, Department of Gynaecology and Obstetrics

Many tumor cells proliferate despite a lack of interaction with the extracellular matrix and without cell-contact inhibition that normally prevents cells from proliferating beyond confluency. This gives tumor cells the advantage to grow into a dense 3-dimensional tissue. As the tumor grows, mechanical stresses arise that depend on proliferation speed, cell contractility, substrate adhesiveness, and cell cohesiveness. They are organized by cells migrating between regions of different mechanical stresses. Here we study how proliferation, adhesiveness and cohesiveness influence the migration of individual tumor cells in rapidly growing 3-dimensional tumor colonies initiated on a 2D substrate. Colonies of highly and weakly adhesive and cohesive cell lines are compared. We also study colonies of embryonic mouse fibroblasts in which focal adhesion kinase was knocked out, which leads to changes in both adhesiveness and cohesiveness involving E-cadherin. In weakly adhesive cell lines, cells close to the border migrate rapidly and persistently in the radial direction. Interestingly, in the central tumor region we also find highly persistent cell migration but in random directions with a spatially and temporally highly correlated migration pattern. Collective cell migration, however, was absent in colonies of high adhesiveness and low cohesiveness.

BP 24.6 Wed 17:30 Poster C

Cell visco-elasticity measured with AFM and optical trap at sub-micron deformations — •Paula Sánchez, Weixing Li, Marie Zeiss, Carina Wollnik, Kai Bodensiek, Florian Rehfeldt, and Iwan Schaap — III. Physikalisches Institut, Faculty of Physics, Georg-August Universität Göttingen, Germany

The elastic properties of cells are widely used as an indicator for differentiation, response to drug treatment, or the effects of the supporting matrix on cell development. We use vertical optical trapping and AFM to measure the cell's visco-elastic response at deformations of 0.2 to 1.2 um. To perform the optical trapping experiments at different speeds we implemented an FPGA based fast force feedback to control the vertical movement of the piezo at speeds up to 50 um/s. We use this combined approach to quantify the visco-elasticity at small and large deformations on both stiff and soft substrates. Deformations up to 0.2 um showed a reversible, thus truly elastic response that was independent of the rate of deformation. At higher indentations, the apparent Young's modulus increased a multifold due to viscous effects that followed a weak power law. Both AFM and optical trapping indentation experiments give consistent results for the cell elasticity. Optical trapping has the benefit of a lower force noise, which allows a more accurate determination of the absolute indentation.

BP 24.7 Wed 17:30 Poster C

Elasticity measurements of fibroblastic cell nuclei by atomic force microscope for characterizing Lamin and TMEM43 mutations — •Tamara Münnich[1], Volker Walhorn[1], Helene Schellenberg[1], Astrid Kassner[2], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Experimental Biophysics, Bielefeld University, Germany — [2]Erich und Hanna Klessmann-Institut, Herz- und Diabeteszentrum Bad Oeynhausen, Germany

Arrhythmogenic right ventricular cardiomyopathy (ARVC) is an inherited heart muscle disease associated with cardiac arrhythmia. It is a major cause of sudden cardiac death in the young and athletes. Mutations of the intermediate filament Lamin and the transmembrane protein 43 (TMEM43) are connected to ARVC. Both proteins are located at the nuclear envelope. As the cell nucleus has to resist strong mechanical stress caused by the contraction of the heart muscle, we suppose that the mutations affect functional mechanical properties of the nucleus. The elastic moduli of the cell nuclei were measured with the atomic force microscope and estimated by the Hertz-model. The measurements were performed with fibroblasts, which serve as a model system for cardiomyocytes. We analyzed a set of Lamin and TMEM43 mutated cells and compared them to a control group consisting of wild type fibroblasts and mutations not associated with ARVC. The TMEM43 mutant showed much higher and widespread elastic moduli, whereas the elasticity of the Lamin mutant is similar to the control group. In the future we will analyze modified fibroblasts expressing no Lamin and TMEM43 respectively.

BP 24.8 Wed 17:30 Poster C

Photo-induced switchable cell adhesion on nanostructured surfaces — •Laith Kadem[1], Qian Li[1], Michelle Holz[2], Rainer Herges[2], and Christine Selhuber-Unkel[1] — [1]Christian-Albrechts-University Kiel, Institute for Materials Science — [2]Christian-Albrechts-University Kiel, Otto Diels-Institute of Organic Chemistry

Cell adhesion (CA) relies on the specific binding of transmembrane proteins to their extracellular ligands. The spacing between individual integrin binding sites in mammalian RGD-integrin CA system controls CA forces and reinforcement as well as cell elasticity. We aim to develop nanostructured surfaces where light-driven switchable CA is feasible. Using Diblock Copolymer Micelle Nanolithography, these nanostructures are introduced on the surface as nanometer-sized monodispersed gold particles ordered in a quasi-hexagonal pattern. The spacing between gold dots can be varied from 20 to 200 nm with nanometer precision. Moreover, we can apply this technique to surfaces with a structured microtopography. Regular microtopographies on surfaces can be obtained with photolithography followed by an etching step. Subsequently, we create patterns of the gold nanodots within the micro-domains. With this protocol, we are able to generate different spacings of gold dots on one single substrate in a single step. The gold dots are functionalized with photoswitchable azobenzene molecules incorporated with RGD peptides in order to mediate specific CA to surfaces through integrins. Using the photoswitching properties of azobenzenes, we aim at switching CA in a spatially and temporally defined fashion.

BP 24.9 Wed 17:30 Poster C

A systems-level model for focal adhesions — •Max Hoffmann[1,2] and Ulrich S. Schwarz[1,2] — [1]BioQuant, Heidelberg University, Heidelberg, Germany — [2]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

Focal adhesions are cell-matrix contacts, which transduce and integrate mechanical as well as biochemical cues from the environment. They are large supra-molecular assemblies with more than 170 types of proteins and more than 700 types of interactions collectively known as the "adhesome". Due to their association with the plasma membrane, focal adhesions are spatially organized in three layers of adhesion receptors, connector and signaling molecules, as well as cytoskeletal proteins. The exact composition and function of focal adhesions is strongly regulated by signaling (including the effect of the small GTPases from the Rho family) and the impact of mechanical force.

Here we present theoretical models, which account for all of these features by describing the assembly process of a generic set of core components. First we introduce a kinetic model that allows us to predict the effect of RNA-interference studies on focal adhesions. Depending on the specific knockdown, focal adhesions can get up or down regulated, in good agreement with recent experimental findings. The impact of force on the assembly and maturation process is investigated for different force models (slip and catch bonds) that can lead to markedly different phenotypes. Second we address the maturation of focal adhesions in spatial detail with a particle-based simulation reflecting the spatial-temporal coordination close to the leading edge of the cell.

BP 24.10 Wed 17:30 Poster C

Measuring viscoelasticity in the extracellular space upon particle binding — •Felix Jünger and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

The cytoskeleton is a highly dynamic structure present in all cells, consisting of various kinds of filaments. It is responsible for movement, shape and division of cells as well as for particle uptake and transport processes inside the cell. Still, many principle questions remain open about the mechanics of particle uptake and the driving forces. What is the role of the membrane, the actin network, the myosin motors and the interplay among them?

Macrophages are essential components of the mammalian immune system, responsible for internalizing pathogens via phagocytosis. In our work we perform micro-rheological experiments on J774 mouse macrophages to investigate the viscous and elastic properties of the extracellular space prior to phagocytosis - parameters that the cell can actively control by reorganizing its actin cytoskeleton. We use photonic force microscopy (PFM) to analyse the temporal fluctuations of an optically trapped bead, which is approached to a cell membrane. The motion of the bead is tracked interferometrically in three dimensions with nanometer precision and on a microsecond time scale. The viscous modulus $G''(\omega)$, but also the elastic modulus $G'(\omega)$ can be obtained by analyzing the fluctuation data on a broad spectral bandwidth ω. We have measured several bead-cell arrangements and developed first simple theoretical models that help explain our experimental findings.

BP 24.11 Wed 17:30 Poster C

Vimentin structure in human mesenchymal stem cells depends on substrate elasticity — •Jennifer Radwitz — Georg-August-Universität, Göttingen, Germany

Human mesenchymal stem cells are multipotent adult stem cells that can differentiate into several cell types, e.g. bone, muscle, cartilage. The differentiation process is usually driven biochemically by growth factors but can also be induced mechanically by changing the elasticity of the microenvironment. Structural integrity and mechanosensing of cells is sustained mainly by the cytoskeleton, which consists of acto-myosin structures, intermediate filaments (IFs) and microtubules. Contributions by microfilaments and microtubules are extensively studied but the class of IFs, in mesenchymal cells represented mainly by vimentin, is lesser explored.

By varying the Young's modulus E of the substrates we mimic different mechanical environments. Cells are transfected to express eGFP-vimentin which can be observed in a fluorescence microscope. In long-term life cell measurements we record the vimentin structure and analyze its dynamics to elucidate its contribution to the mechanical coupling of cell and matrix.

We present data showing that vimentin structure depends on substrate elasticity and develops temporally different than actin fibers, as demonstrated with co-transfected cells. Correlating the structure and dynamics with matrix elasticity will help us to dissect the contribution of vimentin filaments to the complex cytoskeletal network.

BP 24.12 Wed 17:30 Poster C

Increased Stiffness of Neutrophils after Activation by Transfusion Related Acute Lung Injury-Relavant Antibodies — •Michael Glaubitz[1], Tom Berthold[2], Christiane A. Helm[3], Mihaela Delcea[1], and Andreas Greinacher[2] — [1]ZIK HIKE - Centre for Humoral Immune Reactions in Cardiovascular Diseases, University of Greifswald — [2]Department of Transfusion Medicine, University of Greifswald — [3]Department of Physics, University of Greifswald

Transfusion related acute lung injury (TRALI) is a severe adverse effect of blood transfusion. A subgroup of TRALI is induced by antibodies directed against alloantigens on neutrophils, a subgroup of the granulocytes. TRALI is believed to occur in approximately one in every 5000 transfusions. Besides neutrophil aggregation, the neutrophils elasticity could be critical for the development of an acute lung injury, as stiffer neutrophils might get stuck in the narrow microvasculature of the lung. Using colloidal probe or tippless Atomic

Force Microscopy (AFM) cantilevers to compress the cells, the influence of TRALI-relevant antibodies (HNA-3a) on the stiffness (Young's modulus E) of neutrophils is investigated. The AFM indentation measurements are fitted to the Hertz model. The stiffness of neutrophils increased after incubation with HNA-3a. The parameter incubation time was investigated and found to be relevant. These findings give insights in the etiology of TRALI.

BP 24.13 Wed 17:30 Poster C

The actin cytoskeleton of chemotactic amoebae operates close to the onset of oscillations — Christian Westendorf[1], •Jose Negrete Jr[1], Albert Bae[1], Rabea Sandmann[1], Eberhard Bodenschatz[1,2], and Carsten Beta[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen — [2]Laboratory of Atomic and Solid-State Physics, Cornell University, USA — [3]Institute of Physics and Astronomy, University of Potsdam

The rapid reorganization of the actin cytoskeleton in response to external stimuli is an essential property of many motile eukaryotic cells. Here, we report evidence that the actin machinery of chemotactic Dictyostelium cells operates close to an oscillatory instability. When averaging the actin response of many cells to a short pulse of the chemoattractant cAMP, we observed a transient accumulation of cortical actin reminiscent of a damped oscillation. At the single-cell level, however, the response dynamics ranged from strongly to weakly damped oscillations. Furthermore, in a small subpopulation, we observed self-sustained oscillations in the cortical F-actin concentration. To substantiate that an oscillatory mechanism governs the actin dynamics in these cells, we systematically exposed a large number of cells to periodic pulse trains of different frequencies. We propose a model based on a time-delay in the regulatory network of the actin system. The model was quantitatively tested with experiments performed with cells that express GFP-tagged fusion in proteins that enhance the disassembly of actin filaments and thus allow us to estimate the delay time in the regulatory feedback loop.

BP 24.14 Wed 17:30 Poster C

Spatial versus temporal gradient stimuli in eukaryotic chemotaxis — •Alexander Anielski, Eva Pfannes, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Germany

Chemotaxis, the directed movement of a cell in response to a chemical gradient, is a fundamental property that governs numerous essential processes like wound healing, cancer metastasis, and embryonic development. Here, we present for the first time an experimental setup to separately address the dependencies of the chemotactic motion on the average background concentration and on the gradient steepness. In particular, this setup allows us to investigate the role of spatial versus temporal sensing. Our method relies on a computer controlled motorized microscope stage to compensate chemotactic cell movement in response to different stimuli. We use the controlled photolysis of caged compounds in a microfluidic chamber to address single cells with well-controlled concentration signals in space and time (flow photolysis). We show results from experiments with the social amoeba Dictyostelium discoideum to exemplify the role of spatial versus temporal gradient sensing in this widely used model organism of eukaryotic chemotaxis.

BP 24.15 Wed 17:30 Poster C

Amoeboid motion based on membrane folds that are driven by self organized actin waves. — •Matthias Gerhardt, Michael Walz, and Carsten Beta — Institut für Physik und Astronomie, Karl-Liebknecht-Strasse 24/25, 14476 Potsdam, Germany

We observed the movement of small particles enclosed in between the bottom membrane of a large electrofused Dicyostelium cell and the substrate surface. Self-organized waves generated by the actin network inside the cell were reliably pushing the particles forward, indicating that actin waves are generating forces against the cell membrane to push the cell forward. A vertical scan through the self-organized waves revealed that under certain conditions, waves can locally lift the cell membrane to form a small cavity in between the membrane and the substrate surface. These observations led us to propose a novel mechanism for amoeboid motion based on the wave-driven motion of membrane folds across the bottom surface of the cell. We have implemented a simple computer model that consists of a virtual membrane driven by the waves of an excitable FitzHugh-Nagumo system. Depending on the choice of parameters and initial conditions, the virtual membrane was found to move in the direction of wave propagation along either linear or curved trajectories.

BP 24.16 Wed 17:30 Poster C

Dynamics of membrane tubes filled with an active gel — •Dominic Jourdain and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

Cellular systems display a multitude of tubular protrusions, e.g., filopodia, axons or stereocilia. These structures are essentially cylinders delimited by a lipid membrane and filled with cytoskeletal filaments. The intrinsic activity of such protrusions can induce mechanical instabilities. For example, peristaltic shape undulations of axons have been observed subsequent to osmotic perturbations [1]. To further understand possible mechanical instabilities of tubular protrusions, we study the dynamics of active gels inside tubular membranes. Cytoskeletal dynamics are described on a continuum level and on macroscopic length and time scales using a two-fluid hydrodynamic theory. We find that sufficiently large active stresses in the gel induce peristaltic instabilities.

[1] Pullarkat et al., *Phys. Rev. Lett.* **96**, 048104 (2006)

BP 24.17 Wed 17:30 Poster C

Using Scanning-Ion-Conductance-Microscopy to probe the axon initial segment of hippocampal neurons — •Ulrich Fromme[1], Christopher Dilip[2,3], Andreas Neef[2,3], and Christoph Schmidt[1] — [1]Drittes Physikalisches Institut, Fakultät für Physik, Georg-August-Universität, Göttingen — [2]Bernstein Center for Computational Neuroscience, Göttingen — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen

Scanning-Ion-Conductance-Microscopy (SICM) is a scanning-probe-microscopy which allows topographic imaging of living cells with resolutions superior to most optical methods. Its probe consists of an electrolyte-filled glass pipette as used in patch-clamp recordings, so that it can also be used for electrophysiological experiments. By combining SICM with fluorescence microscopy, specific stained structures can be indentified and imaged with SICM. In this work we used fluorescently labeled antibodies against Neurofascin, which is predominantly expressed at the Axon-Initial-Segment (AIS). This allows the identification of the AIS in live, cultured hippocampal neurons so that the surface structure can be imaged with lateral resolutions around 50 nm, and axial resolutions better than 10 nm. Electrophysiological measurements can then be done with the same piezo-driven pipette resulting in the same high precision. This way it is possible to combine structural information with electrophysiological information with high resolution. The shapes of extracellular action potentials can thus be recorded at various positions along the cell, which gives more information on ion current densities and kinetics than standard whole cell recordings.

BP 24.18 Wed 17:30 Poster C

High-speed video microrheology in syncytial Drosophila embryos — •Alok D. Wessel[1], Mahesh.G. Reddy[2], Jörg Grosshans[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Zentrum für Biochemie und Molekulare Zellbiologie, Georg August-Universität Göttingen, Germany

In early development, Drosophila melanogaster embryos are in a syncytial stage, i.e. multiplying nuclei are not yet separated by membranes, but are interconnected by cytoskeletal polymer networks consisting of actin and microtubules. Between division stages 9 and 13, nuclei and the cytoskeletal network form a well-ordered 2D cortical layer.

To understand the underlying mechanical properties and dynamics of this self-organizing "pre-tissue", we measure shear moduli of the interior of the embryo and its cortical layer by high-speed video microrheology. We record position fluctuations of injected micron-sized fluorescent beads with a high-speed camera at kHz sampling frequencies.

The interior of syncytial embryos shows a homogeneous, viscously dominated behavior, whereas in the actin-rich outer parts, near the nuclear layer, we see a viscoelastic response. Furthermore we are able to resolve temporal variations of the shear modulus inside the layer during the coordinated nuclear division cycle, e.g. viscosity becomes about three times higher than during interphase.

BP 24.19 Wed 17:30 Poster C

Bestimmung der Wärmeleitfähigkeit von Pflanzengewebe mit Thermomikrokapillaren — •Waldemar Wedel[1], Miriam Giesguth[2], Haleh Ebrahimian[1], Katharina König[2], Karl-Josef

Dietz[2], Günter Reiss[1] und Simone Herth[1] — [1]Dünne Schichten & Physik der Nanostrukturen, Universität Bielefeld, Deutschland — [2]Biochemie und Physiologie der Pflanzen, Universität Bielefeld, Deutschland

Die Bestimmung der Körpertemperatur ist eine seit Jahrhunderten bekannte Methode. Neu hingegen ist die Messung der Temperatur in einzelnen Zellen. Mittels zwei verschiedener metallbeschichteten Glaskapillaren ist es nun möglich, sowohl lokal Wärme zu erzeugen als auch diese zeitgleich zu messen. **** Diese Thermomikrokapillaren (engl. Thermomicrocapillary, TMC) basieren auf dem Seebeck-Effekt (Messen) bzw. dem Joule-Effekt (Heizen). Die nanometerdicken Metallschichten Ni und NiCr (Typ K) bzw. Ta sind gegenüberliegend als schmale Linien auf der Kapillare aufgedampft. Die TMC macht aufgrund ihrer Spitze das reproduzierbare Einstechen in einzelnen Zellen möglich. In diesem Beitrag wird die Kombination der beiden TMCs zur Bestimmung der Wärmeleitfähigkeit von Pflanzengeweben demonstriert. Dazu wurde eine Heiz- sowie eine Messkapillare in das entsprechende Gewebe eingestochen und eine Spannung an die Heizkapillare angelegt, die zu einer Temperaturerhöhung von 20 °C führte. Der Temperaturverlauf wurde in mehreren definierten Abständen von der Wärmequelle parallel mit der Messkapillare aufgezeichnet und mit mathematischen Methoden ausgewertet.

BP 24.20 Wed 17:30 Poster C

Persistent motion in the crowd - The role of superdiffusivity in cell colony dynamics — •Patrick Krauss, Janina Lange, Claus Metzner, and Ben Fabry — Department of Physics, Biophysics Group, Friedrich-Alexander University, Erlangen, Germany

We study the 3D growth dynamics of circular tumor colonies on planar substrates. By tracking the motion of single cells within dense colonies, cell trajectories were found to have a surprisingly high degree of directional persistence, with a mean squared displacement (MSD) increasing as a fractional power of lagtime. The fractional exponent of the MSD, as well as the distribution of migration directions, depend systematically on the radial position within the colony. This is a qualitative difference to liquid spreading models of tumor growth, were the particles search for a global low energy configuration by non-directional diffusion. Using a generalized Molecular Dynamics method, we study the relation between directional persistence, cell-cell- and cell-surface-interactions, cell proliferation, and the resulting 3D morphology of the colony. Results are compared to experimental data from different cell lines.

BP 24.21 Wed 17:30 Poster C

Plectin contributes to the mechanical stability of keratinocytes and myoblasts — •Navid Bonakdar[1], Achim Schilling[1], Pablo Lennert[1], Michael Kuhn[1], Astrid Mainka[1], Wolfgang Goldmann[1], Gerhard Wiche[2], and Ben Fabry[1] — [1]Biophysics, University of Erlangen-Nuremberg, Germany — [2]Biochemistry and Cell Biology, University of Vienna, Austria

Plectin and its isoforms are promiscuous crosslinkers of actin filaments, microtubules and intermediate filaments (IF) in a wide variety of cell types. In epithelial cells and keratinocytes, it is also found in hemidesmosomes that link the laminin receptor a6b4 with the keratin IFs. Mutations in the plectin gene cause a skin blistering disorder (epidermolysis bullosa) that is also associated with a late-onset of muscular dystrophy. In both disorders, mechanical alterations of the keratinocytes and the myoblasts, respectively, are thought to be ultimately responsible for the pathological manifestation. To test this hypothesis, we measured the mechanical properties of plectin knockout and plectin-expressing mouse keratinocytes and myoblasts with a high force magnetic tweezer device. We found that in plectin-deficient myoblasts, stiffness, tractions, and adhesive strength were about 2-fold reduced, indicating that plectin is important for the mechanical stability of these cells. In contrast, plectin-deficient keratinocytes assessed under similar conditions were found to show other effects. Our results demonstrate that human diseases associated with plectin mutations have a cell mechanical origin, and that plectin affects the cytoskeleton in different cell types in distinct ways.

BP 24.22 Wed 17:30 Poster C

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

It is accepted knowledge that cells sense the mechanical properties of their surroundings, and that many internal cellular processes not only respond to biochemical, but also to mechanical stimuli. Cells generate contractile forces themselves to probe and to adapt to the mechanical properties of their micro-environment. Key players in the generation of contractile forces are acto-myosin structures, such as stress fibers. We aim at elucidating the contributions of acto-myosin fibers to the total force produced by suspending a cell in an idealized geometry between two optical traps. In our setup we attach fibronectin-coated beads to opposite sides of a suspended 3T3 fibroblast cell. We analyze the correlated motion of the two beads at high bandwidth and with pN-resolution by laser interferometry. Using a combination of active and passive microrheology, we can dissect the non-equilibrium fluctuations and simultaneously probe the viscoelastic properties of the cell. Here we present data on contractile forces and elastic properties of the cell. The amount of force fluctuations transmitted to the outside depends on trap stiffness. Biochemical perturbation experiments interfering with the acto-myosin cytoskeleton or microtubules demonstrate the key role of myosin motors for contractile force generation. We used different bead sizes to determine the effect of cell-bead attachment and also tested the cellular response at different temperatures.

BP 24.23 Wed 17:30 Poster C

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 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 under shear stress. Without it (a5b1 fibroblasts) the network is less elastic with a decreased elastic modulus under stress.

BP 24.24 Wed 17:30 Poster C

Dynamics of Stem Cell Stress Fibers — •Carina Wollnik[1], 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

Mechanical cues can be as important to cell behaviour as biochemical ones. Engler et al. demonstrated that varying the substrate stiffness could guide human mesenchymal stem cells (hMSCs) towards different lineages in the absence of additional biochemical cues. The complex differentiation process takes several days up to weeks, but primary characteristic changes of the cytoskeleton can be detected within the first 48 hours. Here the key players are cytoskeletal structures like stress fibers, composed of actin filaments, actin binding- and crosslinking-proteins, and non-muscle myosin motor-proteins. Stress fibers generate and transmit forces within the cell and to the extracellular matrix.

During the initial adhesion and spreading process the cell area changes as well as the cells' aspect ratio and stress fiber structure. We study the dynamics of these processes to gain a deeper understanding of the differentiation initiation steps. In our experiments we use live-cell imaging of RFP-Lifeact transfected hMSCs and trace the acto-myosin stress fibers with novel sophisticated filament tracking algorithms, which enable us to investigate the dynamics of stress fiber formation that leads to a non-monotonic dependence of stress fiber polarization on the Young's modulus of the underlying substrate.

BP 24.25 Wed 17:30 Poster C

Estimation of Local Cellular Tension with Active Cable Models — Philip Guthardt Torres[1], •Jérôme Soiné[1], Christoph Brand[1], Jonathan Stricker[2], Venkat Maruthamuthu[2], Patrick Oakes[2], Margaret Gardel[2], and Ulrich S. Schwarz[1]

— [1]Bioquant and Institute for Theoretical Physics, Heidelberg University, Germany — [2]Institute for Biophysical Dynamics, University of Chicago, USA

The ability to generate intracellular tension is essential for adhesion-dependent tissue cells, allowing them to actively probe and adapt to their mechanical environment. Traction force microscopy on planar elastic substrates has been successfully implemented to reconstruct the cellular traction field, but the correlation with intracellular tension states is largely unexplored. We have developed a procedure to estimate intracellular tension from elastic substrate data by minimizing the difference to the predictions of a theoretical model based on active cable networks. This model has been successfully used before to predict cell shape on micropatterned substrates. We now have extended it to describe not only contractile networks, but also various types of contractile bundles commonly observed in adherent cells. Contractile models are generated from images of adherent cells by segmenting cell shape and actin structures. Subsequent computer simulation of network contraction and parameter optimization allows us to estimate the most likely distribution of tension over the various contractile structures. In the future, our predictions might be compared to experimental results from laser cutting or force-sensitive fluorescent probes.

BP 24.26 Wed 17:30 Poster C

Biologische Neuronen auf elektrischen Leiterbahnen — •Olga Simon[3], Stefan Niehörster[1], Markus Schäfers[1], Marius Schirmer[1], Matthias Schürmann[2], Barbara Kaltschmidt[2], Christian Kaltschmidt[2] und Andy Thomas[1,3] — [1]Universität Bielefeld, Physik, Universitätsstrasse 25, 33615 Bielefeld — [2]Universität Bielefeld, Biologie, Universitätsstrasse 25, 33615 Bielefeld — [3]Universität Hamburg, Angewandte Physik, Jungiusstrasse 11, 20355 Hamburg

Die Synapse ist ein wichtiger Bestandteil in neuronalen Netzwerken, jedoch fehlte bisher ein einfaches, elektrisches Bauteil, welches dieselbe Funktion in einer Schaltung übernehmen kann. Dies erschwert die Entwicklung von Hardware, die die Architektur des biologischen Nervensystems imitiert. Nun haben die Fortschritte auf dem Gebiet der Memristoren das Interesse in künstlichen neuronalen Netzen zusätzlich aufleben lassen. Der Widerstand eines Memristors hängt von seinen bisher eingenommenen Zuständen ab, genau dies kann ausgenutzt werden, um die synaptische Verbindung zwischen zwei Neuronen zu imitieren. Eine Wunschvorstellung wäre die Signalübertragung von einem biologischen Neuron in einen elektronischen Schaltkreis. In diesem Beitrag präsentieren wir erste Ergebnisse zum Wachsen von Nervenzellen auf elektrischen Leiterbahnen. Dabei wird versucht die Biokompatibilität der Unterlage durch geschickte Materialwahl zu beeinflussen. Darüber hinaus wird versucht sicherzustellen, dass nur einzelne Nervenzellen auf die Leiterbahnen aufgebracht werden, um geplant Spike-Detektion den Neuronen zuordnen zu können.

BP 24.27 Wed 17:30 Poster C

Fluctuations and differential contraction during regeneration of Hydra vulgaris tissue toroids — •Claus Fütterer[1,2], Michael Krahe[1], Iris Wenzel[1], Kao-Nung Lin[1], Julia Fischer[1], Joseph Goldmann[3], and Markus Kästner[3] — [1]Institut für Experimentelle Physik I, Universität Leipzig, 04103 Leipzig, Germany — [2]Translationszentrum für Regenerative Medizin (TRM), Universität Leipzig — [3]Institut für Festkörpermechanik, Technische Universität Dresden, 01062 Dresden, Germany

While much is known about the physics of single cells, the mechanics of self-organization and regeneration of cells in tissues and cell assemblies is largely unexplored. We studied regenerating tissue toroids from Hydra vulgaris and relate our macroscopic observations to the dynamics of force-generating mesoscopic cytoskeletal structures. Tissue fragments undergo a specific toroid-spheroid folding process leading to complete regeneration towards a new organism. The time scale of folding is too fast for biochemical signalling or morphogenetic gradients which forced us to assume purely mechanical self-organization. The initial pattern selection dynamics was studied by embedding toroids into hydro-gels allowing us to observe the deformation modes over longer periods of time. We found increasing mechanical fluctuations leading to an instability due to a supra-cellular actin ring destabilizing the toroidal symmetry. We discuss the evolution of their power spectra for various gel stiffnesses. Our observations are related to single cell studies which explain the mechanical feasibility of the folding process. In addition, we observed switching of cells from a tissue bound to a migrating state.

BP 24.28 Wed 17:30 Poster C

Stochastic dynamics of gliding motility — •Thorsten Erdmann[1,2] and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [2]BioQuant, Heidelberg University, Heidelberg, Germany

After being injected into the skin tissue of a vertebrate during a mosquito bite, the sporozoite form of the malaria parasite glides through the tissue in order to reach blood vessels. Experimental trajectories reveal strong fluctuations of the speed of the gliding motility. On the sub-second time scale, sporozoites seem to move in a stick-slip fashion. On longer time scales, gliding is arrested by occasional stationary attachments of the rear of the sporozoite. In order to investigate the stochastic dynamics of gliding motility, we derive a model for the propulsion mechanism, in which specialized adhesion molecules bind to the substrate and are displaced relative to the sporozoite body by small groups of non-processive molecular motors. We study the different regimes of movement in dependence on the binding characteristics of the adhesion molecules, which are described as slip bonds as well as catch bonds, and in dependence on the effective processivity and force-velocity relation characterizing the molecular motors. In order to assess the role of elasticity, we also study the motion of stiff segments of the basic model which are elastically coupled to each other.

BP 24.29 Wed 17:30 Poster C

Bacterial force spectroscopy: the influence of cell wall proteins on the adhesion process of Staphylococci — •Nicolas Thewes, Peter Loskill, and Karin Jacobs — Saarland University, Experimental Physics D-66123 Saarbrücken

Bacterial adhesion to surfaces is a complex process that depends on many factors such as the type of bacterium, the type of surface [1] and the surrounding medium, as well as the composition of the material [2] and the time of contact.

In this study we show the important role of bacterial surface proteins during the adhesion process to an artificial surface.

Using AFM-force spectroscopy, we studied the differences in the adhesion process of two bacterial strains of the Staphylococcus genus, S. aureus and S. carnosus. Measurements with increasing and decreasing surface delay times showed severe differences due to different cell wall protein compositions. To be more precise, pathogenic S. aureus showed a much higher adhesion capability than apathogenic S. carnosus.

In addition, we developed a new set-up to attach single bacteria to an AFM cantilever which now enables adhesion measurements on a single cell level.

BP 24.30 Wed 17:30 Poster C

Automated Optical Stretching — •Roland Stange, Tobias Kiessling, Anatol Fritsch, Susanne Rönicke, and Josef Käs — Institut für Experimentalphysik 1, Leipzig, Deutschland

The mechanical behavior of single eukaryotic cells is known to play a defining role in cell migration, cell division, mechanotransduction, tissue formation and embryogenesis. Thus huge effort was made to develop methods able to test single cell mechanics (e.g.: Optical Stretcher, optical tweezer, atomic force microscope, micropipette aspiration, magnetic beat rheology). Despite the low throughput of these methods it got clear, that cells of the same cell type (e.g. from the same tissue or cell-line) are not mechanically equal, but show a broad, non-Gaussian, asymmetric distribution. To further investigate cell mechanics from a statistical perspective we increased the throughput of the Optical Stretcher technique to 300 cells per hour leading to cell counts of more than 1000 cells for a simple measurement. By measuring fully automated, human bias is drastically reduced and resulting distributions are smooth and reliable due to standard errors smaller than 5%.

BP 24.31 Wed 17:30 Poster C

Novel elastic force sensors for live cell investigations — •Sören Björn Gutekunst, Julia Reverey, and Christine Selhuber-Unkel — Christian-Albrechts-University Kiel, Institute for Materials Science, Germany

Phagocytosis is an essential mechanism found in many cell types. It is of key importance for the functioning of biological systems and tissues and plays a significant role for the immune system. So far, the forces acting during the uptake of target cells and artificial particles are still not known. It can be suggested from electron microscopy that pathogenic amoebae such as Acanthamoebae exert comparably large forces during the phagocytosis of target cells. In order to elucidate the complexity of such force generation events during phagocytosis in

different cellular systems and to gain further insight into the underlying processes, we fabricate elastic polyacrylamide beads (EPABs). To this end, we transfer the concept of traction force microscopy into the third dimension and synthesize fluorescent elastic polyacrylamide beads (EPABs) with incorporated fluorescent nanoparticles by means of inversed emulsion polymerization. The elasticity of the EPABs can be changed by varying the amounts of crosslinker and is characterized with AFM. Our goal is to finally be able to relate changes in particle shape to the forces exerted by cells in a bead deformation assay (BDA). We will in particular use this method to investigate target cell killing and uptake in Acanthamoebae.

BP 24.32 Wed 17:30 Poster C

Blood platelets - a model system for understanding cellular mechanics — •Aishwarya Paknikar, Sarah Schwarz G. Henriques, Rabea Sandmann, and Sarah Köster — Institute for X-Ray Physics, Georg-August-Universität Göttingen, Germany

Platelets get activated during an injury, change their shape and rearrange their actin-myosin cytoskeleton to generate forces, resulting in contraction. The mechanical principles underlying this dynamic process are poorly understood. The average total traction force of a single platelet on a soft polyacrylamide (PAA) substrate (elasticity ~4 kPa), measured by traction force microscopy (TFM) is ~34 nN. Immunostaining experiments also indicate that the platelet cytoskeletal reorganization is dependent on the substrate stiffness and myosin contributes majorly to the total force generation, leading to some open questions. Firstly, the mechanical response of platelets to different substrate stiffness is elusive. We are analyzing this influence of the substrate stiffness on the spreading of single platelets by varying the substrate elasticity within the physiological range (1-100 kPa). Secondly, the extent of contribution of other, myosin-independent forces to the total measured forces is unclear. Hence, we inhibit platelet myosin by blebbistatin, and simultaneously record the platelet force fields by TFM. We have designed an efficient microflow setup that allows for the defined application of blebbistatin to the platelets adhered to PAA substrates during an ongoing TFM recording. Our experimental findings aim at building a mechanical model for platelet activation.

BP 24.33 Wed 17:30 Poster C

Quantification and Simulation of Depletion Induced Red Blood Cell-Cell Adhesion — •Elisabeth Eckle, Richards Grzibovskis, Patrick Steffen, and Christian Wagner — Saarland University, Saarbrücken, Germany

Interactions between cellular components of blood such as aggregation, agglutination or adhesion of cells are observed in a variety of normal and pathological conditions like, for example, rouleaux formation, platelet adhesion and aggregation in both thrombosis and haemostatic clot formation. The aggregation of erythrocytes can be seen if the red blood cells are re-suspended in electrolyte solutions containing neutral macromolecules like dextran. The aggregation of erythrocytes is completely reversible and the disaggregation of these rouleauxs is readily achieved by shearing the suspension. In this study, AFM based single cell force spectroscopy was used to investigate the interaction of single red blood cells in various dextran concentrations. To numerically simulate this interaction, a mathematical model based on free energy minimization was formulated. The equilibrium shape of red blood cell was obtained by means of the minimization of the surface bending energy functional and the interaction supports via the interaction potential. The calculated results have been compared with the experimental results.

BP 24.34 Wed 17:30 Poster C

Mathematical Modelling of the Surface Change of Erythrocytes due to Mechanical Influences — •Elisabeth Eckle and Richards Grzibovskis — Saarland University, Saarbrücken, Germany

Interactions of erythrocytes with artificial surfaces (e.g. specially prepared glass or a mesh of microfibers) and between themselves attract a lot of attention from both experimental and modeling communities. Besides rapid changes in the shape of the cell, these phenomena feature forming of contact areas between the cell and the surface in question or another cell. In spite of the overwhelming biochemical complexity of an erythrocyte, simple bilayer membrane models are widely used to gain an insight into a variety of processes it is involved in. We consider the classical Helfrich model of bilayer membranes with additional contact energy terms as well as total volume and surface area constraints. The equilibrium shapes of the cell are obtained numerically through a proper FEM discretization of the weak formulation of the gradient flow for the resulting energy functional. Computations are performed in three space dimensions. We study properties of the model by exploring its results for different physical parameters, discretizations, and configurations of the artificial surfaces.

BP 25: Posters: Cytoskeleton

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

BP 25.1 Wed 17:30 Poster C

Molecular Motors Can Sharpen the Length Distribution of Treadmilling Filaments — •Christoph Erlenkämper[1,2], Denis Johann[1], and Karsten Kruse[1] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Institut Curie, Paris, France

The assembly of actin filaments and microtubules depends on the hydrolysis of nucleotide tri-phosphates. Together with their structural polarity this can lead to treadmilling, a process during which the filaments, on average, grow at one end and shrink at the other. The distribution of proteins binding to a treadmilling filament increases towards the shrinking end. For proteins affecting the removal rate of filament subunits such a gradient implies an effectively length-dependent depolymerization rate, which can lead to a unimodal length distribution unknown to polymers at equilibrium. Using Monte-Carlo simulations, we show that the width of the length distribution can narrow substantially if the depolymerizing proteins are molecular motors, moving directionally towards the shrinking end. We present expressions for the width of the length distribution in the limits of vanishing and infinite motor speeds.

BP 25.2 Wed 17:30 Poster C

A phase-field model for amoeboid motility — •Alexander Dreher[1], Igor Aronson[2,3], and Karsten Kruse[1] — [1]Theoretische Physik, Universität des Saarlandes, Postfach 151150, D-66041 Saarbrücken, Germany — [2]Materials Science Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, USA — [3]Engineering Sciences and Applied Mathematics, Northwestern University, 21345 Sheridan Road, Evanston, IL 60202, USA

The crawling of eukaryotic cells on substrates is driven by the cytoskeleton. How the cytoskeleton is organized in this process is still poorly understood. It has been suggested that spontaneous polymerization waves provide a possible answer to this question. We examine this possibility theoretically by analyzing a system of treadmilling filaments in presence of nucleating proteins. A challenge arises from the need to describe a moving deformable cell boundary. In this minimal system we treat the cell shape by a phase-field approach. We find spiral waves as well as self-sustained motion of the cell in agreement with experiments on amoeboid motility.

BP 25.3 Wed 17:30 Poster C

A mechanism of stress generation in contractile rings — •Anne Wald[1], Viktoria Wollrab[2], Daniel Riveline[2], and Karsten Kruse[1] — [1]Universität des Saarlandes, Theoretische Physik, Postfach 151150, 66041 Saarbrücken — [2]Laboratory of Cell Physics, ISIS/IGBMC, Université de Strasbourg and CNRS (UMR 7006), 8 allée Gaspard Monge, 67083 Strasbourg, France and Development and Stem Cells Program, IGBMC, CNRS (UMR 7104), INSERM (U964), Université de Strasbourg, 1 rue Laurent Fries, BP10142, 67400 Illkirch, France

Cytokinesis is the final step of cell division during which the mother cell is split into her daughters. In many cell types, this process is driven by the contraction of a ring composed of actin filaments and myosin motors. How the interaction between motor molecules and filaments generates the stress necessary for contraction is still poorly understood. We study a possible mechanism based on the existence of bipolar fila- ment structures. These structures emerge, for example,

when filaments grow into opposite directions from a common nucleator as has been suggested for actin filaments in fission yeast. We study the dynam- ics of dynamic polar filaments in the presence of molecular motors by using a continuum mean-field description. We calculate the stress generated by a homogenous ring in steady state and investigate the stability of this structure against perturbations. Notably, we find that filament assembly can heal defects that might otherwise lead to ring rupture.

BP 25.4 Wed 17:30 Poster C

Depolymerization of Microtubules by Diffusing Motor Proteins — •Emanuel Reithmann, Louis Reese, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Microtubules (MT) are dynamic protein filaments integral to a wide variety of cellular processes such as mitosis, meiosis and cellular transport. Molecular motors moving on the MT play a key role in the control of MT length as they can catalyze depolymerization and polymerization. There is a plethora of molecular motors with different properties such as biased or unbiased movement along the MT. As opposed to depolymerases with a directed motion, only a few theoretical results exist for diffusing motors such as MCAK. Here we investigate a stochastic model for the processive depolymerase activity induced by molecular motors diffusing on the MT. Employing Monte Carlo simulations and analytic mean-field approximation methods we study the depolymerization process. We determine the stationary density profiles of MCAK along microtubules, and show that the concentration of bound motor proteins at the microtubule tip is a critical determinant of the depolymerization rate. Our model agrees well with experimental results [1]. Further, based on this data, predictions of the MCAK off-rate at the MT tip can be made.

[1] J. Cooper, M. Wagenbach, C. Asbury, L. Wordeman, Nat. Struct. Mol. Biol. 17, 77-82 (2010).

BP 25.5 Wed 17:30 Poster C

Dynamics and length distribution of microtubules under force and confinement — Björn Zelinski, •Nina Müller, and Jan Kierfeld — Physics Department, TU Dortmund, Dortmund, Germany

We investigate the microtubule polymerization dynamics with catastrophe and rescue events for three different confinement scenarios: (i) The microtubule is confined by rigid and fixed walls, (ii) it grows under constant force, and (iii) it grows against a linearly increasing force. (i) In confinement, we find exponentially decreasing or increasing stationary microtubule length distributions instead of bounded or unbounded phases and introduce a model for wall-induced catastrophes. (ii) Under a constant force the boundary between bounded and unbounded growth is shifted to higher tubulin concentrations and rescue rates. We determine the critical force f_c which provides the transition from unbounded to bounded growth. (iii) For growth against an elastic obstacle and a non-zero rescue rate, we find a sharply peaked steady state length distribution. The corresponding average length self-organizes such that the average polymerization force equals the critical force f_c for the transition from unbounded to bounded growth.

BP 25.6 Wed 17:30 Poster C

Feedback mechanism for microtubule polymerization regulation — •Maria Zeitz and Jan Kierfeld — Physics Department, TU Dortmund, Dortmund, Germany

We investigate the feedback mechanism in the cell between a polymerizing microtubule and the proteins Rac and stathmin and its role in microtubule length regulation. We use two different approaches to investigate the impact of the feedback mechanism: On the one hand, we construct a homogeneous model, which neglects spatial concentration variations and focuses on the feedback effects in the reaction kinetics. This model can be solved analytically. On the other hand, we introduce a more detailed model which couples reactions to diffusion of stathmin proteins and polymerization dynamics of the microtubule. We investigate the the complex dynamics of all three components by stochastic simulations.

BP 25.7 Wed 17:30 Poster C

Actomyosin Detection at Fluorescence Interference Contrast Checkpoints for Automated Biocomputation Readout — •Mercy Lard[1], Lasse ten Siethoff[2], Malin Persson[2], Alf Månsson[2], and Heiner Linke[1] — [1]The Nanometer Structure Consortium (nmC@LU) and Division of Solid State Physics, Lund University, Lund, Sweden — [2]School of Natural Sciences, Linnaeus University, Kalmar, Sweden

On-chip biotechnologies, which aim to replace microfluidic, driven flow with active molecular-motor driven transport of cytoskeletal filaments include: bio-computation, diagnostics, and drug screening. These applications would benefit greatly from further miniaturization and increased sensitivity. Here we make use of actomyosin in an in vitro motility assay, incorporated in nanostructures, as a platform for biosimulation of the time evolution of motile objects in complex networks, for example in biocomputation. This type of application can require detection of filaments at checkpoints in the device with high signal-to-noise ratio, for example, to record the number and speed of filaments at a specific location. To serve this need, we make use of fluorescence interference contrast (FLIC) at thin gold lines running perpendicular to nano-sized polymer resist channels that guide filament motion. Using cross-correlation at pairs of Au lines, we strongly enhance S/N and counting accuracy. We demonstrate the tracking of single or multiple filaments at these checkpoints, and discuss limits of this technique. Application areas of this technique will be discussed.

BP 25.8 Wed 17:30 Poster C

Single-molecule motility of kinesin-5 motors between crosslinked microtubules — •Alice Wiesbaum[1], Christina Thiede[1], Olga Zaitsava[2], Vladimir Fridman[3], Marcel Janson[2], Larisa Gheber[3], and Christoph Schmidt[1] — [1]Georg-August Universität, Göttingen, DE — [2]Wageningen University, Wageningen, NL — [3]Ben-Gurion University of Negev, Beer-Sheva, IL

During mitosis, a group of several proteins organizes the dynamics of the mitotic spindle midzone. Two essential functions that need to be fulfilled in the midzone are crosslinking and active sliding of antiparallel microtubules (MTs). In S. cerevisiae, crosslinking is done by the protein Ase1, and sliding is powered by the tetrameric kinesin-5 motors Cin8 and Kip1. It is known that kinesin-5 motors are regulated by binding conditions to MTs. X. laevis Eg5 only moves processively when it is bound between two MTs. Cin8 was found to change its directionality when binding between two MTs. On a single MT, Cin8 is minus-end directed and moves processively. When bound between two MTs, Cin8 drives slow, plus-end directed relative sliding. To test if this property is a cooperative phenomenon of multiple motors or a single-motor property, we performed in vitro TIRF single-molecule experiments. In order to ensure bundling even at low motor concentrations, we employed the crosslinking protein Ase1. We found that single Cin8 motors are capable of switching direction when between MTs. In addition, we analyzed the behavior of a Cin8 mutant, Cin8*tail, which lacks the C-terminal tail domain. This mutant still supports sliding of MTs, but lacks a clear directionality switch.

BP 25.9 Wed 17:30 Poster C

Measurement of F-actin localization tubes and their orientation distribution in three dimensions — •Evelin Jaschinski, Inka Kirchenbüchler, Ronald Springer, and Rudolf Merkel — Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52428 Jülich

Under appropriate conditions, the protein actin forms long and semiflexible filaments (F-actin). Due to their large persistence length (~17microns) fluorescently labeled filaments are ideally suited for light microscopic study of conformations and fluctuations. Experiments on labeled test filaments embedded in a non-labeled network enable quantification of the space available, i.e. the well-known localization tube. In recent work our group has analyzed distributions of curvature [1] and diameters of the tubes [2]. These results were analyzed assuming isotropic solutions. However, pronounced and long lasting anisotropy can be induced by sample shear. In order to characterize the impact of directional order of the filaments localization tubes we applied different shear history and measured in three dimension the orientation distributions at different protein concentrations. From them we calculated order parameters and compared the latter to nematic ordering.

[1] J.Glaser, D. Chakraborty, K. Kroy & I. Lauter, M. Degawa, N. Kirchgeßner, B. Hoffmann, R. Merkel, M. Giesen, Phys. Rev. Lett. 105, 037801 (2010)

[2] M. Romanowska, H. Hinsch, N. Kirchgeßner, M.Giesen, M. Degawa, B. Hoffmann, E. Frey, R. Merkel, EPL 86, 26003 (2009)

BP 25.10 Wed 17:30 Poster C

Investigation of desmin intermediate filament assembly

by atomic force microscopy — •Mareike Dieding[1], Volker Walhorn[1], Andreas Brodehl[2], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience, Bielefeld University, Germany — [2]E. & H. Klessmann Institute for Cardiovascular Research & Development, Heart and Diabetes Centre NRW, Ruhr-University Bochum, Bad Oeynhausen, Germany

Arrythmogenic right ventricular cardiomyopathy (ARVC) is a severe heart muscle disease. It is pathologically characterized by predominant dilatation of the right ventricle and arrhythmias often leading to heart failure or sudden cardiac death. ARVC is often associated with mutations in the desmin intermediate filament (IF) protein. It is known from fluorescence microscopy assays that these mutations can inhibit the formation of extended desmin cytoskeletal networks [1].

We used atomic force microscopy (AFM) topography to study the desmin assembly process *in vitro* at different stages of the filament formation. Thereby we were able to reveal various mutation specific structural defects at distinct stages of the filament assembly. Moreover, our results are nicely supported by complementary methods like cell transfection studies [1]. In future measurements we plan to investigate the assembly process on the single molecule level by AFM single molecule force spectroscopy.

[1] A. Brodehl et al., *Dual-color photoactivation localization microscopy of cardiomyopathy associated desmin mutants*, J Biol Chem. 287(19), 2012

BP 25.11 Wed 17:30 Poster C

Keratin 8/18 Networks and their Interplay with Plectin — •Ines Martin[1], Soufi Nafeey[2], Tobias Paust[1], Michael Beil[3], Harald Herrmann[4], and Othmar Marti[1] — [1]Department of Experimental Physics, Ulm University, Ulm, Germany — [2]Central Facility of Electron Microscopy, Ulm University, Ulm, Germany — [3]Clinic of Internal Medicine I, Ulm University, Ulm, Germany — [4]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 some epithelial cells. They are responsible for the stiffness of cells and responses to mechanical stimuli. Keratin filaments can be crosslinked by plectin, a protein that links different parts of the cytoskeleton to each other as well as to hemidesmosomes.

In this work we assembled keratin 8/18 and plectin together in vitro to form crosslinked networks. We checked the resulting networks with Scanning Electron Microscopy (SEM) and Immuno-Gold-Labeling and were able to identify the position of plectin molecules. The viscoelastic network properties were measured by passive microrheology and compared to in vitro assembled networks without crosslinker and with $MgCl_2$ as crosslinker.

BP 25.12 Wed 17:30 Poster C

Investigating Intermediate Filament (dis-)assembly Processes with Microfluidics — •Bernd Nöding, Viktor Schröder, Judith Breuer, Susanne Bauch, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

The cytoskeleton of eukaryotes consists of three different polymer systems: microtubules, actin filaments and intermediate filaments (IFs). While both microtubules and actin filaments are highly conserved, IFs occur in many different variations. A central property of all filament types is the (dis-)assembly mechanism. For vimentin IFs a principal assembly model exists. However, measurements of the assembly process with high time resolution, which would yield insights especially into the early assembly steps, are still largely missing. To approach this problem, we combine microfluidic and fluorescence techniques in two different ways. First, for studying the fast early assembly steps, we use Fluorescence Cross Correlation Spectroscopy (FCCS) in combination with microfluidic flow channels. With this setup, we will be able to characterize the assembly process with a time resolution in the millisecond range. Second, the later assembly stages and the disassembly of IFs can be observed with a different microfluidic design, which employs reaction chambers coupled via diffusion channels to a very well defined buffer reservoir. Thus the IF assembly and dissassembly process can be influenced by minute changes in the buffer system. Trough the combination of both these methods we aim to form a more complete picture of the assembly mechanism of IFs.

BP 25.13 Wed 17:30 Poster C

Passive Microrheology: A model-based approach to determine mechanical properties of assembled networks — •Tobias Paust[1], Ines Martin[1], Michael Beil[2], and Othmar Marti[1] — [1]Institute for Experimental Physics, Ulm University — [2]Department of Internal Medicine I, Ulm University

Macro- and microrheology is extensively used to characterize complex networks of biopolymers. A possible way to describe the mechanical properties of a viscoelastic medium is to measure the thermal motion of a particle embedded in the medium and compute the unilateral transformation.

In a model-based approach the mean squared displacement of the particle motion is divided into three terms describing the different properties of the network - elasticity, viscosity and the motion of the particle in a spatial confinement.

The focus of our work are the measurements of in vitro assembled keratin 8/18 networks to underline the functionality of the model-based approach. Furthermore, Brownian motion simulations of spatially confined beads with the influence of the meshes' elasticity and its drift are performed to allow a comparison to the measurements.

BP 25.14 Wed 17:30 Poster C

Conception and construction of a microfluidic chamber for the optical tweezers — •Samuel Vollmer, Tobias Paust, and Othmar Marti — Institute of Experimental Physics - University Ulm, D-89069 Ulm, Germany

Microfluidics is the science and engineering of systems in which fluid behavior differs from conventional flow theory primarily due to the small length scale of the system. For many measurement systems small length scales are obligatory for the ability to work with small reagent volumes.

It is important to understand the assembly process of Keratin 8/18 networks and their mechanical properties at early times. Therefore we constructed a microfluidic chamber to mix assembly buffer and dialysis buffer at the optical tweezers location to investigate the network mechanics at starting times.

To find the best geometry for our chamber we first have done some simulations using the finite element method. These simulations show the mixing of the two buffers in dependence of the geometry of the chamber.

BP 25.15 Wed 17:30 Poster C

Laser ablation on actomyosin network — •Arnab Saha[1], Guillaume Salbreux[1], Frank Jülicher[1], and Stephan Grill[1,2] — [1]Max Planck Institute for the Physics of Complex Systems Nöthnitzer Straße 38 01187 Dresden Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics Pfotenhauerstr. 108 01307 Dresden, Germany

The cell cortex is a thin layer beneath the membrane that largely consists of cross-linked actin filaments, non-muscle myosin motor protein and a plethora of actin binding proteins (ABPs). Collective dynamics of myosin over actin meshwork (assembled by ABPs), that converts chemical energy to mechanical work by ATP hydrolysis, generates active contractility at large cellular length scales. Contractility can build up mechanical stress in the cortex. Sudden up-or-down regulation of myosin induces spatial inhomogeneity in the stress profile which finally leads to cortical flow.

One need to investigate the flow pattern in order to understand the physical properties of the actomyosin network. Here we describe the actomyosin mesh at a coarse grained level as a viscoelastic, active and contractile gel. We develop a two dimensional hydrodynamic model, valid at long length scales and short to long time scales (incorporating both elastic and viscous regimes), using basic symmetry principles and conservation laws. The description is then used to investigate the spatio-temporal dynamics observed after the laser ablation on actomyosin cable during zebrafish epiboly.

BP 25.16 Wed 17:30 Poster C

Correlating the signaling cascade with movement in Dictyostelium discoideum — •Christoph Blum[1,2], Vladimir Zykov[1,2], Kaumudi Prabhakara[1,3], Marco Tarantola[1,4], and Eberhard Bodenschatz[1,2,3] — [1]Max-Planck-Institu für Dynamik und Selbstorganisation, Göttingen, Germany — [2]Georg-August-Universität, Institut für Nichtlineare Dynamik, Göttingen, Germany — [3]Cornell University, Ithaca, USA — [4]University of California, San Diego, USA

Actin cytoskeletal dynamics provide the fundamental basis of eukaryotic cell motility. The cross-linked actin network at the front of a cell pushes the leading edge of the membrane towards the source of at-

tractant. It is our aim to provide a quantitative understanding of the spatio-temporal dynamics of the actin cytoskeleton within the actin cortex.

We have developed experimental methods to address single Dictyostelium discoideum cells with well-controlled mechanical and chemical stimuli. Our experimental techniques are based on microfluidic devices, such as flattening device and micromixer, and fluorescence microscopy (Confocal, TIRF).

Here we present correlations of an important protein in the signaling cascade(Ras-GTP) with the actin polymerization as well as correlations of Ras-GTP localization with pseudopod dynamics. The localization is visualized by the Ras binding domain(RBD-GFP). The pseudopod formation is analyzed by curvature maps. The polymerization of actin is shown by the filametous actin marker LimE.

BP 25.17 Wed 17:30 Poster C

Rheology of cytoskeletal in-vitro networks — •Meenakshi Prabhune[1], Knut Heidemann[2], Florian Rehfeldt[1], Max Wardetzky[2], and Christoph Schmidt[1] — [1]Third Physics Institute, Georg August University, Göttingen — [2]Department for Numerical and Applied Mathematics, Georg August University, Göttingen

Living cells are governed by active cellular processes such as cell division, adhesion and migration that depend on the cytoskeleton. The cytoskeleton is a composite cross-linked polymer network of cytoskeletal filaments ranging from rod-like microtubules and actin bundles to semi-flexible actin filaments and softer intermediate filaments. 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 and ds DNA via a heterobifunctional cross-linker (sulpho SMCC). DNA as a cross-linker has the unique advantage of having a well-defined length, which we vary in our experiments. We have measured the shear-elastic response in these networks by macrorheology experiments at varying strains and frequencies. The nonlinear response was also characterized using differential stiffness measurements in a macrorheometer. Simultaneously, we compare the experimental data to numerical simulations that we have developed for networks of stiff slender rods connected by semi-flexible linkers (see poster by Knut Heidemann).

BP 25.18 Wed 17:30 Poster C

Biopolymer Networks: Simulations of Rigid Rods Connected by Wormlike Chains — •Knut M Heidemann[1], Meenakshi M Prabhune[2], Florian Rehfeldt[2], Christoph F 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 in cell structure and mechanics. The collective dynamics of these cytoskeletal filaments with different mechanical properties are yet to be understood completely. To model such a strongly heterogeneous composite, we simulate networks of *rigid* rods connected by *flexible* linkers (wormlike chains). We extract elastic moduli by quasistatic deformations at varying filament densities and analyze the crossover between cross-link dominated and rod dominated regimes. In particular, we are interested in the asymptotic stress dependence of the *differential modulus*.

The simulations are accompanied by rheological experiments on networks of *microtubules* (MTs) cross-linked by double-stranded *DNA* of variable length (cf. poster Meenakshi Prabhune).

BP 25.19 Wed 17:30 Poster C

Actin Dynamics in Myosin II-null Dictyostelium Discoideum — Hsin-Fang Hsu[1,4], •Christian Westendorf[1,4], Carsten Beta[2], and Eberhard Bodenschatz[1,3,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [3]Laboratory of Atomic and Solid-State Physics, Cornell University, USA — [4]Institute for Nonlinear Dynamics, Georg-August University, Goettingen, Germany

Starved D. discoideum show chemotaxis to cAMP. The directed migration is driven by the assembly and disassembly of actin filaments. In addition to the actin dynamics the contraction of Myosin II plays an important role in the effective movement. Cells lacking Myosin II show frequent protrusions of the membrane. Here we investigate the dynamics of actin filament (labeled by LimE-GFP) in the AX2 cells without Myosin II heavy chain. We observed Myosin II mutants show spontaneous periodic actin dynamics even without external stimulation of cAMP. We further investigate this phenomenon by perturbing the system with different periodic pulses of cAMP created by flow photolysis. Our observation showed Myosin mutants show more instability of actin networks than wild-type cells.

BP 25.20 Wed 17:30 Poster C

Active Biopolymer Networks — •Adam Walker, Nikta Fakhri, Kerstin von Roden, and Christoph F. Schmidt — Drittes Physikalisches Institut - Biophysik, Georg-August-Universität, Göttingen

Biological cells rely on the cytoskeleton - an active, polymeric structure - to drive essential dynamic processes such as motility, growth and cell division. In contrast to technical materials, a living cell is a non-equilibrium system. This research focuses on the investigation of mechanical properties and dynamics of model biopolymer networks quantitatively using a largely experimental approach centered on both bulk rheology and optical-trapping based microrheology. Non-muscle Myosin IIa motors were characterized using fluorescence microscopy for in vitro actin motility assays and shown to interact with and translocate actin filaments. Initial macro-rheology experiments dealt with model networks constructed purely from actin filaments and allowed us to quantify both the linear- and nonlinear- response of the networks. Networks will be activated using myosin motors and associated crosslinking proteins to better approximate the real cytoskeletal environment.

BP 25.21 Wed 17:30 Poster C

Calmodulin regulates motility, dimerisation and phospholipid-binding of the unique myosin motor in Leishmania, myosin-XXI — •Christopher Batters, Heike Ellrich, Constanze Helbig, Katy Anne Woodall, Christian Hundschell, and Claudia Veigel — Division of Cellular Physiology and CeNS, LMU München, Schillerstrasse 44, 80336 München

The genome of the protozoan Leishmania parasite comprises just two classes of myosin, however only class XXI was shown to be expressed in both stages of the parasites life cycle. Apparently the only myosin motor in Leishmania, myosin-XXI is a unique model system and thought to perform a large variety of functions ranging from membrane anchorage to long-range directed cargo movement. However, nothing is known about the oligomerisation states, motility or cargo-binding of this motor. Using size exclusion chromatography, motility assays and electron microscopy we found that, in the absence of calmodulin, the motor formed immobile dimers. In the presence of calmodulin the motor was monomeric and moved actin filaments at ~15 nm.s-1. The monomers bound to liposomes, while the dimers did not. We identified phospholipid binding domains that overlapped with the dimerisation domains, including a PX-domain overlapping with the converter region. We propose a novel mechanism of myosin regulation where myosin-XXI monomers bind to lipid cargo and act as transporters, while the dimeric form is unable to bind to lipids and acts as an immobile, ATP-dependent crosslinker of actin filaments. Supported by SFB 863, CeNS, Baur-Stiftung

BP 26: Posters: Biomaterials and Biopolymers (joint with CPP)

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

BP 26.1 Wed 17:30 Poster C

Structural design of strategic materials for tissue regeneration — •Maria Helena V. Fernandes — Department of Materials Engineering and Ceramics &

A key factor for the success of tissue engineering targeted for regeneration is the choice of appropriate materials with properties that can fulfill the complex requirements imposed. The structural design of those materials can have a decisive impact on relevant properties, such as, biodegradability, bioactivity, piezoelectricity, cell response.

This talk will be centered on our expertise on some amorphous, semi-crystalline and crystalline strategic materials, namely Si-based bioglasses, Poly-L-Lactic Acid (PLLA) and ZnO nanoparticles to be used in tissue regeneration applications. The materials, in monoliths, films or particles are produced by different processing technologies (melt-quenching, spin coating chemical precipitation) and further characterized in terms of structure, microstructure, degradation, in vitro behavior and cell viability. Relevance will be given to aspects related to the processing technologies employed and to the parameters that can be controlled aiming to obtain tailored structures and custom-made properties in those strategic materials for tissue regeneration purposes, namely of the bone tissue.

BP 26.2 Wed 17:30 Poster C

Artificial hydroxyapatite pellets - mimicking hard tissues with simple surfaces — •Christian Zeitz[1], Samuel Grandthyll[1], Deniz Kahraman[2], Peter Loskill[1], Jörg Schmauch[1], Nicolas Thewes[1], Frank Müller[1], and Karin Jacobs[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Institute for ceramics in engineering, KIT, Karlsruhe, Germany

The interactions of proteins, cells or bacteria with hard tissue surfaces are of utmost importance. On the one hand, characterization of these interactions often employs simplified model surfaces featuring low roughness and controlled surface chemistry (mica, glass, silicon wafers). Thereby specific properties of tissue compounds such as hydroxyapatite are not included. Previous studies showed, however, that hydroxyapatite interacts with attaching proteins in a specific way. On the other hand, the drawback of tissue samples instead of model systems is the lack of controllability or reproducibility. Both approaches are necessary for a comprehensive understanding of the principles on the natural material but limited both in their own way.

Therefore, we have developed substrates consisting of hydroxyapatite featuring a low roughness and defined chemical composition. The local roughness is comparable to the one of silicon wafers. The chemical purity as well as the simple structure allow for controlled characterization of fundamental interactions. Using these samples, we investigate the adhesion of bacteria and adsorption of proteins on natural substrates.

BP 26.3 Wed 17:30 Poster C

Dynamics of vimentin filament aggregation studied in microfluidic drops — •Christian Dammann, Bernd Nöding, Susanne Bauch, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

Studying individual cytoskeletal constituents represents a bottom up approach towards an understanding of cellular mechanics. The structure and function of vimentin intermediate filament networks is influenced – amongst other things – by ions. To perform systematic studies of the influence of ions on vimentin *in vitro*, we use microfluidic devices to encapsulate the protein and multivalent ions in picoliter sized drops. After fast internal mixing, the drops are held in position to image the fluorescently tagged vimentin using fluorescence microscopy. In this trapping mechanism the drops enter a 'U'-shaped constriction that keeps them in position immediately after the protein and ions are in contact for the first time. Thus we directly image the time course of aggregation, *i.e.* how vimentin filaments form connected networks in the drops. The process depends on the ion concentration as well as valence and takes place within the first minutes after drop loading. Since we can resolve individual network features during the aggregation process, our method is promising to shed light on the mechanisms behind the network formation of vimentin in the presence of multivalent ions.

BP 26.4 Wed 17:30 Poster C

Spatio-Temporal Changes in Mechanical Properties of Extracellular Matrix of Hydra Magnipapillata — •Mariam Veschgini[1], Suat Özbek[2], Manfred Burghammer[3], Thomas Holstein[2], and Motomu Tanaka[1] — [1]Physical Chemistry of Biosystems, Physical Chemistry Institut, University of Heidelberg, 69120 Heidelberg, Germany — [2]Center for Organismal Studies, Department of Molecular Evolution and Genomics, University of Heidelberg, 69120 Heidelberg, Germany — [3]European Synchrotron Radiation Facility (ESRF), Grenoble Cedex 9 38053, France)

The extracellular matrix (ECM) of the freshwater polyp hydra, called mesoglea, is one of the early forms of ECM. Hydra mesoglea has a multilayered structure, which is dynamically changed during the development.

The main goal of this study is to investigate the time evolution of local elastic properties of isolated mesoglea by means of nanoindentation with an Atomic Force Microscopy (AFM).

The results indicate a clear change in the elasticity of mesoglea along the main body axis. Furthermore, the analysis of elasticity as a function of budding stage suggests the first sign of a turn-over from "soft" to "stiff" mesoglea during the growth and maturation of buds.

To further gain the local fine structure of mesoglea, the first grazing incidence small angle X-ray scattering experiments on isolated mesoglea were performed with a nano-focused beam (200 nm) at the European Synchrotron Radiation Facility (ESRF).

BP 26.5 Wed 17:30 Poster C

Temperature treatment of protein layers at the solid/liquid interface in different environments - An x-ray reflectivity study — •Irena Kiesel, Michael Paulus, Julia Nase, Sebastian Tiemeyer, Christian Sternemann, and Metin Tolan — Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany

Proteins at solid/liquid interfaces play a key role in technical, biomedical, and food processing applications. The interaction of bacteria and cells with surfaces is influenced by adsorbed proteins. These proteins can lose their functionality when denatured by e.g. heat treatment.

In our experiment we have investigated in situ the denaturation process of different model proteins (lysozyme, RNase A and BSA) induced by increasing temperature (up to 80°C) in two different environments, a pure buffer solution and a protein solution, which represents a protein reservoir. The measurements were performed using the 27 keV x-ray reflectivity setup at beamline BL9 of the synchrotron radiation source DELTA (Dortmund, Germany). The electron density profiles of the layer system and the amount of the adsorbed proteins were obtained by analysing the reflectivities at each temperature.

We observe that in pure buffer solution the proteins desorb with increasing temperature, whereas temperature treatment of protein layers in protein solution results in thicker protein layers and can be explained by additional protein adsorption.

Work was supported by BMBF (05K10PEC) and NRW Forschungsschule.

BP 26.6 Wed 17:30 Poster C

Melting of pectin gels — •Andrea Kramer[1], Romaric Vincent[2], Brad Mansel[3,4], Klaus Kroy[1], and Martin Williams[3,4,5] — [1]Institute for Theoretical Physics, Universität Leipzig, Germany — [2]Institute for Bioengineering of Catalonia, Spain — [3]Institute of Fundamental Sciences, Massey University, NZ — [4]MacDiarmid Institute for Advanced Materials and Nanotechnology, NZ — [5]Riddet Institute, NZ

Pectin gels are the major scaffolding structures responsible for the mechanical stability of plant cells. We have analyzed their slow dynamics and linear and nonlinear viscoelasticity as a function of temperature, using various (micro-)rhelogical techniques and theory. The results are compared to literature data for F-actin and live cells. We find that the linear microrheological and strain-stiffening responses of pectin networks are well-captured by the glassy wormlike chain (GWLC) model. The nonlinear mechanical response is much more sensitive to temperature changes than the linear response, a property that is also observed in F-actin networks and can be accounted for by the model. But the overall sensitivity to temperature changes turns out to be much more

pronounced in actin than in pectin, possibly hinting at a temperature anomaly of actin.

BP 26.7 Wed 17:30 Poster C

Development of hydrogel-based antiviral wound dressings — •Julian Riba and Oliver Lieleg — Zentralinstitut für Medizintechnik, Technische Universität München, Garching, Germany

Mucus is a biopolymer-based hydrogel that lines most of the inner surface in humans and animals and serves as a first layer of protection against pathogenic microorganisms. Recently, it has been shown in vitro that purified porcine gastric mucin biopolymers can act as a broad-spectrum antiviral agent. Yet, the low viscosity of reconstituted mucin solutions hampers their direct application for wound treatment. In this work, we aim to develop a novel mucin-based material for wound dressings. This novel material is supposed to maintain the antiviral properties of mucins while allowing for in situ gelation for easy application on inner wounds. We investigate composites of porcine gastric mucin and other gel-forming polymers such as methylcellulose, alginate, and chitosan so that gelation of the mixed polymer system can be induced by temperature or chemical crosslinking. Sample characterization is performed using macrorheological measurements and optical microscopy.

BP 26.8 Wed 17:30 Poster C

Electrical transport through self-assembled DNA superlattices — •Carlos Paez and Peter Schulz — Universidade Estadual de Campinas, Campinas Brazil

DNA has emerged as a versatile material for self-assembled molecular structures due to its intrinsic characteristics. Several proof concepts of regular two dimensional self-assembled DNA structures have been reported in the literature. Nevertheless, the electronic and transport properties of such systems remain unexplored. In this work we numerically investigate the transport properties of two dimensional square superlattice patterns build from two different DNA sequences (telomeric and random) by means of an effective tight binding model for the electronic structure, while the current is obtained within a Green's function framework. We show that the self-assembled square lattice structures based on telomeric DNA strands show current-voltage characteristics which make the system eligible for nanoelectronic applications. On the other hand, structures based on disordered sequences show currents that quickly go to undetectable ranges with increasing size. The robust plateau structures due to telomeric sequences are superimposed by additional features due to the DNA square superlattice. For the random sequencing case, interesting percolation mechanisms variations are observed, dependent on the competition between the localization length and the distance between the crosses in the self-assembled square superlattice structures.

BP 26.9 Wed 17:30 Poster C

Simulating peptide - ion interactions: choosing a realistic force field — •Jens Kahlen, Davide Donadio, and Christine Peter — Max Planck Institute for Polymer Research, Mainz, Germany

The impact of ions on biomolecules in solution can be tremendous. Classical atomistic simulations are a valuable tool to gain insight into this at a molecular level. However, a prerequisite for meaningful simulation results is a realistic description of the interactions between the different types of solutes. Recent publications (Reif, Hünenberger and Oostenbrink, *J. Chem. Theory Comput.* 2012, **8**, 3705-3723) have shown that a careful reevaluation of the interaction parameters between charged amino acid side chains and ions is necessary. For many force fields, these specific interactions have been only marginally taken into account in the parametrization process. Therefore, well-established force fields may yield significant differences in the description of such systems. In view of the difficulties to directly compare the observed association behavior of the simulated compounds to experimental data, the aim of our work is to identify a systematic way of choosing a force field parametrization, which yields a realistic description. Based on the example of polyglutamate interacting with calcium ions we show how a comparison of simulation results to experimental thermodynamic data and DFT-based calculations can be applied to achieve this aim.

BP 26.10 Wed 17:30 Poster C

Mechanical strength and intracellular uptake of CaCO3-templated layer-by-layer capsules composed of biodegradable polyelectrolytes — Raghavendra Palankar[1], Bat-El Pinchasik[2], Stephan Schmidt[2], Bruno De Geest[3], Andreas Fery[4], Helmuth Möhwald[2], André Skirtach[5,6], and •Mihaela Delcea[1,2] — [1]ZIK HIKE, Ernst-Moritz-Arndt-Universität Greifswald, Greifswald 17489, Germany — [2]Max-Planck Institute of Colloids and Interfaces, Golm 14424, Germany — [3]Laboratory of Pharmaceutical Technology, Department of Pharmaceutics, Ghent 9000 Belgium — [4]Physikalische Chemie II, Universität Bayreuth, Universitätsstrasse 30, D-95447 Bayreuth, Germany — [5]Department of Molecular Biotechnology, Ghent University, Ghent 9000, Belgium — [6]NB-Photonics, Ghent University, Ghent 9000, Belgium

Developing carriers comprised of biomaterials and capable of withstanding significant mechanical pressures, structural deformations and at the same time delivering biomolecules is of high interest for drug delivery. Using colloidal probe AFM combined with fluorescence microscopy, the mechanical and release properties from CaCO3-templated polymeric capsules made of biodegradable polymers are studied in comparison with those of CaCO3-templated capsules composed of synthetic polymers. The influence of the number of polyelectrolyte layers on the mechanical properties and release from biodegradable capsules will be shown. Mechanical deformation of capsules upon their intracellular uptake is determined and the implications for microcapsule design are discussed.

BP 26.11 Wed 17:30 Poster C

Minimization of Errors in the Determination of Elastic Moduli from Indentation Experiments — Michael Glaubitz, Mihaela Delcea, and •Stephan Block — ZIK HIKE, Fleischmannstr. 42 - 44, D-17475 Greifswald, Germany

Atomic force microscopes (AFMs) equipped with colloidal probe (CP) cantilevers allow to determine elastic moduli E with a lateral resolution below 1 μm by indentation experiments. Such experiments were used intensively in the past to study the elastic properties of surface coatings or changes in cell mechanics related to diseases like cancer or cardiomyopathies. Here, we present the first analysis of the Hertz model that allows to calculate the minimum possible error in the determination of E, which depends strongly on measurement noise but also on experimental parameters like spring constant and indentation depth. Scaling laws for these dependencies are analytically derived and supplemented by simulated and real indentation measurements. Our findings allow a systematic optimization of indentation experiments to increase the accuracy in the determination of E.

BP 26.12 Wed 17:30 Poster C

Imaging nanoscale deformation processes in collagen networks of native tendons — •Sebastian Ködel[1], Martin Neumann[1], Anke Bernstein[2], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz, Germany — [2]Department für Orthopädie und Traumatologie, Muskuloskelettales Forschungslabor, Universitätsklinikum Freiburg, D-79106 Freiburg, Germany

A mechanical overload of tendons and ligaments leads often to a restriction of their functionality. To understand the nanoscale deformation processes in tendons under stress and relaxation, we use a microtensile testing device, which allows simultaneous imaging and measurements with atomic force microscopy (AFM) of the mechanical response. With this setup we study the deformation behaviour of individual collagen fibrils within about 10 μm thin slices of human tendons in native conditions. Series of AFM images reveal a large variety of deformation processes and the overall heterogeneous deformation behaviour. Our results show that individual collagen fibrils in a bundle are not permanently connected to each other and rearrange during deformation. AFM subsurface imaging experiments on individual collagen fibrils show evidence of a rearrangement of the tropocollagen molecules at large strain. We discuss the implications of these effects on the macroscopic mechanical properties of tendons.

BP 27: Biotechnology and Bioengineering

Time: Thursday 9:30–12:00 Location: H43

Topical Talk BP 27.1 Thu 9:30 H43

DNA Origami: Applications in Physics and Biotechnology — •Tim Liedl — Center for Nanoscience, LMU, Munich, Germany

DNA Nanotechnology makes use of programmable DNA strands for the construction of self-assembling two- and three-dimensional objects of nano-engineered shapes [1]. Through the introduction of the extremely robust DNA origami technique [2] the field experienced exciting developments during the last years. I will present recent applications of DNA origami in physics and biotechnology and will show, e.g., how the method can be employed for the fabrication of self-assembled plasmonic materials [3, 4]. Through literally nanometer-precise control over the arrangement of nanoparticles, we were able to create chiral plasmonic structures that exhibit pronounced circular dichroism and optical rotatory dispersion. In recent experiments we were able to orient the nanoparticle helices and observe increased optical activity. These results demonstrate the potential of DNA origami for the assembly of plasmonic metafluids with tailored optical properties.

1. N. C. Seeman, "Nanomaterials based on DNA", Annu. Rev. Biochem. 79, 12.1-12.23 (2010). 2. P. W. K. Rothemund, "Folding DNA to create nanoscale shapes and patterns", Nature 440, 297*302 (2006). 3. A. Kuzyk et al., "DNA-based Self-Assembly of Chiral Plasmonic Nanostructures with Tailored Optical Response", Nature 483, 311-314 (2012). 4. D. Smith et al., "Nucleic Acid nanostructures for nanomedicine applications", Nanomedicine 8, in press (2013)

BP 27.2 Thu 10:00 H43

Synthetic ion channels made from DNA — Martin Langecker, Vera Arnaut, Thomas G. Martin, Jonathan List, Hendrik Dietz, and •Friedrich C. Simmel — Physik Department, TU München

We created a new type of synthetic lipid bilayer membrane channel with user-defined geometric specifications that is constructed entirely from DNA. We show that these synthetic channels can be incorporated into lipid bilayer membranes and we study their electrical properties by single-channel electrophysiological measurements. We find remarkable similarities to the behavior of biological ion channels such as "gating" caused by molecular fluctuations within the channel structure. We also demonstrate one of many potential applications of the synthetic ion channels, namely as single-molecule sensing devices.

BP 27.3 Thu 10:15 H43

Diffusion and freezing transition of rod-like DNA origami on freestanding lipid membranes — •Eugene P. Petrov[1,2], Aleksander Czogalla[2], Dominik J. Kauert[3], Ralf Seidel[3], and Petra Schwille[1,2] — [1]Max Planck Institute of Biochemistry, Department of Cellular and Molecular Biophysics, 82152 Martinsried, Germany — [2]Biophysics, BIOTEC, Technische Universität Dresden, 01307 Dresden, Germany — [3]DNA Motors, BIOTEC, Technische Universität Dresden, 01307 Dresden, Germany

During the last decade, DNA origami has become a powerful tool in research at the nanoscale. The relative ease of constructing functionalized DNA origami structures of a defined shape allows for their applications in membrane biophysics. Recently, we have constructed stiff rod-like DNA origami structures consisting of six DNA helixes, which were functionalized with hydrophobic membrane-binding anchors and fluorescently labeled at defined positions [1]. Selective fluorescent labeling allowed us to determine the translational and rotational diffusion coefficients of the DNA origami rods on lipid membranes by fluorescence correlation spectroscopy, which were found to be in a good agreement with the hydrodynamics-based theory of membrane diffusion. Further, we studied the effect of the surface density of membrane-bound origami structures on their Brownian motion. Our results indicate that the 2D membrane hydrodynamics plays an important role in determining the onset of the freezing transition for membrane-bound nanorods.

[1] A. Czogalla, E. P. Petrov, D. J. Kauert, V. Uzunova, Y. Zhang, R. Seidel, and P. Schwille, *Faraday Discuss.* (2013) in press

BP 27.4 Thu 10:30 H43

Biological applications for nano-mechanical detection of molecular recognition — •Andreas Mader[1], Kathrin Gruber[1], Roberto Castelli[2], Peter Seeberger[2], Joachim Rädler[1], and Madeleine Leisner[1] — [1]LMU München, Fakultät für Physik — [2]Department of Biology, Chemistry and Pharmacy, Freie Universität Berlin

Advances in carbohydrate sequencing technologies have revealed the tremendous complexity of the glycome. Understanding the biological function of carbohydrates requires the identification and quantification of carbohydrate interactions with biomolecules. The increasing importance of carbohydrate-based sensors able to specifically detect sugar binding molecules or cells, has been shown for medical diagnostics and drug screening. Our biosensor with a self-assembled mannoside based sensing layer that specifically detects carbohydrate-protein binding interactions (mannoside - ConA), as well as real time interaction of carbohydrates with different E.coli strains in solution. Binding on the Cantilever surface causes mechanical surface stress, that is transduced into a mechanical force and cantilever bending. The degree and duration of cantilever deflection correlates with the interaction's strength. During this study we could establish that carbohydrate-based cantilever biosensing is a robust, label-free, and scalable method to analyze carbohydrate-protein and carbohydrate-bacteria interactions [1]. The cantilevers thereby exhibit specific and reproducible deflection with a high sensitivity range of over four orders of magnitude.

[1] A.Mader et al. NanoLetters, 2012, 12 (1), pp 420-423

15 min break

BP 27.5 Thu 11:00 H43

In-situ electrostatic trapping and manipulation of single nano-objects — •Ji Tae Kim[1,2] and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light, 91058 Erlangen, Germany — [2]Friedrich-Alexander University Erlangen-Nürnberg, 91058 Erlangen, Germany

Direct observation of single molecules in their natural environment is essential for fundamental studies. Many sophisticated trapping methods have been developed to counter the randomizing effect of Brownian motion, but stable trapping of small nanoscopic objects still remains a great challenge. A recent breakthrough showed that charged nano-objects could be trapped in geometry-induced electrostatic potentials on prefabricated nanofluidic chips. Here we extend this technique to in-situ electrostatic trapping that exploits the topological modulations produced by a glass nano-capillary. This arrangement allows us to control and manipulate the nanoparticle dynamically at the nanometer scale. We present our results and discuss the prospects of our work for applications in nanobiophysics.

BP 27.6 Thu 11:15 H43

Membrane protein synthesis in giant vesicles — •Susanne Fenz[1,3], Rita Sachse[2], Stefan Kubick[2], and Thomas Schmidt[3] — [1]Biozentrum, Würzburg, Germany — [2]IBMT, Potsdam-Golm, Germany — [3]Leiden University, Leiden, Netherlands

Interest in the development of biomimetic cell models is driven by its potential to go beyond a purely descriptive picture of cellular processes towards a quantitative understanding and rigorous validation of theoretical modeling.

Recently we introduced a protocol to prepare advanced cell models from giant unilamellar vesicles for studies of membrane processes that involve transmembrane proteins. We further showed that specific functionalization permits to use those biomimetic systems in a lab-on-a-chip scenario. Building on this development, we present here a novel approach that allows us to realize a mimetic cell model that includes in situ protein synthesis and active membrane translocation. Giant unilamellar vesicles were prepared starting from eukaryotic cell lysates containing both the eukaryotic protein synthesis machinery as well as the translocon that is required to integrate proteins into membranes. Our soft methodology for vesicle preparation on agarose-coated surfaces allowed us to keep the translocon fully functional. The advantage of in situ expression and translocation as described here to earlier attempts to produce giant proteo-liposomes is that all proteins are built into the vesicle membrane in the correct orientation. Our novel cell model opens up the possibility to study e.g. protein synthesis in vitro with single-molecule microscopy.

BP 27.7 Thu 11:30 H43

Tailoring substrates for long-term organotypic culture of adult neuronal tissue — •Mareike Zink[1], Valentina

Dallacasagrande[1,2], Alexander Jakob[3,4], Marcus Müller[3], Andreas Reichenbach[2], Josef Käs[1], and Stefan G. Mayr[3,4] — [1]Institut für Experimentelle Physik 1, Universität Leipzig — [2]Paul-Flechsig-Institut, Universität Leipzig — [3]Leibniz Institut für Oberflächenmodifizierung e.V., Leipzig — [4]Translationszentrum für Regenerative Medizin, Fakultät für Physik und Geowissenschaften, Universität Leipzig, Leipzig, Germany

Organotypic tissue cultures establish a highly promising approach for performing in vivo type of studies in vitro. However, very limited survival times of only a few days for adult tissue often limit their application. We propose a novel biotechnological concept, which allows for unprecedented long culture times even in absence of biochemical growth factors. Employing TiO2 nanotube array substrates, whose interaction properties with individual cells and the overall tissue can be tuned by the tube parameters, we verify this concept for different adult neuronal explants, which are successfully cultured for the first time longer than 14 days with no indications of degeneration. It turned out that adequate nanotube diameter, wall thickness and surface roughness vary for successful long-term culture of adult mammalian retinae and brain slices. Additionally, we found that the intrinsic super-hydrophilicity of the substrates allows for a continuous supply of fresh medium without perfusion systems. Our findings pave the way for in vitro drug testing, as well as neuronal tissue regeneration.

BP 27.8 Thu 11:45 H43

Advanced high-throughput SEIRA methodology for multiplexed bioassay assessment — •Andrea Hornemann[1], Sabine Flemig[2], Gerhard Ulm[1], and Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]BAM Bundesanstalt für Materialforschung und -prüfung, Richard-Willstätter-Str.10, 12489 Berlin, Germany

Nanotechnology has an increasing impact in both the design and functionality of biomedical and biodiagnostic devices for a reliable high-performance analysis. High-throughput technological advances in diagnostic assays of high complexity induce requirements on selectivity, sensitivity, and multiplexing capability that will be the main challenges for the prospective assay design. We discuss the capability of surface-enhanced infrared absorption (SEIRA) spectroscopy as versatile diagnostic readout tool for both its potential widespread point-of-care use and application for the multiplexed bioassay assessment. We performed a qualification study on NP-enhanced SEIRA, enabling the readout of tunable assays. We utilized synchrotron radiation as its high brilliance provides an improved quality of spectral datasets and low data acquisition times. Our analysis included a profound study on nanoscaled biolabels that exhibit distinct narrow emission profiles of the incorporated antibody-fluorophore complexes. The molecular fingerprints have been successfully analyzed by multivariate methods with respect to their multiplexing capabilities. This robust spectral encoding by SEIRA signatures is expected to open new opportunities for a fast, reliable and multiplexed high-end screening in biodiagnostics.

BP 28: Focus session: Intracellular Spectroscopy

Organized by Vinod Subramaniam and Malte Drescher, this focus session addresses the biophysical challenges to study biological macromolecules using spectroscopic approaches, in particular in their natural intracellular environment.

Time: Thursday 9:30–13:00 Location: H44

Topical Talk BP 28.1 Thu 9:30 H44

Advanced Fluorescence Methods for Investigating the Lifecycle of Viruses — •Don C. Lamb — Department of Chemistry, Ludwig-Maximilians-Universität München, Munich, Germany

Advances in fluorescence spectroscopy and microscopy make it possible to perform quantitative experiments on biological systems. One of the goals within my group is to develop and apply methods to quantify the details of viral entry and assembly in live cells. To look at the early interactions of the structural HIV protein Gag in the cytosol, we combined pulsed interleaved excitation (PIE) with Raster Image Correlation Spectroscopy. Gag was labeled using fluorescent fusion proteins and PIE-RICS measurements were performed. A slower then expected diffusion of the Gag protein in the cytosol was observed even though no significant oligomerization of Gag was detected. To investigate the origin of the slow diffusion behavior, we measured the mobility of a number of mutant Gag molecules where different interaction sites have been altered. To investigate the fusion of viral particles, we have combined the advantages of single-particle-tracking with image correlation spectroscopy. Individual viruses are tracked in three-dimensions and the signal from the different channels in the volume surrounding the particle are cross-correlated. Using the TRacking Image Correlation analysis (TRIC), we detected multiple fusion events of Foamy Virus. The analysis revealed a novel intermediate step during the fusion process where the envelope and capsid are still connected although they are separated by several hundred nanometers.

BP 28.2 Thu 10:00 H44

Quantifying the milieu of organelles in living cells via fluorescence lifetime imaging — Nisha Pawar, Saeedeh Aliaskarisohi, and •Matthias Weiss — Experimental Physics I, University of Bayreuth, Germany

Compartmentalization is a hallmark of eukaryotic cells. A diverse set of organelles is dynamically maintained by eukaryotes to provide biochemical reaction vessels with a distinct milieu. Prominent examples are the endoplasmic reticulum (ER) and the Golgi apparatus, both of which are major constituents of the cell's secretory pathway. Along this pathway, about 10,000 different protein species are sorted and eventually sent to their final destination. It has long been hypothesized that the lumenal milieu of the ER and the distinct cisternae of the Golgi apparatus provide important cues for these sorting processes, yet assessing their milieu in a living cell has been a challenge. Using fluorescence lifetime imaging (FLIM), we have monitored the milieu of the Golgi apparatus and the ER under various conditions. We find a significant change in the Golgi milieu towards that of the ER when adding perturbative drugs. Moreover, following the trajectory of proteins from the ER through the Golgi, we can attribute distinct milieus to the individual sub-compartments along the secretory pathway, e.g. Golgi cisternae.

BP 28.3 Thu 10:15 H44

Protein motion in crowded solutions on fast time scales: diffusion and internal dynamics — •Felix Roosen-Runge[1], Marcus Hennig[1,2], Fajun Zhang[1], Tilo Seydel[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]Institut Laue-Langevin, Grenoble, France

Protein function depends on the complex interplay of structure, dynamics and the aqueous, but crowded cellular environment. We present a comprehensive experimental study accessing the full hierarchy of protein dynamics in solutions, e.g. vibrations, interdomain motions and diffusion of the entire protein. Quasi-elastic neutron and dynamic light scattering experiments have been performed and compared to theoretical predictions. In crowded solutions, both self diffusion D_s and collective diffusion D_c of protein solutions are well described by colloidal concepts, with D_s reduced to 20% at $\approx$ 20% volume fraction [1,2]. Separating the motion of the entire protein molecule, the internal motions are accessed under native conditions [3]. We studied the dynamics before, during and after thermal denaturation, supporting the notion of protein unfolding with subsequent chain entanglement. In the denatured, gel-like state, long-range motions are strongly *reduced*, while the local flexibility is *enhanced*. Using the analysis frameworks, neutron backscattering is well-suited to address the relation of protein function and dynamics under native conditions at fast time scales.

[1] F. Roosen-Runge, M. Hennig et al., PNAS 108 (2011) 11815; [2] M. Heinen, F. Zanini et al., Soft Matter 8 (2012) 1404; [3] M. Hennig, F. Roosen-Runge et al., Soft Matter 8 (2012) 1628

BP 28.4 Thu 10:30 H44

Labelfree coherent Raman scattering microspectroscopy: A new intracellular spectroscopy tool in lipidomic research — •Gregor Hehl[1], Margot Grandl[2], Alexander Kovalev[1],

Markus Peer[2], Gerhard Liebisch[2], Gerd Schmitz[2], and Andreas Volkmer[1] — [1]3rd Institute of Physics, University of Stuttgart, 70569 Stuttgart, Germany — [2]University Hospital Regensburg, 93053 Regensburg, Germany

A series of technological advances have made coherent Raman scattering (CRS) microscopy a highly sensitive and chemically selective imaging tool for the noninvasive analysis of biological cells. To facilitate a spectral identification and quantitative analysis of intracellular lipid species of a priori unknown composition by CRS microscopy, we developed the technique of hyperspectral coherent anti-Stokes Raman scattering (CARS) imaging. Here, we report on its exemplifying applications in lipidomic research. We investigated the uptake mechanism of atherogenic model lipoproteins into THP-1 macrophages. We observed a decrease of the degree of acyl unsaturation within individual lipid droplets in those cells, which have been loaded with oxidized lipoproteins, compared to the unperturbed cell. Furthermore, we addressed the question: Can an intracellular Raman-based spectroscopy selectively identify and detect minor molecular structure differences between the different lipid oxidation pathways in the living cell? Corresponding mass spectra of the respective cellular lipid contents were compared and correlated with our results obtained from Raman and CRS microscopy, and will also be presented.

BP 28.5 Thu 10:45 H44

Mapping lipid membrane molecular properties via vibrational imaging of vesicular systems — •Hilton B. de Aguiar and Andreas Volkmer — 3. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Probing the physical properties and chemical composition of lipid membranes is of fundamental importance to understand their role on biological cell functioning. Unlike in conventional fluorescence-based microscopies of membranes, which require specific labeling and may perturb the molecular properties of interest, Raman microspectroscopy directly probes the intrinsic vibrational spectral response of the membrane lipids offering the advantage of both chemical specificity and sub-micron spatial resolution in a noninvasive manner. Here, we report on the spatially resolved Raman spectroscopy of vesicular model membranes (Giant Unilamellar and Multilamellar Vesicles). We observe distinct Raman image patterns of an individual vesicle for distinct vibrational modes. We successfully model this sensitivity of the Raman image contrast to the physical properties of the lipids by taking the higher order optical nature of Raman scattering into account. Remarkably, the image patterns turn out to be very sensitive on molecular orientation and order parameters offering the opportunity of membrane structure analysis by label-free Raman microscopy. Furthermore, we demonstrate how the Raman spectral response can be readily used to distinguish between thermodynamic phases (liquid/gel state) and domain composition of membrane lipids.

BP 28.6 Thu 11:00 H44

Plasmonic Nanoantennas for SERS on Supported Membranes — •Paul Kühler, Theobald Lohmüller, and Jochen Feldmann — Chair for Photonics and Optoelectronics, LMU München

We utilize plasmonically coupled gold triangles for Surface enhanced Raman scattering (SERS) measurements of a fluid lipid bilayer. First, large arrays of plasmonic nanoantennas made of gold triangles are prepared on a solid support by an improved colloidal lithography technique. Then, a fluid supported membrane is formed on the intervening glass substrate by vesicle fusion. We demonstrate the applicability of this platform for spectroscopic investigations by performing SERS measurements of molecules that are constituents of a fluid supported phospholipid membrane. Our method offers a tool to analyze lipid membranes and membrane components under physiological conditions without fluorescent labeling or static entrapment of the membrane molecules.

15 min break

Topical Talk BP 28.7 Thu 11:30 H44

Looking at proteins inside live cells with atomic resolution: Science fiction or science reality? — •Phil Selenko — FMP Berlin

A protein's structure and its dynamic behavior are inherently dependent on its physiological environment. While most proteins function inside live cells, our knowledge about them is largely based on experiments that bear little resemblance to the physical and biological properties of a cell. A new approach in liquid-state NMR spectroscopy, in-cell NMR, now offers convenient means to directly study proteins at atomic resolution inside live cells. In this lecture, I will introduce the basic concepts behind in-cell NMR spectroscopy and provide examples of the structural and dynamic characteristics of a human amyloid protein in five different mammalian cell types, including dopaminergic neurons.

BP 28.8 Thu 12:00 H44

Inhibition of amyloid formation is impeded at the phospholipid interface — •Michael Schleeger[1], Corianne van den Akker[2], Maarten Engel[2], Tobias Weidner[1], Gijsje Koenderinke[2], and Mischa Bonn[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany — [2]FOM Institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

Several severe human diseases (including Alzheimer's, Parkinson's disease and type 2 diabetes mellitus) are characterized by the deposition of proteins as insoluble fibrils, also called amyloids. Amyloids fibrils are formed by self-assembly of peptide or protein precursors, which aggregate spontaneously into highly well-defined polymeric structures. The formation of amyloids can be inhibited by polyphenols, as has been previously shown in bulk studies. However, recent studies have shown that amyloid fibrils assemble and exert their cytotoxicity at cellular membranes, rather than in bulk solution. We therefore investigated the inhibitor activity specifically at the phospholipid membrane interface. We show, using surface-specific sum frequency generation (SFG) spectroscopy, that the commonly used amyloid inhibitor epigallocatechin gallate (EGCG) is a much less efficient inhibitor of amyloid formation at a lipid interface than in bulk solution. Moreover, we demonstrate that EGCG is not able to disaggregate existing amyloid fibrils at a lipid interface, in contrast to its behavior in bulk. Clearly, inhibitors are much less effective at membrane surfaces, which should be considered during the design and testing of novel amyloid inhibitors.

BP 28.9 Thu 12:15 H44

Calculation of the CD spectrum of a flexible peptide — •Zlatko Brkljača[1], Karmen Čondić-Jurkić[1,2], Momir Mališ[2], David M. Smith[2,3], and Ana-Sunčana Smith[1] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Ruđer Bošković Institute, Zagreb, Croatia — [3]Computer Chemie Centrum, Universität Erlangen-Nürnberg, Erlangen, Germany

Circular dichroism (CD) spectroscopy is a standard experimental method employed in the structural characterization of optically active chiral molecules, such as proteins and peptides. Because the CD spectrum of a molecule is an ensemble average over its entire conformational phase space, the interpretation of the experimental data is challenging. This is particularly true for highly flexible peptides, where the spectra cannot be unambigously interpreted without theoretical modelling. However, so far there has been no accurate theoretical approach to predict peptide CD spectra. We address this problem by developing a method that combines replica exchange molecular dynamics to generate the conformational phase space, and TDDFT to calculate the electronic transitions. Thereby we systematically treat the solvent induced polarization of the peptide. We validate our method on an example of the CD spectrum of the opioid growth factor (Met-enkephalin). On the level of the single conformation we compare TDDFT with high level ab-initio calculations (RI-CC2), while on the level of the ensemble we make a comparison with the experimentally measured spectrum. Good agreement is obtained in both cases.

BP 28.10 Thu 12:30 H44

CD-Spectroscopic Assessment of Potential Antigenicity of Negatively Charged Biopharmaceuticals — •Sven Brandt[1], Krystin Krauel[1], Kay Gottschalk[2], Christiane Helm[3], Andreas Greinacher[4], and Stephan Block[1] — [1]ZIK HIKE - Humorale Immunreaktionen bei kardiovaskulären Erkrankungen, Fleischmannstr. 42-44, D-17475 Greifswald, Germany — [2]Institut für Experimentelle Physik, Universität Ulm, D-89069 Ulm, Germany — [3]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany — [4]Institut für Immunologie und Transfusionsmedizin; D-17475 Greifswald, Germany

Platelet factor 4 (PF4), a protein with a high positive surface charge forms complexes with natural or artificial polyanions (PA). It is known that such complexes exhibit an antigen of the adverse drug reaction heparin induced thrombocytopenia (HIT) and that their antigenicity is three fold: (i) the molar ratio between PF4 and the PA, (ii) the

charge density of the PA, and (iii) the chain length of the PA. To the best of our knowledge, we show for the first time by circular dichroism (CD) spectroscopy that the secondary structure of the protein is altered when complexes which are known to be antigenic are formed. Here we correlate the changes in the proteins secondary structure determined using CD spectroscopy with HIT antigenicity determined by ELISA. This allows us to assess potential antigenicity of negatively charged biopharmaceuticals without the necessity of in vivo studies or the use of antibodies isolated from immunized patients specific for the antigenic epitopes.

BP 28.11 Thu 12:45 H44

Ribonuclease A: A model system to study intrinsically unfolded proteins — •Jennifer Fischer[1], Ralf Biehl[1], Bernd Hoffmann[2], and Dieter Richter[1] — [1]ICS-1, FZ-Jülich, Jülich, Germany — [2]ICS-7, FZ-Jülich, Jülich, Germany

Structure and dynamics play the key role in protein function, but roughly 30% of eukaryotic proteins are partially or even completely unfolded [1]. Nevertheless, intrinsically unfolded proteins are functional and involved in several biological processes. To get further insight into disordered structures and their dynamics, we use Ribonuclease A (RNase A) as a model system, as it is a well known protein denaturing reversibly upon heating. Additionally, by varying the buffer conditions by different pH values, several states can be prepared. A detailed study of the structure and dynamics using Small Angle Neutron and X-ray Scattering (SANS, SAXS) as well as Neutron Spin Echo Spechtroscopy (NSE) and Circular Dichroism Spectroscopy is presented. The combination of these techniques allows us to observe large-scale internal dynamics of subdomains or of unfolded protein strands that operate on the same length scale as rotational diffusion. However, the timescale can be different and depends on the protein structure and internal interactions. [1] A. L. Fink, Current Opinion in Structural Biology 2005, 15:35-41

BP 29: Symposium Computational Challenges in Scale-Bridging Modeling of Materials (SYMM, joint with CPP, DY and MM)

Time: Thursday 9:30–12:00 Location: H1

Invited Talk BP 29.1 Thu 9:30 H1

Challenges for first-principles based computation of properties of oxide materials — •Karsten Albe — TU Darmstadt, FB 11, FG Materialmodellierung, Petersenstr. 32, D-64287 Darmstadt

Calculations based on density functional theory (DFT) have been the mainstay of theoretical studies of the properties of semiconductor and oxide materials over the past few decades. Despite of their significant successes, challenges remain in adapting these methods for predictive simulations that are quantitatively useful in predicting complex device properties. Increasing computing power and improved theoretical methods taking advantage of ever more powerful computer hardware offer the possibility that computational modelling may finally allow a virtual materials design by truly predictive simulations. In this contribution, I will give examples for successes and failures in calculating bulk, point defect and surface properties of transparent conducting as well as ferroelectric oxides and describe the remaining challenges.

Invited Talk BP 29.2 Thu 10:00 H1

Deformation and Fracture of Solids: Tough Nuts at Atomic and Continuum Scales — •Peter Gumbsch[1,2], Matous Mrovec[1,2], Kinshuk Srivastava[1], and Daniel Weygand[1] — [1]Institut for Applied Materials IAM, Karlsruhe Institute of Technology KIT — [2]Fraunhofer IWM, Freiburg

Multiscale modeling of deformation processes in crystalline materials poses several challenges although the basic physical process, the motion of dislocations, is well understood. I will use the deformation of single crystalline alpha-iron to illustrate these challenges.

To feed dislocation dynamics with realistic atomistic information requires a reliable and computationally efficient description of the atomic interactions. We use a recently developed magnetic bond-order potential (BOP). Dislocation mobility laws for discrete dislocation dynamics (DDD) studies of large dislocation ensembles then require consideration of the full local stress state in a mesoscopic mobility law since it turned out that the effect of non-glide stresses and orientation of the applied loading is crucial for capturing the non-Schmid behavior.

Averaging the behavior of discrete dislocations into continuum mechanical equations is even more difficult. It requires a homogenization of the dislocation fields including a description of their multiplication and mutual interaction. The mathematical framework for such a continuum field theory is still not available. I will present a kinematically consistent continuum description of the dynamics of curved dislocation systems as a first approach to such a continuum field theory.

Invited Talk BP 29.3 Thu 10:30 H1

Crucial Issues and Future Directions of Through-Process Modeling — •Guenter Gottstein — RWTH Aachen University, Institut of Physical Metallurgy and Metal Physics, Aachen, Germany

Computer simulation of materials processing and properties has advanced to an established field and indispensible research topic in materials science and engineering during the past decade. Moreover, it has grown to a powerful and accepted tool for commercial alloy and process development. While the general theory has been laid out, physics based scale-bridging modeling approaches have been developed and are currently employed also in industrial environments, flexible interfacing has become available and automated simulation is currently being tested, there are still bottlenecks that impede the ease of application and the predictive power of these tools and urgently need to be addressed. Such needs include reliable experimental databases, the bridging of knowledge gaps on critical phenomena like nucleation, interacting microstructural evolution processes that require vastly different computation times, inverse modeling algorithms etc. Finally, despite of the remarkable advances in available computer power, computer simulation still suffers from too low computational speed to address statistically significant system sizes and to lend itself to process control. More recent concepts will be introduced, in particular in view of the changing philosophy of computer architecture and the increasing availability of massively parallel computing power, which may actually require a departure from conventional and established modeling concepts.

Invited Talk BP 29.4 Thu 11:00 H1

Adaptive Resolution Simulations for Soft Matter: Applications and New Developments — •Kurt Kremer — Max Planck Institute for Polymer Research

The relation between atomistic structure, architecture, molecular weight and material properties is a basic concern of modern soft matter science. A typical additional focus is on surface and interface aspects or the relation between structure and function in nanoscopic molecular assemblies. Here computer simulations on different levels of resolution play an increasingly important role. To progress further, adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution. The lecture will concentrate on these methods to couple particle based simulations. In addition first approaches to connect particle based simulations to continuum as well as to include quantum effects will be presented. Furthermore the extension to open systems MD as well as new recent methodology advances will be explained. A general review on the first part can be found in M. Praprotnik, L. Delle Site, and K. Kremer, Ann. Rev. Phys. Chem. 59, (2008) and recent advances in S. Fritsch et al. Phys. Rev. Lett. 108, 170602 (2012)

Invited Talk BP 29.5 Thu 11:30 H1

Materials by design — •Markus Buehler — MIT, 77 Mass. Ave, Cambridge, MA 02139

Biological materials are synthesized, controlled and used for an astonishing variety of purposes including structural support, force generation, mass transport, catalysis, or energy conversion. By incorporating concepts from biology and engineering, computational modeling has led the way in identifying the core principles that link the molecular structure of biomaterials at scales of nanometers to physiological scales at the level of tissues. The use of the world's fastest supercomputers allows us to predict properties of complex materials from first prin-

ciples, realized in a multiscale modeling approach that spans massive ranges in scale. Combined with experimental studies, such in silico models allow us to simulate disease, understand catastrophic failure of tissues, and enable us to translate concepts from the living world into material designs that blur the distinction between the living and non-living systems. We discuss challenges and opportunities in new methods of scale bridging.

BP 30: Tissue

Time: Thursday 15:00–17:30 Location: H43

Invited Talk BP 30.1 Thu 15:00 H43

Inversion and perversion in biomechanics: from microscopic anisotropy to macroscopic chirality. — •Alain Goriely — Mathematical Institute, University of Oxford

One of the fundamental problems of bio-physics is to understand the relationship between a microscopic structure and its overall macroscopic response. A paradigm for this problem is chirality. How does a right-handed structure behaves under loads? A simple example motivated by the study of DNA is the extension of a right-handed spring under pure axial load. Would it rotate clockwise or counter-clockwise? Similarly, many plant structures are fibre-reinforced and the problem is to connect the chirality of the fibre with the chirality of the rotation induced by change in pressure. Motivated by different biological experiments on active gels, DNA, plant cell walls, and fungi, I will show that biological systems, through a combination of internal stresses and nonlinear responses offer many puzzling and often counter-intuitive chiral behaviour leading to the interesting possibility of perversion, an inversion in chirality under load or remodeling.

BP 30.2 Thu 15:30 H43

Interplay of tissue extension and pattern formation during vertebrate segmentation — •David J. Jörg[1], Luis G. Morelli[2], Andrew C. Oates[3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Departamento de Física, FCEyN UBA and IFIBA, Conicet; Pabellón 1, Ciudad Universitaria, 1428 Buenos Aires, Argentina — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany

During embryonic development of vertebrates, the elongating body axis is segmented into somites, precursors of the vertebrae, which appear sequentially. This process is coordinated by a tissue level patterning system based on cell-autonomous genetic oscillators, the segmentation clock. We develop a continuum theory of coupled phase oscillators that takes into account position-dependent tissue extension. This tissue extension corresponds to a cell flow field that enters the description of the phase dynamics through a convective term. We show that our theory can account for the key features of dynamic gene expression patterns observed in experiments.

BP 30.3 Thu 15:45 H43

Mechanically driven interface propagation between cellular populations — •maryam aliee[1], Jonas Ranft[2], Jacques Prost[3], Jean-François Joanny[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Institut Curie, 26 rue d'Ulm, 75248 Paris cedex 05, France — [3]ESPCI ParisTech, 10 rue Vauquelin, 75231 Paris cedex 05, France

Many biological tissues consist of different cell types. The interface between two cell populations can evolve in time due to the interplay of cell dynamics and tissue mechanics. Here we introduce a continuum description of tissues with two cell types. The balance of cell numbers and the conservation of momentum include source terms, which account for the effects of cell division and apoptosis. We study the case where two cell populations with different homeostatic pressure are separated by an interface. The difference in the homeostatic pressures of two cell types drives the propagation of the interface, corresponding to the invasion of one cell type into the other. The dynamics of the system is described by a generalized version of the Fisher wave equation, which takes into account the coupling between cell number balance and tissue mechanics. We calculate the profile of the moving interface and its velocity as a function of relevant parameters. By linearizing the equations near the unstable front, we can compare our numerical results to analytical solutions. We show that both pulled and pushed front solutions occur, depending on parameter values.

BP 30.4 Thu 16:00 H43

***Physarum polycephalum* Percolation as a Paradigm for Topological Phase Transitions in Transportation Networks** — •Adrian Fessel[1,2], Christina Oettmeier[1,2], Erik Bernitt[1,2], Nils Gauthier[2], and Hans-Günther Döbereiner[1,2] — [1]Institut für Biophysik, Universität Bremen — [2]Mechanobiology Institute, National University of Singapore

As a foraging strategy, the slime mold *Physarum polycephalum* spans an extended vein network. If grown from disconnected pieces, evenly distributed in size, a giant component develops. Using tools from graph theory, this process can be understood as a percolation transition, driven by the distribution of node degrees (Fessel, PRL 109, 2012).

We present two analytical solutions for this topological transition, a two-dim. phase diagram representing the transition as a function of two node degree ratios and a one-dim. solution suitable for our system. Neither biological nor other constraints are taken into account, making the solutions universal for transportation networks, given local connectivity is low.

An experimental indication for universality can be found in vasculogenesis. Various malignant tissues mimic embryos which derive their blood vessels by fusing blood islands, i.e., aggregates of newly differentiated angioblast cells. This process can be studied in vitro by observing the behavior of plated endothelial cells. Reanalyzing such an experiment (Serini, EMBO 22, 2003) we find the same transition.

Due to the universal character of this process we conclude that percolation might serve as a gauge in anti-angiogenic theraphies.

Invited Talk BP 30.5 Thu 16:15 H43

A noisy path to order: refinement of a developing tissue — •Buzz Baum — LMCB, UCL, London, WC1E 6BT, UK

The remarkable complexity we see in the macroscopic biosphere is generated during development. Even though cellular processes are inherently noisy, the complex order we see in multicellular organisms is generated by the actions of semi-autonomous cells working in constant dialogue with one another. Here, I will use two examples from our work in the fly notum that reveal ways in which noise at the cellular level can contribute to the refinement of patterning and cell packing at the tissue scale.

BP 30.6 Thu 16:45 H43

Morphogenesis and ageing of MDCK epithelial tissues depend on substrate elasticity — •Sara Kaliman[1], Christina Jayachandran[2], Damir Vurnek[1], Florian Rehfeldt[2], and Ana-Sunčana Smith[1] — [1]Institute for Theoretical Physics, University Erlangen-Nürnberg, Germany — [2]3^{rd} Institute of Physics-Biophysics, University ofGöttingen, Germany

Morphogenesis of epithelial tissues is the key to understanding tissue development and regeneration, or tumour growth. It is believed to be dominated by intercellular interactions, and hence, independent of substrate rigidity. However, here we show that different regimes of growth occure on soft and hard substrates. Substrates with a rigidity higher than 5 kPa promote radially growing clusters, which in early stages expand exponentially with a persistantly low density of cells. When the cluster radius exceeds 5 mm, its area increases linearly in time. During that period, a bulk tissue of higher density forms in the center of the cluster, whereas the edge remains at a constant low density, independently of the cluster size. On 1 kPa substrates the cells initially form small multilayered dropplets that, if sufficiently large, nucleate a very dense and well structured monolayer in its center. These clusters expand to macroscopic sizes by adopting irregular shapes, while mantaining the initial monolayer morphology. In both cases, tissues age, the signature of which are (i) an inhomogeneous density, and (ii) nuclei that deform strongly due to the substrate sensitive restructuring of the actin cortex. Furthermore, dome-like and tubule-like structures are found on hard substrates, while soft substrates promote anoikis.

BP 30.7 Thu 17:00 H43

Cell Shape and Dynamics on micropatterned Substrates — •Philipp J. Albert and Ulrich S. Schwarz — Institute of Theoretical Physics, University of Heidelberg

Micropatterned substrates have been used for cell normalization and to quantitatively study the relation between cell shape and function. In order to design micropatterns, models to predict shape and dynamics of cells are needed. To this end, we combine two previously introduced models. The tension elasticity model (TEM) [1] focuses on strongly contracted shapes which can be predicted correctly on dot pattern substrates. However, the TEM cannot predict dynamical changes, like the movement from one pattern to the next. A two-dimensional cellular Potts model (CPM) [2] combined with directional persistence is used to account for the dynamics of cells on micropatterned substrates. In contrast to earlier applications of the CPM in the context of tissues, in our case the area of cells is not fixed as they can exchange material with the third dimension. We modify the energy function of previous formulations of the CPM to account for this feature as well as to include insights from the TEM and to represent the effect of the adhesive micropattern. We use our model to predict the dynamics of cell shape, spreading and division, and to identify promising patterns for experiments.

[1] I.B. Bischofs, F. Klein, D. Lehnert, M. Bastmeyer and U.S. Schwarz, Biophys. J. **95**, 3488 (2008).

[2] F. Graner and J.A. Glazier, Phys. Rev. Lett. **69**, 2013 (1992).

BP 30.8 Thu 17:15 H43

On the Relevance of Cellular Adhesion for Compartmentalization — •Steve Pawlizak, Anatol Fritsch, and Josef A. Käs — University of Leipzig, Institute for Experimental Physics I, Soft Matter Physics Division, Linnéstraße 5, 04103 Leipzig, Germany

Compartmentalization is a fundamental organization process of cells, which can be demonstrated *in vitro* by means of a simple model system: When two different populations of suspended cells are mixed, the mixture will eventually segregate into two phases, whereas mixtures of the same cell type will not. Nowadays, the concept of compartmentalization is coming more and more into focus of cancer research because it has been observed that even tumor cells are confined to their original compartment for a relatively long time in their development. For that reason, the understanding of the mechanical principles underlying this process is of great importance. The *differential adhesion hypothesis* by Malcolm S. Steinberg gives a first explanation by differences in surface tension and adhesiveness of the interacting cells. We are investigating whether cellular adhesion is in fact a necessary or even sufficient factor to characterize compartmentalization and tumor spreading. For our studies, we use healthy and cancerous breast cell lines of different malignancy as well as primary cells from human cervical carcinoma. We apply a broad set of techniques to study their mechanical properties and interactions, including 3D segregation experiments in droplet cultures, *optical stretching* for whole cell rheology, and *AFM* to directly measure cell-cell-adhesion forces. The combination of these techniques will help to shed some new light on the role of cellular adhesion.

BP 31: Statistical Physics in Biological Systems III (joint with DY)

Time: Thursday 15:00–17:30 Location: H46

BP 31.1 Thu 15:00 H46

On the Fourier spectra of fitness Landscapes — •Johannes Neidhart, Ivan Szendro, and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Deutschland

Fitness Landscapes are a well established tool in the analysis of evolutionary precesses. In order to extract important information, graph theoretical Fourier decomposition has proven to be very useful. In order to compare experimental data with stochastic models, we analyse several models, amongst others Kauffmann's *LK* model and present exact results for the Fourier spectra as well as a comparison to experimental data.

BP 31.2 Thu 15:15 H46

On the existence of accessible paths in trees — •Stefan Nowak and Joachim Krug — Institute for Theoretical Physics, University of Cologne

The study of accessible paths is a new type of percolation problem which is inspired by evolutionary biology. To each node of the underlying graph a random number is assigned and a path through the graph is called accessible if all random numbers along the path are in ascending order. We will give an exact expression for the second moment of the number of accessible paths from the root to the leafs in n-trees and an asymptotic expression for the probability that there is at least one accessible path. Furthermore, we will show that there is a percolation threshold if the random variables are Gumbel distributed and a linear drift is added.

BP 31.3 Thu 15:30 H46

A new evolutionary food web model — •Korinna T. Allhoff[1], Daniel Ritterskamp[2], Christian Guill[3], and Björn C. Rall[3] — [1]Institute of Condensed Matter Physics, TU Darmstadt — [2]Institute for Chemistry and Biology of the Marine Environment, Carl von Ossietzky University of Oldenburg — [3]J. F. Blumenbach Institute for Zoology and Anthropology, Georg-August-University Göttingen

Understanding the conditions that are required for complex ecosystems to persist despite changes in species composition and anthropogenic perturbations, is of utmost importance in order to conserve these systems. Evolutionary food web models provide a mechanistic tool to understand how complex ecosystems emerge and how they react to changes in their composition. We present such an evolutionary food web model, where each species is characterized by three key traits: its own body mass, its preferred prey body mass, and the width of its potential prey body mass spectrum. The model contains allometric effects on feeding and competition interactions and determines dynamically whether a species is viable or goes extinct. The evolutionary processes that enable new species to enter the system as mutants of already existent ones, also follow allometric rules. The food web structure emerges as a highly nontrivial result from the combined effect of population dynamics and evolution. We present computer simulations of different model modifications and show how they influence network structure and stability.

BP 31.4 Thu 15:45 H46

The influence of chaos on the stability of small food webs — •Fanny Groll and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Germany

Ecological networks can show different types of dynamics. Experiments have demonstrated that they can actually be governed by deterministic chaos. In that case the population numbers evolve along a chaotic attractor; they show large fluctuations but do not go extinct.

We examine a mathematical model of a simple food web consisting of two prey and one predator population. In this model a control parameter triggers the onset of chaos via bifurcation. Such dynamics have already been observed in an aquatic system of few competing species.

In studying this system we aim to find a catalogue of techniques to approach such a system and to analyze its features. Starting from a general master equation approach we have explored routes to chaos in few-species ecological systems. Emphasis has been put on the mechanisms leading to chaotic attractors. Under ambient conditions ecological systems are subject to demographic and environmental fluctuations. We explore the stability and persistence of populations in chaotic regimes compared to more regular types of dynamics.

BP 31.5 Thu 16:00 H46

The effect of migration between patches on the stability of foodwebs — •Sebastian Plitzko and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Germany

During recent years, several factors that stabilize food webs have been identified. Among these are allometric scaling of metabolism with body size and adaptive foraging. So far, food web models rarely take space into account. However, it is known that being distributed over several spatial patches can have positive as well as negative effects on the stability of metacommunities.

Using computer simulations for the population dynamics of sys-

tems with many species, we investigate the stability of food webs that are distributed over several patches that are connected by migration. We evaluate species persistence in dependence of food-web complexity, patch arrangement, and migration rule. In particular, we study conditions under which migration alone, without the above-mentioned additional stabilizing factors, can increase food-web stability. We also determine whether food webs that already have a high stability can gain further by being distributed over several patches.

BP 31.6 Thu 16:15 H46

The effect of predator limitation on the dynamics of simple food chains — •Christoph Schmitt[1], Stefan Schulz[1], Jonas Braun[1], Christian Guill[2], and Barbara Drossel[1] — [1]Physics Department, TU Darmstadt — [2]Institute for Zoology and Anthropology, University of Göttingen

We investigate the influence of competition between predators on the dynamics of predator-prey systems and of tritrophic food chains. Competition between predators is implemented either as interference competition, or as a density-dependent mortality rate.

With interference competition, the paradox of enrichment is reduced or completely suppressed, but otherwise the dynamical behavior of the system is not fundamentally different from that of the Rosenzweig-MacArthur model, which contains no predator competition.

In contrast, with density-dependent predator mortality the predator-prey system shows a surprisingly rich dynamical behavior. In particular, decreasing the density regulation of the predator can induce catastrophic shifts from a stable fixed point to a large oscillation. Furthermore, the model shows several other types of nonlocal bifurcations, the coexistence of several attractors, and different types of regime shifts. In tritrophic food chains chaos can occur in both models.

BP 31.7 Thu 16:30 H46

Score statistics of multiple sequence alignments — •Pascal Fieth and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

Optimally aligned sequences of amino acids [1] can be studied numerically [2] in the biologically relevant high scoring region by means of parallel tempering simulations [3]. Preceding studies have shown that the scores of gapped pairwise sequence alignments of finite-length sequences follow a Gumbel extreme value distribution, modified by a Gaussian correction [4] rather than a simple Gumbel extreme value distribution as previously predicted for ungapped pairwise alignments. In this study these methods are applied to the case of multiple sequence alignment (MSA). Here the distributions of the sum-of-pair scores of the MSA of more than two sequences are studied. In particular the distribution of protein MSA-scores using different common substitution matrices (BLOSUM and PAM) are analysed for protein background frequencies of real sequences.

[1] R. Durbin et al., *Biological sequence analysis*, (Cambridge University Press, 1998)
[2] A.K. Hartmann, *Practical Guide to Computer Simulations*, (World Scientific, 2009)
[3] A.K. Hartmann and Heiko Rieger, *Optimization Algorithms in Physics*, (Wiley-VCH, 2001)
[4] S. Wolfsheimer et al., *Local Sequence Alignments Statistics: Deviations from the Gumbel Statistics in the Rare-Event Tail*, (Algorithms for Molecular Biology, 2007)

BP 31.8 Thu 16:45 H46

Understanding evolutionary conserved contacts by structure based models. — •Abhinav Verma[1], Benjamin Lutz[1], Martin Weigt[2], and Alexander Schug[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Université Pierre et Marie Curie, Paris, France

The evolution of a protein family leaves a fingerprint in databases of protein sequences. In a recent study, Direct Coupling Analysis (DCA) has been shown to accurately identify co-evolving residue pairs preserved as spatial contacts in their three dimensional fold [1]. Such DCA-derived contacts can be combined with molecular dynamics simulations to predict experimentally inaccessible transiently occupied active states [2]. Only a fraction of a contact map, however, is identified by DCA. Here we attempt to understand the evolutionary constraints leading to the conservation of these specific contacts by native structure based models [3]. We compare simulations with DCA derived contact maps to randomly chosen subsets of contacts.[unpublished data]

[1] Marcos et. al. , PNAS, 2011, 108, E1293
[2] Dago et. al. , PNAS, 2012, 109, E1733
[3] Whitford et al. Proteins, 2009 75, 430

BP 31.9 Thu 17:00 H46

Symmetry Breaking of Sequence Information in Catalytic Polymer Soups — •Shoichi Toyabe and Dieter Braun — Systems Biophysics,Ludwig-Maximilians-University Munich, Munich

One of the most distinguished properties of living systems is that they sustain genetic information and reproduce it. However, its origin remains elusive; how can information emerge in the chaotic molecular soup in the prebiotic earth? We discuss models and preliminary experiments to show the emergence of order in a catalytic polymer solution. We argue that template-directed copolymerization of diverse polymers is a promising route. Autocatalytic copolymerization extends polymers stochastically. Interestingly, a numerical simulation shows that the polymers self-organize into an ordered state where a stochastically chosen small set of sequence motifs become dominant. This spontaneous symmetry breaking occurs because autocatalytic chain reactions in the reaction network interact competitively and amplify strands beyond exponential growth. This amplifies spontaneous fluctuations and sustains it by Darwinian selection against other sequences. The transition to the ordered state is accompanied by a population inversion, i.e. the length distribution of polymers was biased to the longer side at the ordered state. In order to demonstrate the symmetry breaking by experiments, we performed ligase chain reactions of DNA strands with semi-random sequences. Under nonequilibrium driving of material flux and temperature cycles, we observed a population inversion, which implies the breaking of the symmetry. Furthermore, we analyzed the sequences to confirm the symmetry breaking by on the basis of PCR.

BP 31.10 Thu 17:15 H46

Characteristics of the formation of oligomers in a primordial broth — •Sabrina Scherer — Biologische Experimentalphysik, Universität des Saarlandes

We analyse the energetically driven emergence of spontaneous and dynamic states of order in prebiotic, complex systems. We perform Miller-Urey-type experiments: simple anorganic molecules driven by electric discharges and form complex, organic reaction mixtures. The process is analysed by real-time mass spectroscopy. The spectra reveal the formation of a time-dependent order of molecules in the reaction mixture. The peak intensities of several oligomeric molecules oscillate over time. Some oligomers vanish after their first occurence to reform again later. The increase and decrease of these intensities follow exponential and sigmoid courses. This points towards autocatalytic processes. In contrast to the original Miller-Urey-experiment which consists of the constituents methane, ammonia, hydrogen and water, we add other biologically relevant elements like phosphor and sulfur to observe their influence on the stability of the oligomer oscillations.

BP 32: Cell Adhesion and Mechanics

Time: Friday 9:30–13:00 Location: H43

BP 32.1 Fri 9:30 H43

Mechanics as second messenger in signal transduction — Roger Hardie and •Kristian Franze — University of Cambridge, Department of Physiology, Development and Neuroscience

Fly eyes have the fastest visual responses in the animal kingdom, but how they achieve this has long been an enigma. Phototransduction in Drosophila microvillar photoreceptors is mediated by a G-protein coupled phospholipase C (PLC) cascade culminating in activation of 'transient receptor potential' (TRP) and TRP-like (TRPL) channels by a still unresolved mechanism. Here we show that these light-sensitive channels are not ligand but mechanically gated. Using atomic force microscopy we found that light exposure evoked rapid contractions of the photoreceptor cells. These contractions were even faster than

the cell's electrical response and appeared to be caused directly by PLC activity. Photoreceptor light responses were facilitated by membrane stretch and inhibited by amphipaths, which alter lipid bilayer properties. When we replaced the native light-sensitive channels with mechano-sensitive channels, photoreceptors still generated electrical signals in response to light. These results indicate that splitting of the membrane lipid PIP2 by PLC reduces the membrane area, which leads to an increase in membrane tension, and ultimately causes the contractions of the cells. They furthermore suggest that the resultant mechanical forces contribute to gating the light-sensitive channels, thereby introducing the concept of mechanical force as an intermediate or 'second messenger' in metabotropic signal transduction.

Reference: Roger C. Hardie and Kristian Franze, Photomechanical Responses in Drosophila Photoreceptors, Science 338: 260-263, 2012.

BP 32.2 Fri 9:45 H43

Mechanical Properties & Active Fluctuations of Primary Cilia — •Christopher Battle and Christoph F. Schmidt — Drittes Physikalisches Institut, Georg-August Universitaet, Goettingen, Germany

Recent studies have shown that the primary cilium, long thought to be a vestigial cellular appendage with no function, is involved in a multitude of sensory functions. One example, interesting from both a biophysical and medical standpoint, is the primary cilium of kidney epithelial cells, which acts as a mechanosensitive flow sensor. Genetic defects in ciliary function can cause, e.g., polycystic kidney disease (PKD). The mechanical properties of these non-motile, microtubule-based 9+0 cilia, and the way they are anchored to the cell cytoskeleton, are important to know if one wants to understand the mechano-electrochemical response of these cells, which is mediated by their cilia. Using optical traps and DIC/fluorescence microscopy we probe the mechanical properties, cellular anchoring conditions, and dynamics of the cilia of canine kidney epithelial cells (MDCK), finding evidence for non-equilibrium, active fluctuations.

BP 32.3 Fri 10:00 H43

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 University, Germany — [2]Max Planck Institute of Biochemistry, Department of Molecular Medicine, 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.

BP 32.4 Fri 10:15 H43

Influence of the Subsurface Composition of a Material on the Adhesion of *Staphylococci* — •Christian Titus Kreis[1], Peter Loskill[1], Nicolas Thewes[1], Mathias Herrmann[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, 66041 Saarbruecken, Germany — [2]The Institute of Medical Microbiology and Hygiene, Saarland University, Homburg/Saar, 66421, Germany

Controlling the interface between bacteria and solid materials has become an important task in biomedical science. For a fundamental and comprehensive understanding of adhesion it is necessary to seek quantitative information about the involved interactions. Most studies concentrate on the modification of the surface (chemical composition, hydrophobicity, or topography) neglecting, however, the influence of the bulk material, which always contributes to the overall interaction via van der Waals forces. We applied AFM force spectroscopy and flow chamber experiments to probe the adhesion of *Staphylococcus carnosus* to a set of tailored Si wafers, allowing for a separation of short- and long-range forces. We provide experimental evidence that the subsurface composition of a substrate influences bacterial adhesion. A coarse estimation of the strength of the van der Waals forces via the involved Hamaker constants substantiates the experimental results. The results demonstrate that the uppermost layer is not solely responsible for the strength of adhesion. Rather, for all kinds of adhesion studies, it is equally important to consider the contribution of the subsurface.

P. Loskill et al. *Langmuir* **28** (2012) 7242

BP 32.5 Fri 10:30 H43

Actin and membrane contributions to the micromechanics of cell adhesions — •Konrad Berghoff[1,2,3], Yoko Nakano[2,3], Patricia Dankers[2,3], Leo van IJzendoorn[2,3], Bert Meijer[2,3], and Holger Kress[1,2,3] — [1]University of Bayreuth, Germany — [2]Eindhoven University of Technology, The Netherlands — [3]Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands

Adhesion to extracellular structures is import for a cell's ability to anchor itself in its environment and for receiving information from this environment. Understanding the mechanics of adhesion bonds and associated cellular structures will help to understand how cell adhesions fulfill their role as anchors and messengers. We investigate the mechanics of extracellular and intracellular adhesion bonds as well as the mechanics of associated cytoskeleton and membrane structures by using optical traps. We investigate the binding properties of microparticles functionalized with the integrin-binding RGD peptides to fibroblasts, and measure intracellular and extracellular rupture forces of adhesion bonds. Furthermore we investigate the viscoelastic properties of the actin network and the cell membrane which are associated with the adhesion area. Force-deformation measurements enable us to discriminate between permanent and reversible changes of the cellular mechanics. Our work provides an experimental basis for testing and improving recent models of cell membrane and cytoskeletal mechanics. It will help to improve our understanding of the mechanics of cell adhesions and associated structures.

BP 32.6 Fri 10:45 H43

Fluctuations of adhesion forces during cellular migration — •B. Sabass[3], S. V. Plotnikov[1], C. M. Waterman[1], and U. S. Schwarz[2] — [1]Nat. Heart Lung and Blood Inst., NIH — [2]Inst. f. Theo. Phys., U Heidelberg — [3]-

Migration of endothelial cells is based on the concerted dynamics of intracellular structures and adhesion sites. The continuous formation and dissociation of adhesion sites leads to observable fluctuations of the transmitted force. In order to elucidate the connection between force fluctuation and cellular migration we recently performed traction measurements for integrin-based adhesions. The force fluctuation magnitude is seen to decrease monotonously for increasing substrate stiffness. However, the speed of cellular migration shows a pronounced maximum for intermediate stiffnesses around 8 kPa. The occurrence of stiffness-guided migration (durotaxis) is promoted by the presence of force fluctuations. Therefore, force fluctuations can be interpreted as dynamical sampling of extracellular stiffness to guide durotaxis.
We here suggest a quantitative interpretation of these results with a simple model for a cell-wide force balance. The adhesion sites are described by a stochastic model that predicts a non-linear relationship between extracellular rigidity and adhesion stability (1). The model is also employed to compare measured effects of biochemical perturbations of the Paxillin module with predicted changes in the cellular mechanics.

(1) B. Sabass and U. S. Schwarz. J. Phys. Condensed Matter, 22, 2010.

BP 32.7 Fri 11:00 H43

Reaction-diffusion binding of a membrane to an underlying scaffold — •Timo Bihr[1,2], Ana-Suncana Smith[1], and Udo Seifert[2] — [1]Institut für Theoretische Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnber — [2]II. Institut für Theoretische Physik, Universität Stuttgart

Adhesion between cells plays a key role in a number of biological processes. It involves the formation of domains consisting of a large number of ligand-receptor bonds. The dynamics of domain growth has been studied on cells and vesicles over the last two decades, whereby a number of different growth behaviours and a variety of domain morphologies have been characterized. However, a comprehensive theoretical framework accounting for these observations is largely missing. We here develop a coarse-grained, kinetic Monte Carlo scheme that accounts for the discrete and the stochastic nature of the ligand-

receptor recognition, the diffusion of binders, and the membrane mediated, long-ranged interactions. Exploring this rich parameter space allowed us to recover all observed types of growth patterns, including the transition from the reaction to the diffusion limited dynamics, as well as the formation of radially growing or fractal patterns as well as ring-shaped domains. Last but not least, we are able to rationalize a number of those regimes by analytic arguments.

15 min break

BP 32.8 Fri 11:30 H43

Microfluidic Shear Alters Network Dynamics 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. They play a key role in cell mechanics, providing cells with compliance to small deformations and reinforcing them when large stresses are applied. Here, we present a study of fluorescent keratin intermediate filament networks in living cells with respect to their behavior in the presence of external forces by exposing the cells to controlled microflow. The response of the keratin network to this shear stress is investigated *in situ*. We track the nodes in the keratin network to deduce the dynamic behavior of the network as a function of the external shear forces. The investigation of the time tracks as well as image-to-image cross-correlations show that the network fluctuations are reduced upon the application of flow leading to a more persistent network. We conclude that cytoskeletal cross-talk between the keratin and the actin network is involved in this response to shear stress.

BP 32.9 Fri 11:45 H43

Impact of Temperature on Cell Nuclei Integrity — •Enrico Warmt, Tobias Kiessling, Roland Stange, Anatol Fritsch, and Josef Käs — Universität Leipzig, Germany

The deformation of cells in Optical Stretcher experiments is considered to be caused exclusively by the deformation of the cellular cytoskeleton. However, the visual appearance of certain cell types during the stretching process implicates events taking place in the cell organelles, especially the cell nucleus. To obtain a more detailed view into the cell we dyed the nucleus in different cell lines and stretched many cells to examine the behavior of the nucleus. At a certain laser power, we observe an abrupt restructuring of the nucleus of MCF-7 cells. This restructuring is irreversible and does not occur during a second stretch of the same cell. Interestingly, the intensity of the restructuring differs between cell lines in a highly reproducible way: While MCF-7 and HMEC show a significant restructuring, less or almost no restructuring is observed on MDA-MB-231, MDA-MB-436 and MCF-10A cells. By controlling the ambient temperature, we show that restructuring is triggered by a laser-induced increase in temperature during measurement and occurs at 45 to 55 °C. It is known that the nuclear matrix as well as the nuclear lamina is thermolabile and some proteins denature in this temperature range, which potentially causes the observed nuclear restructuring and probably leads to cell death. The underlying physical processes and the origin of the variations among cell lines have to be clarified.

BP 32.10 Fri 12:00 H43

Viscoelastic properties of differentiating blood stem cells evolve to suit their functions — •Andrew Ekpenyong[1,3], Graeme Whyte[1], Kevin Chalut[1], Stefano Pagliara[1], Chii Jou Chan[1,3], Stephan Paschke[2], Ulrich F. Keyser[1], and Jochen Guck[1,3] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, CB3 0HE, UK. — [2]Department of Surgery, University of Ulm, 89075 Ulm, Germany. — [3]Biotechnology Center, Technische Universität Dresden, 01307 Dresden, Germany

It has become clear that stem cells can alter their mechanical properties during differentiation. But understanding of the functional relevance of such alterations is incomplete. Here, we show that during the differentiation of human myeloid precursor cells into three different lineages, the cells modulate their viscoelastic properties to suit their fates and functions. Myeloid cells circulating in blood have to be advected through constrictions in blood vessels, engendering the need for compliance at short time-scales. Intriguingly, only the two circulating myeloid cell types have increased short time-scale compliance and flow better through microfluidic constrictions. Furthermore, all three differentiated cell types show a reduction in steady-state viscosity, enabling them to migrate better through tissue-like pores, compared to undifferentiated cells. Moreover, we find similar fate-specific differences in compliance between primary human CD34+ stem cells and the differentiated cells. Our results indicate that the mechanical properties of cells define their function, can be used as a differentiation marker and could serve as target for new therapies.

BP 32.11 Fri 12:15 H43

Cell plasticity is tightly linked to elastic stresses in the cytoskeleton — •Richard Gerum, Navid Bonakdar, Michael Kuhn, Achim Schilling, Anna Lippert, Marina Spörrer, Astrid Mainka, and Ben Fabry — Biophysics, University of Erlangen-Nuremberg, Erlangen, Germany

Cells show pronounced non-linear visco-elastic and visco-plastic properties under large deformations and forces. We used a high-force magnetic tweezer setup to deliver unidirectional forces of up to 30nN to fibronectin-coated magnetic beads bound to cell surface adhesion receptors. To probe cells with bidirectional forces, the cell culture plate was placed on a rotational/translational stage such that the magnetic bead remained at a constant distance to the magnetic tweezer tip after a 180° rotation. Bead displacements were measured during application of force steps (creep response) and after the force was removed (recovery response). With increasing force magnitude, the recovery became increasingly incomplete, indicating the emergence of plastic behavior. This plasticity was a constant fraction (~20%) of the total bead displacement, regardless of duration and magnitude of force application. The plastic behavior is attributable to a buildup of excess slack in the cytoskeletal fibers. The creep and the recovery response were fully characterized by a simple power-law vs. time, indicating that plastic energy dissipation during cell deformations is tightly linked to elastic stress dissipation.

BP 32.12 Fri 12:30 H43

The Power of a Flagellar Beat — •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

In the microscopic world, where inertia cannot be used for propulsion, most of our everyday strategies of self-propulsion do not work. One class of parasites that knows its way around, the flagellate Trypansoma, manage to navigate in blood, which flows a lot faster than the Trypanosomes' own propulsion velocity. There, the Trypanosomes are constantly attacked by their host's immune response. Yet, they survive and even penetrate the blood-brain-barrier, which actually should be too tight to enter. Although Trypanosomes are known for more than 100 years, their motility strategies are not completely elucidated yet. Using high-speed microscopy combined with optical tweezers in microfluidic devices and analyzing the recorded data, new light has been shed on the motility of these parasites. Our results show that Trypanosomes can be optically trapped and dragged through microfluidic devices without harming them. Once caught in an optical trap, they rotate in elaborate patterns. By analyzing the power-spectra for our high-speed image-series we have discovered two main rotation frequencies. Furthermore, we probe the impact of their chemical environment and of objects in close proximity, such as particles, red blood cells and other Trypanosomes, by analyzing their motility behaviour.

BP 32.13 Fri 12:45 H43

Hydrodynamic simulations of platelets in blood flow — •Kathrin Müller, Dmitry A. Fedosov, and Gerhard Gompper — Institute of Complex Systems , Forschungszentrum Jülich, 52425 Jülich, Germany

The bleeding through an injured vessel wall can be stopped by blocking the opening with a plug primarily formed by platelets. For an immediate response to the injury, the platelets must be located close to the vessel wall. A decrease of the volume fraction of red blood cells (hematocrit) leads to a reduced concentration of platelets near the wall. This can result in a considerable increase of the bleeding times [1]. Numerical simulations of blood flow help us better understand this complex process.

Blood flow simulations are performed in idealized geometries using the Dissipative Particle Dynamics method [2], a mesoscale hydrodynamic simulation technique. The blood is modelled as a fluid with suspended red blood cells and platelets, which are constructed using viscoelastic spring networks [3]. In order to identify the conditions

for an efficient migration of platelets towards the wall (margination), their distribution in flow is monitored with respect to hematocrit, shear rate, their shape and deformability. Furthermore, possible mechanisms which are responsible for the platelet margination will be discussed.

References
[1] Reininger, *Haemophilia* **14** (Suppl. 5), (2008)
[2] Hoogerbrugge and Koelman, *Europhys. Lett.* **19**, (1992)
[3] Fedosov, Caswell, and Karniadakis, *Biophys. J.* **98**, (2010)

BP 33: Statistical Physics in Biological Systems IV (joint with DY)

Time: Friday 9:30–12:45 Location: H44

BP 33.1 Fri 9:30 H44

Range expansions in heterogeneous environments — •Wolfram Möbius[1], Andrew W. Murray[2], and David R. Nelson[1] — [1]Department of Physics and FAS Center for Systems Biology, Harvard University, Cambridge, MA, USA — [2]FAS Center for Systems Biology and Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA, USA

How species invade new territories and how these range expansions influence a population's genetic diversity are important questions in the field of population genetics. While the majority of work addressing these questions focuses on well-mixed environments, populations on a set of islands, or spatially uniform environments, much less is known about the consequences of an expanding population encountering obstacles such as lakes or mountain ranges.

We employ both experimental and theoretical methods to better understand range expansions in such types of environments. In particular, we established a system of bacteriophage T7 and *E. coli* as a bench-scale model system: The bacteriophage population spreads on a lawn of susceptible bacteria while a region of resistant bacteria poses an obstacle to the population wave and determines its shape. We use reaction-diffusion modeling and a phenomenological description to complement the experimental results. In addition, stochastic modeling allows us to study the fate of individual alleles in the course of the range expansion.

BP 33.2 Fri 9:45 H44

Chemical Warfare and Survival Strategies in Bacterial Range Expansions — Gabriele Poxleitner[1], •Markus Felix Weber[2], Elke Hebisch[1], Erwin Frey[2], and Madeleine Leisner[1] — [1]Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, D-80539 Munich, Germany. — [2]Arnold-Sommerfeld Center for Theoretical Physics and Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 Munich, Germany.

Bacterial communities represent complex and dynamic ecological systems. Different environmental conditions as well as bacterial interactions determine the establishment and sustainability of bacterial diversity. We study the competition of three Escherichia coli strains during range expansions on agar plates. In this bacterial model system, a colicin E2 producing strain C competes with a colicin resistant strain R and with a colicin sensitive strain S for new territory. Genetic engineering allows us to tune the growth rates of the strains and to study distinct ecological scenarios. These scenarios may lead to either single-strain dominance, pairwise coexistence, or to the coexistence of all three strains. In order to elucidate the survival mechanisms of the individual strains, we developed a stochastic agent-based model to capture the ecological scenarios in silico. In a combined theoretical and experimental approach we are able to show that the level of biodiversity depends crucially on the composition of the inoculum, on the relative growth rates of the three strains, and on the effective reach of colicin toxicity.

BP 33.3 Fri 10:00 H44

Efficacy of ribosome-targeting antibiotics determined by a non-linear molecular race — •Philip Greulich[1,2], Martin R. Evans[2], and Rosalind J. Allen[2] — [1]Cavendish Laboratory, University of Cambridge — [2]School of Physics and Astronomy, University of Edinburgh

Many antibiotics in current clinical use target bacterial ribosomes. We present a dynamical model for the response of a cell to a ribosome-targeting antibiotic. In this model, the efficacy of the antibiotic is determined by a non-linear "molecular race" between binding of the antibiotic to ribosomes and net production of new ribosomes. The model points to a non-trivial growth-rate dependence of the minimum inhibitory concentration (MIC) and predicts a discontinuous transition at the MIC when the antibiotic concentration is varied: the growth rate abruptly drops to zero at this point. Furthermore, the efficacy of an antibiotic treatment depends on both its intensity and duration, and we can determine the relation to critical pharmacokinetic/-dynamic parameters for cell killing.

BP 33.4 Fri 10:15 H44

Information-theoretic vs. thermodynamic entropy production in autonomous sensory networks — •Andre Cardoso Barato and Udo Seifert — Universität Stuttgart, II. Institut für Theoretische Physik, Pfaffenwaldring 57 / III, D-70550, Stuttgart, Deutschland

Acquiring and processing information about the instantaneous state of the environment is a prerequisite for survival for any living system. Sensory and signal transducting networks have evolved to achieve this task under a variety of external conditions as, e.g., the work on bacteria like Escherichia coli has demonstrated so beautifully [1,2].

We determine the rate with which sensory networks acquire information about the changing external conditions. Comparing this rate with the thermodynamic entropy production that quantifies the cost of maintaining the network, we show that there is no universal bound restricting the rate of obtaining information to be less than this thermodynamic cost. These results obtained within a general bipartite model consisting of a stochastically changing environment that affects the instantaneous transition rates within the system are illustrated with a simple four-states model motivated by cellular sensing. On the technical level, we require and justify a new conjecture on the mutual information rate involving a non-Markovian process.

[1] H. C. Berg and M. Purcell, Biophys. J. 20, 193 (1977).
[2] G. Lan, P. Sartori, S. Neumann, V. Sourjik, and Y. Tu, Nature Phys. 8, 422 (2012).

BP 33.5 Fri 10:30 H44

Optimality principles for bacterial quorum sensing — •Bastian Drees and Ilka Bischofs — BioQuant, Center for Quantitative Analysis of Molecular and Cellular Biosystems at Heidelberg University, Heidelberg

Bacterial signaling networks have to meet the challenge of gathering information from noisy biochemical signals. We introduce a theoretical framework to quantify the accuracy of a signaling process in the presence of noise by defining the resolving power R, the minimal difference between two inputs that is required to separate two outputs. We show that many natural quorum sensing systems - which regulate cell density dependent behavior in bacteria - tend to optimize R at their switching points. We furthermore study how differences in the physical network design affect R as a function of input strength. We find different network architectures to optimize R in different input regimes, which could explain the diversity of quorum sensing architectures that is observed in nature. Together our results suggest the existence of a physics-driven optimal design principle for quorum sensing networks, which could be exploited to facilitate rational design choices in synthetic biology applications.

BP 33.6 Fri 10:45 H44

In vivo facilitated diffusion model — •Maximilian Bauer[1,2] and Ralf Metzler[1,3] — [1]Institute for Physics and Astronomy, Potsdam University, Germany — [2]Physics Department, Technical University of Munich, Germany — [3]Physics Department, Tampere University of Technology, Finland

In vitro transcription factors (TFs) alternate between three-dimensional bulk diffusion and sliding along DNA in order to quickly find their target on DNA. Recent experiments showed that also in the crowded interior of living cells TFs employ this facilitated diffusion mechanism. For a theoretical description of the situation in vivo we use a simple model of the bacterial genome embedded in an experimentally identified subvolume of the cell. Explicitly taking into account

the configuration of DNA, our findings agree with experimental results and suggest that cells operate near to conditions which are optimal for target localization.

References: M. Bauer and R. Metzler, Biophys. J. 102, 2321 (2012) and submitted (2012)

BP 33.7 Fri 11:00 H44

Random walks of bacteria: How the motility pattern affects diffusion and chemotaxis — •Johannes Taktikos[1,2], Holger Stark[2], and Vasily Zaburdaev[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Institut für Theoretische Physik, Technische Universität Berlin

The motility patterns of many bacterial species can be described with the help of random walk models. Swimming *E. coli* bacteria alternate almost straight runs with tumbling events, which randomize the direction of cell motion but keep a certain persistence. The majority of marine bacteria fully reverse their swimming direction after a tumbling event. However, the swimming strategy of the marine bacterium *V. alginolyticus* was recently discovered to consist of a strict sequence of reversal and completely randomizing flick events between the runs [Xie *et al.*, PNAS **108**, 2246 (2011)]. Remarkably, all these bacteria are capable to undergo chemotaxis – the ability to adjust their swimming direction to the concentration gradient of certain chemicals. We propose a generalized random walk model describing these motility patterns and use it to characterize the diffusion process of bacteria moving in chemically neutral environments. In the presence of a small gradient of a signaling chemical we calculate the chemotactic drift velocity along the gradient and analyze how it depends on the particular motility pattern. Our calculations show that the motility pattern alone cannot explain experimentally observed differences in the chemotactic behavior of *E. coli* and *V. alginolyticus* bacteria. This result suggests that the chemotactic internal response function of both bacteria differ.

15 min break

BP 33.8 Fri 11:30 H44

Impact of the cell division cycle on the dynamics of gene expression — •Veronika Bierbaum and Stefan Klumpp — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Am Mühlenberg 1, 14476 Potsdam

Cell growth and division are elementary processes that influcence gene expression: While proteins are being synthesized, the change in cell volume due to cell growth leads to a dilution of protein concentration. To maintain a stable amount of protein, the protein content has to be doubled during the cell cycle. In this way, upon division, each daughter cell initiates the new cycle with the same amount of each protein. Protein synthesis and cell growth are typically not synchronous, such that the protein concentration varies over the cell division cycle. This variation may have an impact on the function of gene regulatory circuits.

We have developed a theoretical description of genetic regulatory systems that explicitly considers the cell division cycle to investigate its impact onto both simple and regulated systems of gene expression. We calculate the cell-to-cell variations in protein content of cells at different stages in the division cycle, and discuss to which extent these variations contribute to the extrinsic noise observed in single-cell experiments. While positive autoregulation can amplify the variation in protein concentration over the division cycle, negative autoregulation buffers against such variation. In addition, we investigate how the variability in the concentration influences the stability phases of bistable autoregulated systems.

BP 33.9 Fri 11:45 H44

Deducing underlying mechanisms from protein recruitment data — •Laurin Lengert and Barbara Drossel — TU Darmstadt, Hessen

The technique of fluorescently labelling proteins made it possible to visualize cellular proteins and to measure their distribution and dynamics within the cell. We focus on protein recruitment to a region in the cell following a triggering event, such as irradiation. Often mechanistic models are used to fit the recruitment data. In such models, differential equations describe the changes in the concentrations of activated or bound proteins in the region of interest. The aim of such mechanistic models consists in evaluating rate constants, in identifying the proteins and reactions that are essential for the investigated process, and in obtaining evidence for processes that are not directly visible. By analyzing in a systematic way the recruitment curves generated by different simple models, we explain how the features of the recruitment curves reflect the properties of the underlying processes. This analysis also shows that a distinction between different models is not always possible from a given set of data. However, in many cases it is possible to suggest additional experiments with different protein concentrations that allow to distinguish between different models.

BP 33.10 Fri 12:00 H44

Scaling behaviour of knotted polymer rings in semidilute solutions — •Benjamin Trefz and Peter Virnau — Johannes Gutenberg Universität Mainz

Recently, the study of ring polymers and in particular their scaling behaviour in semidilute solutions [1, 2] has attracted considerable attention as a potential model system for the organization of DNA in chromosome territories. Building upon these studies, we investigate the influence of topology in melts of rings, which contain a certain knot type. These molecular dynamics simulations typically require around half a million particles as well as long run times and have been performed on graphic cards. Just like their unknotted counterparts, knotted rings form crumpled globules in the large N-limit. Knots tend to take up a large fraction of the chain for small rings, but become localized in the thermodynamic limit.

[1] J. Halverson, W. Lee, G. Grest, A. Grosberg, and K. Kremer, "Molecular dynamics simulation study of nonconcatenated ring polymers in a melt. I. Statics," The Journal of chemical physics, vol. 134, p. 204904, 2011.

[2] D. Reith, L. Mirny, and P. Virnau, "GPU Based Molecular Dynamics Simulations of Polymer Rings in Concentrated solution: Structure and Scaling," Progress of Theoretical Physics Supplement, vol. 191, pp. 135-145, 2011.

BP 33.11 Fri 12:15 H44

Molecular knots can pass through each other — •Peter Virnau and Benjamin Trefz — Uni Mainz

We propose a novel mechanism in which two molecular knots can pass through each other and effectively swap positions along a polymer strand. Associated free energy barriers in our molecular dynamics simulations only amount to a few k_BT, which may enable the interchange of knots on single DNA strands.

BP 33.12 Fri 12:30 H44

Sequence depending membrane-activity of amphiphilic polymers — •Marco Werner[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

Using the bond fluctuation model with explicit solvent we investigate self-assembled bilayer membranes interacting with random copolymers of hydrophilic/-phobic monomers under variation of the fraction of hydrophobic monomers, H. Our simulation data indicates that polymers localize at the membrane-solvent interface for values of $H \gtrsim 1/2$, where the polymer forms excess blobs in the solvent- and lipid tail phases to increase the number of preferred contacts to both environments. Excess blobs with hydrophobic majority are inhibited to freely expand in the lipid tail phase due to the self-organized packing of lipids. Therefore, the number of preferred polymer-environment contacts is balanced on both sides for values of H slightly larger than $H = 1/2$. Here, the polymer shows the largest membrane-activity as indicated by a maximum of polymer-induced permeability for solvent. Testing a larger population of random polymer sequences we demonstrate that heterogeneity of the amphiphilic components of the polymer on a scale smaller than the lipid tail length is a key feature for polymer-induced bilayer perturbations. This seems to be confirmed by testing polymers with alternating sequences with hydrophobic blocks of size smaller than the lipid tail length, for which the polymer-induced membrane permeability for solvent is larger than on average for the population of random copolymers.