

Biological Physics Division Fachverband Biologische Physik (BP)

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Overview of Invited Talks and Sessions

(lecture rooms H43 and H45; Posters B1 and B2)

Plenary Talks related to BP

PV I	Mon	8:30– 9:15	H1	Response of live cells to mechanical stress — ●SAMUEL SAFRAN
PV V	Tue	8:30– 9:15	H1	NMR and MRI: Basic Physics for the Sake of Society — ●RICHARD R. ERNST
PV X	Thu	8:30– 9:15	H1	Complex Networks: From Statistical Physics to the Cell — ●ALBERT-LASZLO BARABASI

Invited Talks

BP 2.1	Mon	10:15–10:45	H43	Probing Cellular Events with Single Quantum Dot Imaging — ●MAXIME DAHAN
BP 3.1	Mon	14:00–14:30	H43	Exciting positional control with DNA Origami: Onwards nanoscale gadgets for Science and Technology. — ●HENDRIK DIETZ
BP 4.1	Mon	14:00–14:30	H45	Nonlinear dynamics and control of migraine waves — ●MARKUS DAHLEM
BP 9.1	Tue	9:30–10:00	H43	Mechanics of Cellular Aggregates — ●FRANÇOISE BROCHARD-WYART, CHRISTOPHE CLANET, DAMIEN CUVELIER, SYLVIE DUFOUR, DAVID GONZALEZ-RODRIGUEZ, KARINE GUEVORKIAN
BP 13.1	Tue	14:00–14:30	H45	Carbon nanotubes fluids: simple or complex? — ●MATTEO PASQUALI
BP 14.1	Tue	14:00–14:30	H44	Stochasticity and specificity in DNA repair — ●THOMAS HÖFER, MARTIJN LUIJSTERBURG, GESA VON BORNSTAEDT, ROEL VAN DRIEL
BP 21.1	Wed	14:00–14:30	H43	Deconstructing hearing: mechanisms and molecules — BJÖRN NADROWSKI, THOMAS EFFERTZ, ●MARTIN GÖPFERT
BP 23.1	Thu	10:00–10:30	H43	Single-molecule Fluorescence Studies of RNA Folding and Function — ●GERD ULRICH NIENHAUS
BP 26.1	Thu	14:00–14:30	H43	Molecular misfolding investigated by mechanically unzipping nucleic acids — ●FELIX RITORT
BP 37.1	Fri	10:00–10:30	H43	Pearls and Feathers: New Concepts and Inspiration for Plant's Design — ●INGRID WEISS, EDUARD ARZT, HELMUT KIRCHNER

Invited talks of the joint symposium SYMR

See SYMR for the full program of the Symposium.

SYMR 4.1	Tue	9:30–10:00	H1	NMR with a Magnetic Resonance Force Microscope — ●BEAT H. MEIER, KAI EBERHARDT, JOSS ROSMARIE, TOMKA IVAN
SYMR 4.2	Tue	10:00–10:30	H1	Probing Novel Electronic States in Strongly Correlated Electron Materials Using NMR and NQR — ●NICHOLAS CURRO
SYMR 4.3	Tue	10:30–11:00	H1	Interplay of Structure and Dynamics in Macromolecular and Supramolecular Systems as Revealed by NMR Spectroscopy — ●HANS WOLFGANG SPIESS
SYMR 4.4	Tue	11:15–11:45	H1	Big times for small NMR — ●BERNHARD BLÜMICH
SYMR 4.5	Tue	11:45–12:15	H1	Traveling-Wave MRI — ●KLAAS PRÜSSMANN

SYMR 4.6 Tue 12:15–12:45 H1 **Life on the Edge: The Origins and Proliferation of Protein Misfolding Diseases** — •CHRISTOPHER M. DOBSON

Invited talks of the joint symposium SYMM

See SYMM for the full program of the Symposium.

SYMM 1.1 Wed 9:30–10:00 H1 **Magnetic resonance imaging: an ongoing success story** — •JENS FRAHM
 SYMM 1.2 Wed 10:00–10:30 H1 **Biomedical nanomagnetism: A spin through new possibilities** — •KANNAN KRISHNAN
 SYMM 1.3 Wed 10:30–11:00 H1 **Recent SQUID applications in medicine** — •HANS KOCH
 SYMM 1.4 Wed 11:00–11:30 H1 **Biomedical Magnetic Resonance using Hyperpolarized Gases and Liquids** — •LAURA SCHREIBER
 SYMM 1.5 Wed 11:30–12:00 H1 **Recent Developments in Healthcare Biomagnetics** — •QUENTIN PANKHURST
 SYMM 1.6 Wed 12:00–12:30 H1 **SQUIDS for Noninvasive Magnetogastrography** — •ALAN BRADSHAW, LEO CHENG, ANDREW PULLAN, WILLIAM RICHARDS

Invited talks of the joint symposium SYAT

See SYAT for the full program of the Symposium.

SYAT 1.1 Wed 14:30–15:00 H1 **Aging, ergodicity breaking and universal fluctuations in continuous time random walks: Theory and (possible) experimental manifestations** — •IGOR SOKOLOV
 SYAT 1.2 Wed 15:00–15:30 H1 **Distinguishing anomalous from simple diffusion in crowded solutions and in cells with fluorescence correlation spectroscopy** — •CECILE FRADIN, DANIEL BANKS, SHYEMAA SHEHATA, FELIX WONG, ROBERT PETERS
 SYAT 1.3 Wed 15:30–16:00 H1 **Exploring Diffusion in Nanostructured Systems with Single Molecule Probes: From Nanoporous Materials to Living Cells** — •CHRISTOPH BRÄUCHLE
 SYAT 2.1 Wed 16:30–17:00 H1 **The Lorentz model: a paradigm of anomalous transport** — •FELIX HÖFLING
 SYAT 2.2 Wed 17:00–17:30 H1 **Viscoelastic subdiffusion: from anomalous to normal** — •IGOR GOYCHUK
 SYAT 2.3 Wed 17:30–18:00 H1 **Phase transitions, liquid micro-compartments, and embryonic patterning** — •CLIFFORD BRANGWYNNE, JÖBIN GHARAKHANI, ANTHONY HYMAN, FRANK JÜLICHER

Sessions

BP 1.1–1.10 Mon 10:15–13:00 H45 **Statistical Physics of Biological Systems I (joint BP, DY)**
 BP 2.1–2.9 Mon 10:15–13:00 H43 **New Technologies**
 BP 3.1–3.9 Mon 14:00–16:45 H43 **DNA, RNA and Associated Enzymes**
 BP 4.1–4.10 Mon 14:00–17:00 H45 **Statistical Physics of Biological Systems II (joint BP, DY)**
 BP 5.1–5.41 Mon 17:15–20:00 Poster B1 **Posters: Biopolymers and Biomaterials**
 BP 6.1–6.11 Mon 17:15–20:00 Poster B1 **Posters: DNA and DNA Enzymes**
 BP 7.1–7.11 Mon 17:15–20:00 Poster B1 **Posters: Biological Machines, Motor Proteins**
 BP 8.1–8.6 Tue 9:30–12:45 H1 **SYMR: Nuclear Magnetic Resonance: From Applications in Condensed Matter Physics to New Frontiers**
 BP 9.1–9.11 Tue 9:30–12:45 H43 **Physics of Cells I**
 BP 10.1–10.5 Tue 9:30–11:00 H44 **Evolutionary Game Theory I (joint SOE, BP)**
 BP 11.1–11.5 Tue 11:15–12:30 H44 **Evolutionary Game Theory II (joint SOE, BP)**
 BP 12.1–12.10 Tue 13:45–16:15 H48 **Nuclear Magnetic Resonance: Frontiers and Applications (joint CPP, BP)**
 BP 13.1–13.8 Tue 14:00–16:30 H45 **Nanoparticles and Viruses**
 BP 14.1–14.7 Tue 14:00–16:00 H44 **Evolutionary Game Theory III (joint SOE, BP)**
 BP 15.1–15.9 Tue 14:30–17:00 H43 **Physics of Cells II**
 BP 16.1–16.6 Wed 9:30–12:30 H1 **SYMM: Magnetism and Medicine**
 BP 17.1–17.6 Wed 9:30–11:00 H38 **Anomalous Transport I (joint BP, DY)**
 BP 18.1–18.7 Wed 11:15–13:15 H38 **Anomalous Transport II (joint BP, DY)**

BP 19.1–19.10	Wed	10:00–12:45	H43	Membranes and Vesicles
BP 20.1–20.9	Wed	10:15–12:45	H44	Networks: From Topology to Dynamics I (joint DY, BP, SOE)
BP 21.1–21.10	Wed	14:00–17:00	H43	Neurobiophysics and Sensory Transduction
BP 22.1–22.1	Thu	9:30–10:15	H44	Networks: From Topology to Dynamics II (joint DY, BP, SOE)
BP 23.1–23.10	Thu	10:00–13:00	H43	Biopolymers
BP 24.1–24.10	Thu	10:15–13:00	H44	Networks: From Topology to Dynamics III (joint DY, BP, SOE)
BP 25.1–25.5	Thu	11:00–12:45	H45	Focus: Charge Effects in Soft and Biological Matter I (joint CPP, BP, ST)
BP 26.1–26.11	Thu	14:00–17:15	H43	From Single-Molecule to Tissue Dynamics
BP 27.1–27.7	Thu	14:00–16:00	H44	Networks: From Topology to Dynamics IV (joint DY, BP, SOE)
BP 28.1–28.12	Thu	14:00–17:45	H37	Focus: Charge Effects in Soft and Biological Matter II (joint CPP, BP, ST)
BP 29.1–29.9	Thu	14:30–17:00	H45	Biomolecular Spectroscopy
BP 30.1–30.5	Thu	16:00–17:15	H44	Networks: From Topology to Dynamics V (joint DY, BP, SOE)
BP 31.1–31.18	Thu	17:15–20:00	Poster B1	Posters: Membranes and Vesicles
BP 32.1–32.49	Thu	17:15–20:00	Poster B1	Posters: Physics of Cells
BP 33.1–33.7	Thu	17:15–20:00	Poster B1	Posters: Neurobiophysics
BP 34.1–34.16	Thu	17:15–20:00	Poster B2	Posters: New Technologies
BP 35.1–35.15	Thu	17:15–20:00	Poster B2	Posters: Statistical Physics, Evolution, and Networks
BP 36.1–36.11	Thu	17:15–20:00	Poster B2	Posters: Tissue Dynamics, Charge Effects, and Anomalous Transport
BP 37.1–37.10	Fri	10:00–13:00	H43	Biomaterials
BP 38.1–38.6	Fri	10:15–12:00	H45	Focus: Charge Effects in Soft and Biological Matter III (joint CPP, BP, ST)

Annual General Meeting of the Biological Physics Division

Wednesday 18:30–19:30 H45

- Bericht
- Verschiedenes

BP 1: Statistical Physics of Biological Systems I (joint BP, DY)

Time: Monday 10:15–13:00

Location: H45

Invited Talk

BP 1.1 Mon 10:15 H45
Noise during rest enables the exploration of the brain's dynamic repertoire — ●VIKTOR JIRSA — Theoretical Neuroscience Group CNRS, ISM UMR6233, Marseille Luminy, France

At rest certain cortical regions of the human brain consistently show temporally coherent activity. In humans, these resting state networks have been shown to greatly overlap with functional architectures present during consciously directed activity, which motivates the interpretation of rest activity as day dreaming, free association, stream of consciousness, and inner rehearsal. Here, we show that comparable resting state networks emerge from a stability analysis of the network dynamics using biologically realistic primate brain connectivity, although anatomical information alone does not identify the network. We specifically demonstrate that noise and time delays via propagation along connecting fibres are essential for the emergence of the coherent fluctuations at rest. The combination of anatomical structure and time delays creates a space-time structure of the couplings in which the neural noise enables the brain to explore various functional configurations representing its dynamic repertoire.

BP 1.2 Mon 10:45 H45
Constrained Branching Random Walks as a minimal model for adaptive evolution — ●OSKAR HALLATSCHKEK — Biologische Physik und Evolutionäre Dynamik, MPI DS, Goettingen

Models of both sexual and asexual adaptation in well-mixed populations usually lead to solitary waves of adaptation. This means that the fitness distribution of the population assumes the form of a wave and moves to higher fitness at a certain speed of adaptation. This nonequilibrium steady state is easy to obtain in simulations but usually hard to analyze due to lack of detailed balance. Here, we introduce an analytically tractable minimal model that captures the essence of fitness waves of adaptation: i) a branching random walk of genotypes. ii) a global constraint that keeps the populations size finite. We show that for certain constraints an exact solution can be found. This exact solution, which can be summarized as a deterministic PDE with a peculiar cutoff, also turns out to approximate conventional models of adaptation in an unprecedented accuracy.

BP 1.3 Mon 11:00 H45
The number of adaptive paths in fitness landscapes with sign epistasis — ●JASPER FRANKE¹, ALEXANDER KLOEZER¹, JOACHIM KRUG¹, and J. ARJAN G.M. DE VISSER² — ¹Institut für Theoretische Physik, Universität zu Köln — ²Laboratory of Genetics, Wageningen University

A mutation of an organism's (genotypic or phenotypic) configuration has a higher probability of becoming fixed in the population if it increases the mutant's degree of adaptation to the environment (the organism's 'fitness'). A sequence of fitness-improving mutations forms an adaptive path along which the population can evolve. This concept of accessible paths plays an important role in determining the possible configurations that can be reached by evolutionary adaptation.

Since the mapping from configuration to fitness is biochemically only partially understood, several statistical models have been proposed trying to capture the essential features.

In this contribution, we consider the expected number of accessible paths and the probability of not having any accessible paths at all. We present analytic and numerical results for three statistical models for fitness landscapes and compare these results to data for the fitness landscape of the fungus *Aspergillus niger*.

BP 1.4 Mon 11:15 H45
Active Transport on Biological Networks — ●INES-KRISTIN WEBER¹, PHILIP GREULICH^{1,2}, and LUDGER SANTEN¹ — ¹Department of Theoretical Physics, Saarland University, 66041 Saarbrücken — ²Department of Theoretical Physics, Cologne University, 50937 Cologne

Active transport processes are vital for living cells. They are used, e.g. for structure formation, cell signaling and motion of cells. An large number of transport processes is carried out by molecular motors, i.e. specialized proteins that are able carry cargo along the cytoskeleton. The cytoskeleton is an inhomogeneous network of polar filaments which determines the cell shape and guides the motion of molecular motors.

In this work we investigate the relation between network structure and dynamics of molecular motors, whereat we consider computer generated filament networks as well as realistic structures of the cytoskeleton. The real cytoskeleton structures are obtained from light microscopy images which are preprocessed by automated image analysis procedures to localize fluorescent marked microtubules. Molecular motors are modeled as stochastic self-driven particles. By means of computer simulations and a phenomenological approach we investigate the formation of clusters on the different kinds of networks. We observe cluster formation at all size scales, even for small particle densities [1].

[1] P. Greulich, L. Santen, arXiv:0904.3890v1

BP 1.5 Mon 11:30 H45
Estimating molecule numbers based on fluctuations — ●ANDREAS RUTTOR and MANFRED OPPER — Technische Universität Berlin

Microarray experiments and other methods used to analyze biochemical systems are often not calibrated, so that results are given in arbitrary units. In this case the actual amount of molecules involved in the reactions remains unknown. However, fluctuations visible in the data set can be used to estimate it. For that purpose we use a diffusion model based on stochastic differential equations, which describe the dynamics of the reaction system. Here, two sources of fluctuations have to be taken into account: Observation noise, caused by the measurement process, is usually independent of the state of the system. But internal noise is the result of discrete reaction events occurring at random points in time. Therefore its size is directly related to the number of molecules per arbitrary unit, which is included in the model as a parameter. By solving the backward Fokker-Planck equation of the diffusion model in the weak noise limit, it is possible to calculate the likelihood of all observations. Maximizing this quantity with respect to the parameters leads to an estimate of the molecule numbers per arbitrary unit. Additionally, the uncertainty of this calibration can be obtained by calculating the Laplace approximation of the marginal posterior distribution.

BP 1.6 Mon 11:45 H45
Clustering in self-propelled particle systems — ●FERNANDO PERUANI¹ and MARKUS BAER² — ¹Service de Physique de l'Etat Condense, CEA Saclay, 91191 Gif-sur-Yvette, France — ²Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

Self-propelled particle systems exhibit a rich irreversible clustering dynamics. Independently of the initial condition, these systems reach a steady state cluster size distribution which depends on particle density and noise intensity. We show that the aggregation process can be described by a set of Smoluchowski equations whose functional form is independent of the symmetry of the velocity alignment rule or interaction forces. For a given density (noise intensity) there is always a critical noise intensity (density) at which the cluster size distribution becomes critical, with a exponent 4/3. Below the critical point, the cluster size distribution is exponential and the system exhibits a characteristic cluster size. Above the critical point, the cluster size distribution can be well fitted by a power-law with a second peak at large cluster sizes. The exponent of the power-law is a function of the noise intensity, resp. of particle density.

BP 1.7 Mon 12:00 H45
A Colloidal Approach to Protein Adsorption — ●OLAF LEIDINGER and LUDGER SANTEN — Fachrichtung Theoretische Physik, Universität des Saarlandes

We investigate the unspecific adsorption of proteins, which are modeled as polydisperse colloidal particles. The particle-particle interactions are described in the framework of the DLVO theory, including steric repulsion, electrostatic and van der Waals interactions. Furthermore we introduce internal degrees of freedom representing different conformations of the model proteins at the surface.

By means of extensive Monte Carlo simulations we reproduce the experimentally observed characteristics of the biofilm-formation[1,2]. The adsorption kinetics can be divided into three intervals: Initially the adsorption is limited by the flux of particles to the surface. At low concentrations the proteins spread at the surface in order to opti-

mize the binding to the surface. At higher concentrations the adsorbed proteins are compacted due to particle-particle interactions and finally the surface coverage saturates. These dynamical regimes can be identified in experimental and theoretical investigations of the adsorbed amount. The comparison between experimentally and theoretically generated biofilms is completed by a detailed analysis of the point patterns connected to the adsorbed particles, which is carried out by means of integral measures.

[1] A. Quinn et al 2008 EPL 81 56003 (6pp)

[2] M Bellion et al 2008 J. Phys.: Condens. Matter 20 404226 (11pp)

BP 1.8 Mon 12:15 H45

All-or-none protein-like folding transition of a flexible homopolymer chain — ●WOLFGANG PAUL¹, MARK TALOR², and KURT BINDER³ — ¹Institut für Physik, Martin-Luther-Universität, 06099 Halle — ²Department of Physics, Hiram College, Hiram, Ohio 44234, USA — ³Institut für Physik, Johannes-Gutenberg-Universität, 55099 Mainz

We report a first-order all-or-none transition from an expanded coil to a compact crystallite for a flexible polymer chain. Wang-Landau sampling is used to construct the complete density of states for square-well chains up to length 256. Analysis within both the microcanonical and canonical ensembles shows a direct freezing transition for finite length chains with sufficiently short-range interactions. This type of transition is a distinctive feature of "one-step" protein folding and our findings demonstrate that a simple homopolymer model can exhibit protein-folding thermodynamics. We also discuss how this finding depends on the range of the attractive interaction. Chains assume an expanded coil conformation at high temperatures and a crystallite structure at low temperatures. For large well diameters, with decreasing temperature a chain undergoes a continuous coil-globule (collapse) transition followed by a discontinuous globule-crystal (freezing) transition. For small well diameters the collapse transition is preempted by the freezing transition and thus there is a direct first-order coil-crystal phase transition.

BP 1.9 Mon 12:30 H45

Genome Folding at the 30 nm Scale — ●PHILIPP M. DIESINGER¹ and DIETER W. HEERMANN² — ¹Institute of Theoretical Physics, Heidelberg, Germany / MIT, Cambridge, USA — ²Institute of Theoretical Physics, Heidelberg

We present a Monte Carlo model for genome folding at the 30-nm scale

with focus on linker-histone and nucleosome depletion effects. Depletion of linker histones and nucleosomes affects, massively, the flexibility and the extension of chromatin fibers. Increasing the amount of nucleosome skips can lead either to a collapse or to a swelling of chromatin fibers. We show that depletion effects may even contribute to chromatin compaction. Furthermore, we find that predictions from experimental data for the average nucleosome skip rate lie exactly in the regime of maximum chromatin compaction.

We determine the nucleosome pair distribution function of chromatin. We show that chromatin nanostructure might in principle be accessible by 2D high-resolution light microscopy: Our simulations show that even in the case of fibers with depletion effects and after a projection, the main dominant peaks can still be identified.

Furthermore, we compare our simulations with 5C data of a gene desert as well as FISH data and find that only fibers with random depletion of linker histones or nucleosomes can explain the probability of random chromatin contacts on small length scales that play an important role in gene regulation. Missing linker histones and nucleosomes might not just be randomly occurring simple unavoidable defects but instead they might even play a regulatory role in gene expression.

BP 1.10 Mon 12:45 H45

Statistical aspects of trypanosome's motility — ●VASILY ZABURDAEV^{1,2}, SRAVANTI UPPALURI³, THOMAS PFOHL^{3,4}, MARKUS ENGSTLER⁵, HOLGER STARK², and RUDOLF FRIEDRICH⁶ — ¹Harvard University, Cambridge, USA — ²Technical University of Berlin, Berlin, Germany — ³MPI for Dynamics and Self-Organization, Göttingen, Germany — ⁴University of Basel, Basel, Switzerland — ⁵University of Würzburg, Würzburg, Germany — ⁶University of Münster, Münster, Germany

Trypanosome is a parasite causing the sleeping sickness. The way it moves in the blood stream and penetrates various obstacles is the area of active research. Our goal was to investigate a free trypanosomes' motion in the planar geometry. Our analysis of trypanosomes' trajectories reveals that there are two correlation times - one is associated with a fast motion of its body and the second one with a slower rotational diffusion of the trypanosome. We propose a system of Langevin equations to model such motion. One of its peculiarities is the presence of multiplicative noise predicting higher level of noise for higher velocity of the trypanosome. Theoretical and numerical results give a comprehensive description of the experimental data such as the mean squared displacement, velocity distribution and auto-correlation function.

BP 2: New Technologies

Time: Monday 10:15–13:00

Location: H43

Invited Talk

BP 2.1 Mon 10:15 H43

Probing Cellular Events with Single Quantum Dot Imaging — ●MAXIME DAHAN — Ecole normale supérieure, Paris, France

In the past years, experiments on membrane molecules have demonstrated the potential of single quantum dot (QD) tracking to decipher the dynamics of complex events and to study biochemical reactions at the single molecule level, directly in live cells. Here I will discuss the principles, methods and challenges of single QD tracking. In particular, I will present our current effort to go beyond membrane dynamics and make QD imaging a standard imaging technique in cell biology. First, I will discuss how QDs can be internalized into live cells, how their colloidal properties affect their intracellular behavior and how QDs can be targeted to specific biomolecules or organelles. Next, I will show the results of recent experiments on the motion of molecular motors kinesin and myosin V in the cytoplasm of live cells. These experiments give access to important parameters such as the velocity, the processivity or stepping characteristics of the motor, directly in its cellular environment. Finally, I will present the challenges that need to be met to improve the properties of QDs as biological probes and the strategies that we are implementing to prepare small functional nanoparticles with controlled valency using peptide-coated QDs. Overall, the combination of tracking measurements, single-molecule counting methods and emerging high-resolution imaging techniques offer exciting possibilities to probe the composition, structure and dynamics of supramolecular assemblies in live cells.

BP 2.2 Mon 10:45 H43

Near-fields in Fluorescence Microscopy - Absolute Determination of z-positions in the Nanometer Range — ●MICHAEL BERNDT¹, MIKE LORENZ¹, JÖRG ENDERLEIN², and STEFAN DIEZ¹ — ¹Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany — ²III. Institute of Physics, Georg-August-University, Göttingen, Germany

Typical processes in molecular biology take place on a nanometer range and are too small to be resolved by conventional light microscopy. To though reveal information from such systems, techniques are required which access information on the nanometer scale. Here, we present a novel near-field based method to precisely determine absolute heights on the length scale of 0-100 nm above surfaces. We make use of distance dependent quenching processes fluorophores undergo in the proximity to conductive interfaces and measure the influence on the fluorescence lifetime by wide-field fluorescence lifetime imaging microscopy [1]. We use theoretical computations based on the CPS theory to scale the determined lifetimes to absolute heights [2]. We apply our method to fluorescently labeled microtubules elevated to different heights by several spacer molecules. Hence we demonstrate a technique to measure molecule geometries with nanometer precision.

References: [1] M. Lorenz, RNA 15, 97-103 (2009), [2] R.R. Chance, A. Prock, R. Silbey, Advances in Chemical Physics XXXVII, 1-65 (1978)

BP 2.3 Mon 11:00 H43

Robust measurement of diffusion with scanning FCS — ●ZDENĚK PETRÁŠEK, SUSAN DERENKO, and PETRA SCHWILLE —

Biophysics group, Biotechnologisches Zentrum, Technische Universität Dresden, Tatzberg 47/49, 01307 Dresden, Germany

We present a simple modification of Fluorescence Correlation Spectroscopy (FCS), where the position of the measurement volume is not stationary, but is scanned along a circle of a diameter comparable to the volume size. The known scan radius serves as an internal spatial standard, meaning that the exact volume size need not be known to determine the diffusion coefficient. In this way the method gains robustness against optical distortions that may uncontrollably enlarge the measurement volume, or affect its shape.

The oscillations, introduced into the measured correlation curve by scanning, favourably constrain the fit of a model to the data. Therefore, a relatively narrow range of the autocorrelation is sufficient to obtain a stable fit. Consequently, the correlation values at short lag times, that may be influenced by complicated photophysics of the dye or suffer from a poor signal-to-noise ratio, or the values at long correlation times, that may be affected, for example, by depletion due to photobleaching, can be excluded from the analysis, contributing to the robustness of the method.

The implementation of scanning FCS based on a two-dimensional piezo scanner has been applied to studies both in bulk solution and on surfaces — supported lipid bilayers and giant unilamellar vesicles.

BP 2.4 Mon 11:15 H43

Which parameters influence resolution in optical sub-diffraction imaging? — •THORBEN CORDES^{1,2}, CARSTEN FORTHMANN¹, CHRISTIAN STEINHÄUER¹, JAN VOGELSANG¹, and PHILIP TINNEFELD¹ — ¹Applied Physics - Biophysics, LMU München, Amalienstr. 54, 80799 München, Germany — ²Biological Physics Research Group, Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX1 3PU, United Kingdom

In this contribution we will discuss imaging resolution of recently developed superresolution approaches from two different perspectives: (i) At first we reconsider those factors that are actually responsible for the achievable resolution limit of all superresolution techniques - either using subsequent localization of single-fluorophores (STORM, PALM)[1] or targeted readout (STED, SSIM)[1] - by incorporating the photostability of the emitter. (ii) In a second step we experimentally investigate the dependence between resolvable fluorophore density and photophysical parameters that determine the actual imaging speed in a method termed Blink-Microscopy[2]. We therefore employed single-molecule cut-and-paste[3], a method that enables molecule-by-molecule assembly of structures with features below the diffraction limit. Then complex or regular structures with patterns below the diffraction limit were used as calibration structures to characterize how parameters, such as the ON/OFF-time ratio, influence resolution and imaging speed. References: [1] S. W. Hell, *Nature Methods* 6 (2009) 24-31. [2] C. Steinhäuer, et al. *JACS* 130 (2008) 16840-16841. [3] S. K. Kufer, et al. *Science* 319 (2008) 594-596.

15 min. break

BP 2.5 Mon 11:45 H43

A Pore-Cavity-Pore Nanodevice to Trap and Optically Investigate Single Molecules — •MARTIN LANGECKER, DANIEL PEDONE, and ULRICH RANT — Walter Schottky Institut, TU München

Single engineered nanopores in solid state membranes have attracted broad attention in recent years as a tool to study single biological molecules like DNA or proteins. Here we introduce a novel solid-state device which comprises two stacked nanopores defining the in- and outlet of a pico liter cavity. This pore-cavity-pore (PCP) architecture allows for the electrical as well as optical examination of single molecules. The PCP device is fabricated by structuring nanopores into a sandwich SiN/Si/SiN wafer using e-beam lithography, wet chemical etching, and feedback controlled electrochemical etching steps. The in- and outlet nanopores of the fabricated PCP-devices are characterized by transmission electron microscopy, evidencing that the pore diameters may be controlled independently down to 10 nm. Through electric potential control we are able to inject and eject nano-objects into and out of the device. We present fluorescence experiments of single DNA molecules and nm-sized polystyrene beads inside the PCP device. We study the potential-dependent loading and unloading of the cavity with 40 nm fluorescently labeled beads and analyze the diffusion of single particles within the cavity by particle tracking. We find that the apparent diffusion coefficients inside the cavity deviate from values obtained for free diffusion in solution and correlate the deviation with

the confinement effect of the cavity. Moreover, we present experiments showing the trapping and translocation of fluorescently labeled DNA.

BP 2.6 Mon 12:00 H43

Scanning Ion Conductance Microscopy vs. Atomic Force Microscopy in Cell Imaging — •JOHANNES RHEINLAENDER and TILMAN E. SCHÄFFER — Lehrstuhl für Angewandte Physik, Universität of Erlangen-Nürnberg, Staudtstr. 7, Bau A3, 91058 Erlangen, Deutschland

We performed a direct comparison of AFM and SICM by imaging the same fibroblast cell with both techniques in series. We thereby show the advantages and disadvantages of both techniques with respect to topography imaging of soft samples. The finite imaging force applied to the cell by the AFM tip causes vertical and lateral cell indentations, which we analyzed quantitatively. SICM imaging, on the other hand, is based on a non-contact imaging mechanism and provides true topography data. We show that thin, loosely-bound filopodia can be imaged with SICM at high resolution.

Rheinlaender, J. and T.E. Schäffer, *J. Appl. Phys.*, 2009. 105(9): p. 094905

BP 2.7 Mon 12:15 H43

Quantitative biological imaging by ptychographic x-ray diffraction microscopy — •KLAUS GIEWEKEMEYER¹, PIERRE THIBAUT², SEBASTIAN KALBFLEISCH¹, ANDRÉ BEERLINK¹, CAMERON M. KEWISH³, MARTIN DIEROLF², FRANZ PEIFFER², and TIM SALDITT¹ — ¹Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, Germany — ²Department Physik (E17), Technische Universität München, Garching, Germany — ³Paul Scherrer Institut, Villigen PSI, Switzerland

Mesoscopic structures with specific functions are abundant in many cellular systems and have been well characterized by electron microscopy in the past. However, the quantitative study of the three-dimensional structure and density of subcellular components remains a difficult problem.

In this contribution we show how these limitations could be overcome in the future by the application of recently introduced and now rapidly evolving coherent x-ray imaging techniques for quantitative biological imaging on the nanoscale. More specifically, we report on a recent scanning (ptychographic) diffraction experiment on unstained and unsliced freeze-dried cells of the bacterium *Deinococcus radiourans* using only a pinhole as beam defining optical element [1]. As a result quantitative density projections well below optical resolution have been achieved. [1] Giewekemeyer et al. *PNAS* (2009), in press.

BP 2.8 Mon 12:30 H43

The Nanofocus Endstation of the MiNaXS Beamline at PETRA III — •CHRISTINA KRYWKA¹, STEPHAN ROTH², RALPH DÖHRMANN², and MARTIN MÜLLER³ — ¹Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstraße 19, D-24098 Kiel — ²DESY, Notkestraße 85, D-22603 Hamburg — ³GKSS Forschungszentrum Geesthacht, Max-Planck-Straße 1, D-21502 Geesthacht

The former PETRA storage ring of DESY (Hamburg) was refurbished into PETRA III, one of the most brilliant x-ray sources worldwide. All beamlines of the new 3rd generation synchrotron radiation source are currently in their final state of completion.

The Micro- and Nanofocus X-ray Scattering beamline (MiNaXS) is equipped with two endstations, out of which the farthest is designed to provide a high flux, monochromatic x-ray beam (8-25 keV) focused to a size of about 100nm * 100nm.

Due to the low divergent, sub-micron sized focus experiments with a superior spatial resolution and a flux sufficiently high to study both biological and synthetic materials will very soon become routinely available for nanodiffraction experiments at this endstation of MiNaXS.

This contribution presents the current status of the nanofocus endstation and future extensions. Along with the latest commissioning measurements exemplary and potential applications of nanofocused x-rays are shown. Their applicability to life and materials science is demonstrated on the basis of the availability of high flux density and coherence; both being key-features of the new PETRA III source.

BP 2.9 Mon 12:45 H43

Programmable Lab on a Chip System for single cell analysis — •STEFAN THALHAMMER¹ and ACHIM WIXFORTH² — ¹Helmholtz Zentrum München, Institut für Strahlenschutz, Ingolstädter Landstrasse 1, 85764 Neuherberg — ²Universität Augsburg, Experimental

Physik I, Universitätsstrasse 1, 86159 Augsburg

The collection, selection, amplification and detection of minimum genetic samples became a part of everyday life in medical and biological laboratories, to analyze DNA-fragments of pathogens, patient samples and traces on crime scenes. Here, a multifunctional programmable Lab-on-a-Chip driven by nanofluidics and controlled by surface acoustic waves (SAW) is presented. This system combines serial DNA-isolation-, amplification- and array-detection-process on a modified glass-platform. The fluid actuation is controlled via SAW by interdigital transducers implemented in the chemical modified chip surface.

The chemical surface modification allows fluid handling in the sub-microliter range. Minute amount of sample material is extracted by laser-based microdissection out of e.g. histological sections at the single cell level. A few picogram of genetic material are isolated and transferred via a low-pressure transfer system (SPATS) onto the chip. Subsequently the genetic material inside single droplets, which behave like "virtual" beaker, is transported to the reaction and analysis centers on the chip surface via surface acoustic waves, mainly known as noise dumping filters in mobile phones. At these "biological reactors" the genetic material is processed, e.g. amplified via polymerase chain reaction methods, and genetically characterized.

BP 3: DNA, RNA and Associated Enzymes

Time: Monday 14:00–16:45

Location: H43

Invited Talk

BP 3.1 Mon 14:00 H43

Exciting positional control with DNA Origami: Onwards nanoscale gadgets for Science and Technology. — ●HENDRIK DIETZ — Laboratory for Biomolecular Nanotechnology, Physik Dept, Technische Universität München - Garching, Germany

Scaffolded DNA Origami (1) is a molecular self-assembly method that enables folding a multiple-kilobase 'back-bone' DNA molecule into complex nanoscale shapes by introducing interactions between different segments on the backbone molecule. Interaction patterns are expressed by sets of synthetic 'staple' molecules that are added to the much longer back-bone molecule. Based on this concept we have developed a general approach to the construction of custom three-dimensional shapes that can be conceptualized as creating custom-crossection bundles of DNA double helices (2) where the number, arrangement, and lengths of helices can be freely designed. We further enabled building yet more sophisticated shapes that also twist and bend in desired ways (3). Importantly, DNA origami retains spatial registry over each of thousands of DNA bases that are installed in a constructed shape. These methods thus afford truly unique positional control on the nanoscale. Our current efforts are now centered around taking advantage of this positional control in the form of nanoscale "gadgets" for applications in the molecular biosciences.

(1) PWK Rothmund: NATURE 2006

(2) SM Douglas, H Dietz, T Liedl, B Hogberg, F Graf, W Shih: NATURE 2009

(3) H Dietz, SM Douglas, W Shih: SCIENCE 2009

BP 3.2 Mon 14:30 H43

Effect of DNA sequence variation on the dynamics of backtracking during RNA transcription — ●ABIGAIL KLOPPER^{1,2}, JUSTIN BOIS^{1,2}, and STEPHAN GRILL^{1,2} — ¹Max Planck Institute for the Physics of Complex Systems — ²Max Planck Institute of Molecular Cell Biology and Genetics

The transcription of information encoded in the genome is facilitated by RNA polymerase, a macromolecular machine which steps along a DNA template, assembling and extruding a complementary RNA transcript. The process is typically marked by pausing events which have been linked to an inactive backtracked state, involving diffusive excursions of the polymerase along the template. In this state, the polymerase cannot elongate the RNA transcript, and productive synthesis only resumes once the polymerase has realigned with the RNA, effectively stepping out of the backtrack. Inability to recover can lead to cleavage of the transcript or termination of the process. We investigate the notion that sequence variation along the template influences the average time required for unassisted recovery. We perform simulations and numerical calculations using a hopping model with DNA sequence-specific transition rates. Motivated by results from single molecule experiments in which the polymerase is subject to mechanical force, we compute the sequence-averaged distribution of force-dependent pause recovery times. We show that DNA sequence variation rescales the distribution associated with a simple random walk and renders the polymerase less sensitive to the applied force.

BP 3.3 Mon 14:45 H43

Transcription of ribosomal RNA - a central task for rapid bacterial growth — ●STEFAN KLUMPP¹ and TERENCE HWA² — ¹Max-Planck-Institut fuer Kolloid- und Grenzflaechenforschung, 14424 Potsdam — ²Center for Theoretical Biological Physics, UC San Diego, La Jolla CA, USA

Synthesis of ribosomes is essential for rapid cell growth and fast growing cells, from bacteria to cancer cells, devote a substantial fraction of their transcriptional activity to making ribosomal RNA (rRNA). Transcription of rRNA is typically characterized by dense traffic of RNA polymerases (RNAPs) along the rRNA genes, very different from the typical situation for mRNA-encoding genes, which have low transcription rates. As dense traffic is susceptible to traffic jams which may arise inevitably due to stochastic pausing of the polymerases, we asked whether there are specific constraints that govern transcription in a dense traffic situation. This perspective allows us to propose novel functions for termination/antitermination systems in bacterial rRNA transcription [1]. More general, the theoretical analysis of rRNA synthesis from a "traffic viewpoint" provides a unique perspective towards the physiological constraints and regulatory principles governing ribosome synthesis in bacterial and eukaryotic cells [1,2].

[1] S. Klumpp and T. Hwa PNAS 105, 18159 (2008)

[2] S. Klumpp and T. Hwa RNA Biol. 6, 392 (2009)

BP 3.4 Mon 15:00 H43

Human Telomeric Quadruplex Conformations studied by pulse EPR — MYKHAILO AZARKH, SINGH VIJAY, HARTIG JÖRG, and ●DRESCHER MALTE — University of Konstanz, 78457 Konstanz, Germany

The Emmy-Noether group at the department of Physical Chemistry in Konstanz is engaged in developing and applying methods in Electron Paramagnetic Resonance (EPR) to study structure and dynamics of disordered materials.

Here we present for the first time distance measurements in quadruplex sequences based on pulsed EPR measurements (DEER) of double-nitroxide spin labeled DNA oligonucleotides. Telomeric quadruplex sequences have attracted much attention since a biological function of these unusual folds is anticipated. The human telomeric repeat is able to form structures that differ drastically in strand orientation and loop connectivity. Although it has been an important quest to decipher the physiologically relevant quadruplex topologies, the exact structures contributing to the mixtures present in potassium-rich solutions are still discussed controversially.

Our measurements demonstrate the presence of the all-parallel (so called propeller) and the all-anti-parallel (called basket) conformation in K⁺ solution, adding an important piece of evidence to the current debate.

15 min. break

BP 3.5 Mon 15:30 H43

Integrative investigation of DNA supercoiling under tension — ●ROBERT SCHÖPFLIN¹, HERGEN BRUTZER², RENÉ STEHR¹, RALF SEIDEL², and GERO WEDEMANN¹ — ¹University of Applied Sciences Stralsund, 18435 Stralsund, Germany — ²Biotechnology Center Dresden, University of Technology Dresden, 01062 Dresden, Germany

Recent studies of high resolution single molecule experiments yielded detailed information of DNA supercoiling under applied tension. Here, an approach integrating experimental, numerical and analytical methods was used to understand these data. Linear DNA was investigated with magnetic tweezers under different concentrations of monovalent ions over a range of pulling forces and added supercoils. According to this we performed Monte Carlo (MC) simulations with a coarse-grained DNA model considering stretching, bending, twisting and electrostatic

ics. The simulations reproduce well the experimentally observed behavior: A force and salt dependent abrupt buckling at the onset of the plectonemic phase is followed by a linear length decrease with added turns. The buckling transition is accompanied by an abrupt DNA length decrease depending on the ionic conditions. Beyond an overall qualitative agreement, the MC simulations reproduce quantitatively many of the experimental parameters. These include the slope and torque of the linear decrease after buckling as well as the jump size and the torque change during abrupt buckling. Moreover, we developed an analytical model for the description of DNA supercoiling. This model describes well both data from experiment and simulation when incorporating a reduced DNA charge.

BP 3.6 Mon 15:45 H43

Diffusion Based Looping Of Chromatin — •DIETER HEERMANN and MANFRED BOHN — Universität Heidelberg, Institut für Theoretische Physik, Heidelberg, Germany

Chromatin folding inside the interphase nucleus of eukaryotic cells is done on multiple scales of length and time. Despite recent progress in understanding the folding motifs of chromatin, the higher-order folding still remains elusive. Fluorescent in situ hybridization reveals a tight connection between genome folding and function as well as a folding into a confined sub-space of the nucleus. The folding state of chromatin reveals distinct differences from a compact conformation. A previously published model, the random loop (RL) model, explains the folding state by the formation of random loops, which themselves seem to be an ubiquitous motif of transcriptional regulation. However, it remains a crucial question what mechanisms are necessary to make two chromatin regions become co-located, i.e. have them in spatial proximity.

The model presented here bridges the gap between statistical polymer models and an effective description of the dynamic process of loop formation mediated by the nuclear environment. Without assuming long-range forces or any active transport mechanisms, this model assumes that the formation of contacts or loops is done solely on the basis of random collisions. The probabilistic nature of the formation of temporary contacts mimics the effect of e.g. transcription factors in the solvent. Although only basic interactions are taken into account, this model is in agreement with recent experimental data.

BP 3.7 Mon 16:00 H43

An accurate approximation for the end-to-end distance distribution of worm-like chains of arbitrary stiffness — •NILS B BECKER¹, ANGELO ROSA², and RALF EVERAERS¹ — ¹Labo de Physique and Centre Blaise Pascal de l'ENS de Lyon, Université de Lyon, CNRS UMR 5672, Lyon, France — ²Institute for Biocomputation and Physics of Complex Systems (BIFI), Zaragoza, Spain

The thermal conformations of semiflexible macromolecules are generically described by the worm-like chain model. To date, the model's fundamental quantity, the end-to-end distance distribution, is not known in closed form. We give an overview of the available approximations

and exact limiting results for this distribution. We then combine all relevant exact limits into an explicit, generally applicable interpolation formula. The proposed expression accurately reproduces, at no computational cost, high-precision Monte-Carlo data, covering the full range from stiff to flexible chains and from looped to stretched configurations. Some applications are discussed.

BP 3.8 Mon 16:15 H43

Orientation Defined Stretching and Immobilization of DNA by AC Electrokinetics — •VENKATESH ALAGARSWAMY GOVINDARAJ¹, SIMONE HERTH¹, ANKE BECKER^{1,2}, and GÜNTER REISS¹ — ¹Thin Films & Physics of Nanostructures, Bielefeld University, Universitätsstr. 25, 33615 Bielefeld. — ²Molecular Genetics, Institute for Biology III, Albert-Ludwigs-Universität Freiburg, Schänzlestr. 1, 79104 Freiburg.

DNA based single molecule studies, nano-electronics and nano-cargos require a precise placement of DNA in an orientation defined manner. Until now there is a lack of orientation defined stretching and immobilization of DNA for gaps smaller than several micrometers. However, this can be realized by designing bi-functionalized DNA with thiol at one end and (3-Aminopropyl) triethoxy silane on the other end, which specifically bind to gold and SiO₂ layer after or during stretching. The electrode assembly consists of platinum as electrode material for applying the AC voltage and islands of gold and silicon dioxide fabricated at a distance of about 500-800 nm. The orientation defined stretching and covalent fixing of DNA was carried out at different frequency ranges of the applied electric field and observed after metallization of DNA by palladium ions in a Field Emission Scanning Electron Microscopy (FESEM).

BP 3.9 Mon 16:30 H43

DNA-DNA electrostatic frictional forces: magnitude and biological implications — •ANDREY CHERSTVY — IFF-2, FZ Jülich, Germany

We estimate theoretically the strength of DNA-DNA electrostatic frictional forces emerging upon dragging one DNA molecule over another one in a close parallel juxtaposition [1]. For ideally helical DNA duplexes, this friction occurs due to correlations in electrostatic potential near DNA surfaces. The latter originate from intrinsic helicity of DNA phosphate charges on the scale of 3.4 nm along DNA axis that produces a positive-negative charge interlocking along the DNA-DNA contact. For realistic, non-ideally helical DNAs, where electrostatic potential barriers become decorrelated due to accumulation of "sequence mismatches" in DNA structure, DNA-DNA frictional forces are strongly impeded. We calculate DNA-DNA frictional forces in both cases and describe their implications for sequence recognition of DNA duplexes that takes place in vivo upon cell division. We also discuss the possibilities of probing DNA-DNA intermolecular interactions in strongly confined DNA superhelical plies as obtained in single-molecule dual optical trap experiments.

[1] A. G. Cherstvy, J. Phys. Chem. B, 113 5350 (2009).

BP 4: Statistical Physics of Biological Systems II (joint BP, DY)

Time: Monday 14:00–17:00

Location: H45

Invited Talk

BP 4.1 Mon 14:00 H45

Nonlinear dynamics and control of migraine waves — •MARKUS DAHLEM — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany
Migraine is a dynamical disease. A mechanism is presented by which traveling wave patterns, which cause migraine, are formed in the 2D folded human cortex. The predicted wave is maintained only transiently but with a characteristic form (shape and size). Such patterns contradict the established image of a migraine wave engulfing one cortical hemisphere, but we found that they are in agreement with our results obtained from a study using functional magnetic resonance imaging. The mechanism is based on an unstable particle-like wave solution that exists in generic reaction-diffusion media of activator-inhibitor type. This solution can vanish in a saddle-node bifurcation if excitability is globally controlled. This creates a bottleneck region in phase space that sucks in all sufficiently largely perturbed cortical states (ignition phase in migraine). While, as a consequence, recovery is slowed down, a pattern with universal space and time scales

emerges. Our bifurcation analysis is also supported by numerical simulations. Moreover, it is shown analytically that such confined waves favor certain cortical geometries. Consequences are discussed for the design and application of biomedically engineered devices that can be used in therapeutic approaches to intelligently target migraine waves by changing the bottleneck passage time and thus more quickly revive the physiological state of the cortex.

BP 4.2 Mon 14:30 H45

Using GFRD to Study Pattern Formation due to the Interplay of Active and Passive Transport — •THOMAS SOKOLOWSKI, NILS BECKER, LAURENS BOSSEN, THOMAS MIEDEMA, and PIETER REIN TEN WOLDE — FOM Institute AMOLF, Science Park 113, 1098 XG Amsterdam, The Netherlands

Cells exploit the interplay of active transport along cytoskeletal tracks and cytosolic passive diffusion to establish a wide range of spatial patterns of functional proteins, mRNA and specialized organelles. Such systems are not well-stirred, so standard simulation techniques can be very expensive while coarse-graining may be inappropriate.

Green's function reaction dynamics (GFRD) is an exact event-driven chemical simulation scheme based on analytical solutions of the Smoluchowski equation with appropriately chosen boundary conditions. For sufficiently low particle concentrations up to 1 μ M it allows for spatially resolved stochastic simulations of many-particle-systems with an efficiency orders of magnitude higher as compared to common Brownian dynamics schemes.

Based on GFRD we develop a framework which allows for a spatio-temporal stochastic simulation of both active and diffusive movement in different geometries to study pattern formation arising from the interplay the two transport types.

BP 4.3 Mon 14:45 H45

Prokaryotic Chromosome Organization in the Context of Entropy, Confinement and Tethering Interactions — ●MIRIAM FRITSCHÉ and DIETER W. HEERMANN — Institute for Theoretical Physics, University of Heidelberg, Philosophenweg 19, 69120 Heidelberg, Germany

Prokaryotic chromosomes are physically organized and condensed into an intricately structured DNA-protein complex called a nucleoid. The large-scale physical structure might arise from protein mediated interactions that can form both inter and intra-chromosome tethers as well as anchoring the chromosome to the membrane of the nucleoid or to protein scaffolds [1]. Motivated by recent experiments that capture *E. coli* nucleoid structure using three spectrally distinct, fluorescently-labeled genetic loci [2], we analyze single-locus and two-locus positioning distributions in the theoretical framework of a coarse-grained polymer model taking into account excluded volume, confining geometries as well as tethering interactions therewith shedding light into the mechanisms governing *E. coli* nucleoid structure between replication cycles.

[1] W.F. Marshall, *Current Biology* 12, 158 (2002)

[2] P.A. Wiggins, K. Cheveralls, J.S. Martin, R. Lintner, J. Kondev, private communication

BP 4.4 Mon 15:00 H45

Velocity distributions of foraging bumblebees in the presence of predators — ●FRIEDRICH LENZ¹, THOMAS C. INGS², LARS CHITTKA², ALEKSEI V. CHECHKIN³, HOLGER KANTZ⁴, and RAINER KLAGES¹ — ¹Queen Mary University of London, School of Math. Sci., UK — ²Queen Mary University of London, School of Biol. & Chem. Sci., UK — ³Inst. for Theo. Physics, NSC KIPT, Kharkov, Ukraine — ⁴Max Planck Institute for the Physics of Complex Systems, Dresden

We analyse changes in the flight behaviour of foraging bumblebees under varying environmental conditions, measured in a laboratory experiment by Ings and Chittka[1]. We estimate parameters for different plausible velocity distributions by maximising their likelihood and compare their goodness of fit by applying the Akaike Information Criterion. Using Quantile-Quantile-plots we check for deviations between the estimated probability distributions and the data. We also discuss differences in these distributions for different individual bumblebees. On this basis, we look for systematic changes of the distributions due to the presence of different kinds of artificial spiders.

[1] Thomas C. Ings and Lars Chittka. *Current Biology*, 18(19):1520-1524 (2008)

BP 4.5 Mon 15:15 H45

Modelling a flexible sheet swimmer with stochastic rotation dynamics — ●SUJIN BABU and HOLGER STARK — Institut für Theoretische Physik Technische Universität Berlin

The dynamics of microorganisms in a viscous fluid has recently received considerable attention in the physics community. It has been reported that some microorganisms (such as the African Trypanosome) make use of hydrodynamic flow fields to evade attack from antibodies. The flexible cell body of the African Trypanosome possesses some bending rigidity due to its cytoskeleton. To mimic the cell body of such an organism, we introduce a flexible sheet that is impenetrable to the surrounding fluid. The flow fields around such a sheet are simulated by stochastic rotation dynamics. I will explain how we couple the flexible sheet to the viscous fluid. Then I will discuss the drag coefficients of the sheet and investigate how it swims under the influence of appropriately applied forces.

15 min. break

BP 4.6 Mon 15:45 H45

The first passage problem for diffusion through a cylindrical pore with sticky walls — ●NICHOLAS A. LICATA^{1,2} and STEPHAN W. GRILL^{1,2} — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

We calculate the first passage time distribution for diffusion through a cylindrical pore with sticky walls. A particle diffusively explores the interior of the pore through a series of binding and unbinding events with the cylinder wall. Through a diagrammatic expansion we obtain first passage time statistics for the particle's exit from the pore. Connections between the model and nucleocytoplasmic transport in cells are discussed.

BP 4.7 Mon 16:00 H45

A growth model for bacterial flagella — ●MAXIMILIAN SCHMITT, REINHARD VOGEL, and HOLGER STARK — Institut für Theoretische Physik, TU Berlin

Bacterial flagella of e.g. *E. coli* consist of up to 30000 flagellin molecules which are arranged in a hollow tube with outer and inner diameters of 20nm and 3nm, respectively, and a length of up to 20 μ m. When the flagellum grows, flagellin molecules are transported through the hollow core of the filament and attached at its tip.

As a model for this growth process, we extend one model system of non-equilibrium statistical mechanics, the ASEP (Asymmetric Simple Exclusion Process), to an exclusion process on a growing lattice. In this one-dimensional model, particles enter the lattice with rate α , travel forward with jump rate q and backward with rate p . At the tip particles can transform into a new lattice site with rate γ .

Monte Carlo simulations and mean-field approximations both give the same phase diagram in (α, γ) phase space with distinct low density, high density and maximal current phases. In case of symmetric dynamics ($q = p$) both low density and high density phase vanish, which is in agreement with the SSEP (Symmetric Simple Exclusion Process). Special attention is put on the tip velocity with which the length L of the flagellum grows. It shows an unstable fixed point at $q = p$. For $q > p$ the model is ballistic with $\langle L^2 \rangle \sim t^2$, for $q = p$ diffusive with $\langle L^2 \rangle \sim t$, and for $q < p$ sub-diffusive with a tip velocity slower than single-file diffusion: $\langle L^2 \rangle \sim t^{1/6}$.

BP 4.8 Mon 16:15 H45

Long-range protein coupling mediated by critical low-energy modes of tubular lipid membranes — SYLVAIN MONNIER^{1,3}, SERGEI B. ROCHAL², ●ANDREA PARMEGGIANI³, and VLADIMIR L. LORMAN¹ — ¹LPTA, CNRS, University of Montpellier II, 34095 Montpellier, France — ²Physical Department, South Federal University, 344090 Rostov-on-Don, Russia — ³DIMNP, CNRS, University of Montpellier II, 34095 Montpellier, France

Tubular lipid membranes (TLMs) are nanoscopic cylindrical assemblies that play a fundamental role in many intracellular and intercellular processes like protein trafficking, signaling and organelle morphogenesis. TLMs can be generated by a sum of mechano-chemical actions, ranging from mechanical forces produced by motor proteins pulling at one TLM-end up to the specific chemical activity of membrane proteins.

We develop a theory of TLM instabilities under longitudinal force and pressure difference constraints. Two qualitatively different critical low-energy modes are shown to define the stability domain boundaries. The analysis allows to introduce a new framework describing TLM-protein coupling, adsorbed protein-protein interaction and protein cluster nucleation on a TLM. In particular, bare TLM mechanical instabilities strongly influence protein-TLM coupling and protein desorption from the TLM. Model predictions can be directly tested in experiments involving nanomechanical devices extracting TLM over a large spectrum of mechanochemical conditions.

BP 4.9 Mon 16:30 H45

Protein folding trajectories and free energy landscapes in a coarse-grained model — ●KATRIN WOLFF¹, MICHELE VENDRUSCOLO², and MARKUS PORTO¹ — ¹Institut für Festkörperphysik, TU Darmstadt, Germany — ²Department of Chemistry, University of Cambridge, UK

We study protein free energy landscapes and folding dynamics from completely unfolded to folded structures using a coarse-grained model biased towards the native state. Proteins are modeled as a chain of uniform thickness with bending rigidity (tube model [1]) with a bias towards the native structure based on a one-dimensional representation

of the structure (structure profile). This approach is conceptually very different from those relying on the assumption of minimal frustration (such as Gō-models) since it does not favour the formation of contacts between specific residues but mediates ‘connectivity’ of residues, that, much like hydrophobicity, describes a residue’s propensity to form contacts. We show that the ‘effective connectivity’ profile [2] constitutes a suitable bias towards the native structure [3] and investigate free energy landscapes, heat capacity curves and typical folding trajectories and compare our results to experimental folding behaviour and results from (much more computationally expensive) molecular dynamics simulations.

[1] T.X. Hoang *et al.*, Proc. Natl. Acad. Sci. USA **101**, 7960 (2004).

[2] U. Bastolla *et al.*, Proteins **73**, 872 (2008).

[3] K. Wolff, M. Vendruscolo, and M. Porto, PMC Biophysics **1**, 5 (2008)

BP 4.10 Mon 16:45 H45

Intrinsic fluctuations in stochastic delay models of gene regulation — ●TOBIAS GALLA — Theoretical Physics, School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, UK

We study the effects of intrinsic noise on stochastic delay systems within an expansion in the inverse system size. It is shown that the stochastic nature of the underlying dynamics can induce sustained quasi-cycles in parameter ranges where the deterministic system does not show oscillatory behaviour. We compute the power spectra of these stochastic oscillations analytically, in good agreement with simulations. The theory is applied to a simple gene regulatory system representing the basic motif of an auto-inhibitory feedback loop and motivated by its relevance to somite segmentation. Such systems often contain only a small number of molecules, leading to significant fluctuations in mRNA and protein concentrations, and the proposed mechanism of enhanced stochastic oscillations may therefore be applicable.

Reference: Tobias Galla, Phys. Rev. E 80 (2009) 021909

BP 5: Posters: Biopolymers and Biomaterials

Time: Monday 17:15–20:00

Location: Poster B1

BP 5.1 Mon 17:15 Poster B1

Interactions between proteins and thermoresponsive microgels — ●NICOLE WELSCH¹ and MATTHIAS BALLAUFF^{1,2} — ¹Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin — ²Department of Physics, Humboldt University Berlin, 12489 Berlin

The interface of materials science and biology is emerging as a major research focus and especially nanomaterials in medicine and biotechnology are considered to accelerate the progress in these fields. However, nanoparticles entering the bloodstream initially become coated with proteins and the contact to these particles may induce misfolding of the protein structure and the perturbation of the function of the bound proteins. Therefore, this ‘nano-bio’ interface has to be understood in detail for new applications to evolve. Particles based on poly(N-isopropylacrylamide) (PNiPA) exhibit lower critical solution behaviour close to the physiological temperature and therefore have potential to be applied in biotechnology. For deeper insight into the interactions of biomolecules to PNiPA microgels the adsorption of proteins with different surface properties is investigated. Thereby, SAXS experiments elucidate the spatial distribution of the proteins within the polymer network. Furthermore, the activity of immobilized enzymes is investigated temperature-dependent to analyse the impact of the immobilization on the catalytic activity. By using FT-IR spectroscopy changes of the secondary structure of adsorbed proteins and the formation of interactions towards the carrier particles can be analysed.

BP 5.2 Mon 17:15 Poster B1

Probing the components of nacre by contact angle measurements — ●MALTE LAUNSPACH, FABIAN HEINEMANN, and MONIKA FRITZ — Pure and Applied Biomineralisation, Biophysics Institute, University Bremen, Germany

Nacre of some molluscs is a highly structured polymer/mineral composite, which has been brought to perfection by evolution over millions of years. Densely packed mineral platelets are interdispersed by a few nanometer of organics. The order and the dimension of the platelets lead to astonishing mechanical properties. Soluble and insoluble proteins are involved in the formation of the aragonite platelets; some are attached to a chitin core - the organic matrix. Here the surface energy properties are probed by contact angle measurements to quantify the adhesive strength between the mineral and organic phase and to investigate the relevance of the organic matrix during platelet formation. Measurements were conducted with a home-made device. The demineralised insoluble organic matrix in a native state and after enzymatic treatment were probed as well as the (001) surface of geological aragonite. The (001) surface of aragonite is not a cleavage plane and had to be processed in a special way. The surface free energy of the organic matrix was calculated using semi-empirical approaches. Three different models yield a total surface free energy between 40 and 44 mJ/m² for the native matrix and a value between 51 and 59 mJ/m² after enzymatic treatment. In the case of the minerals the obtained values could not be used for further calculations since the influence of

the preparation process was to dominant.

BP 5.3 Mon 17:15 Poster B1

Phase behaviour and structure of enzyme containing skin friendly microemulsions for decontamination — ●RALF STEHLE¹, CHRISTOPH SCHULREICH¹, STEFAN WELLERT², CHRISTINA DIEDERICH¹, ANDRE RICHARDT³, MARC-MICHAEL BLUM⁴, and THOMAS HELLWEG¹ — ¹Universität Bayreuth, Physikalische Chemie I, Universitätsstr. 30, D-95444 Bayreuth — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Glienicker Str. 100, D-14109 Berlin — ³Armed Forces Scientific Institute for NBC-Protection, Humboldtstr. 1, D-29633 Munster — ⁴Bundeswehr, Wissenschaftliche Dienste, Ledererstr. 23, D-80331 München

Microemulsions are promising media for decontamination. Various toxic chemicals and most chemical warfare agents are hydrophobic and can only be solubilized in organic solvents, while most degradation agents are water soluble. Microemulsions allow both, the solubilisation of the lipophilic toxins and their corresponding hydrophilic degradation reagents. For human skin decontamination microemulsions have to be skin friendly.

In this contribution, a system composed of a sugar surfactant and an oil, commonly used in cosmetics, is presented.

Unlike other systems based on skin friendly oils, the bicontinuous phase of this microemulsion contains much lower concentration of sugar surfactant. The phase behaviour is studied and the structure of the bicontinuous phase is characterized by small angle neutron scattering (SANS), and dynamic light scattering (DLS). Properties of the enzyme and its effect on the microemulsion are investigated.

BP 5.4 Mon 17:15 Poster B1

Deep UV Raman spectroscopy on sensory rhodopsin — ●ANDREAS BRÖERMANN, NILS PRIESNITZ, BERND WALKENFORT, JOHANN KLARE, HEINZ-JÜRGEN STEINHOFF, and SEBASTIAN SCHLÜCKER — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

The light-driven membrane pigment sensory rhodopsin II (SR II) consists of the protein opsin and the cofactor retinal. SR II is responsible for the negative phototaxis of halobacteria. Incident photons induce an isomerization of the retinal chromophore, which leads to a conformational change of opsin and, by means of a signalling cascade, finally controls the flagellar motor and thereby the swimming behavior of the cells.

The nano- to millisecond conformational dynamics of SR II can be probed by time-resolved UV resonance Raman scattering (UV RR) in a pump(VIS)-probe(deep UV) experiment with kHz repetition rate. The sample is excited by a frequency-doubled Nd:YAG laser (532 nm, 10 ns pulse length). After a variable time delay, the photo-excited SR II molecules are probed with deep UV laser radiation (195 nm, 10 ns pulse length). The deep UV Raman spectrum is recorded by a triple monochromator equipped with a gated image intensifier.

BP 5.5 Mon 17:15 Poster B1

Optical properties of light-harvesting systems determined by molecular dynamics simulations — ●CARSTEN OLBRICH¹, JÖRG LIEBERS¹, MICHAEL SCHREIBER², and ULRICH KLEINEKATHÖFER¹ — ¹Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — ²TU-Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz, Germany

Harvesting sun light to gain energy for life is initially done by light-harvesting antenna complexes containing chlorophyll and carotenoid molecules. Starting from the available crystal structure of the light-harvesting systems 2 (LH2) of purple bacterium, we applied all-atom classical molecular-dynamics (MD) simulations to the LH2 ring embedded in a membrane. Thus obtained thermal fluctuations of the nuclear positions provide the input for quantum chemical calculations. To obtain the energies of the Q_y excited states of the single Bacteriochlorophyll (BChl) molecules, the semi-empirical ZINDO/CIS method is used to be able to analyze longer time series as was previously possible with the CIS method [1,2]. To include solvent effects to the excited state dynamics, the surrounding atoms of the BChls are treated as classical point charges in the QM calculations. Using the nuclear motion and the obtained energy differences between ground and Q_y excited states with a time-dependent Hamiltonian, we are able to calculate optical properties of the analyzed system.

[1] A. Damjanovic, I. Kosztin, U. Kleinekathöfer, and K. Schulten, *Phys. Rev. E* 65, 031919 (2002)

[2] L. Janosi, I. Kosztin, and A. Damjanovic, *J. Chem. Phys.* 125, 014903 (2006)

BP 5.6 Mon 17:15 Poster B1

Coarse Grained Simulations of a Small Peptide: Effects of Finite Damping and Hydrodynamic Interactions — ●TIHAMER GEYER — Zentrum für Bioinformatik, Universität des Saarlandes, D-66123 Saarbrücken

In the coarse grained Brownian Dynamics simulation method the many solvent molecules are replaced by random thermal kicks and an effective friction acting on the particles of interest. For Brownian Dynamics the friction has to be so strong that the particles' velocities are damped much faster than the duration of an integration timestep. Here we show that this conceptual limit can be dropped with an analytic integration of the equations of damped motion. In the resulting Langevin integration scheme our recently proposed approximate form of the hydrodynamic interactions between the particles [1] can be incorporated conveniently, leading to a fast multi-particle propagation scheme, which captures more of the short-time and short-range solvent effects than standard BD. Comparing the dynamics of a bead-spring model of a short peptide, we recommend to run simulations of small biological molecules with the Langevin type finite damping and to include the hydrodynamic interactions [2].

We also present our recently released "Brownmove" simulation package for coarse-grained many-particle simulations incorporating the above explained propagation techniques.

[1] Geyer, Winter, *J. Chem. Phys.*, 130 (2009) 114905

[2] Winter, Geyer, *J. Chem. Phys.* 131 (2009) 104102

BP 5.7 Mon 17:15 Poster B1

Microhydration of two polyalanine-based peptides — ●SUCISMITA CHUTIA, MARIANA ROSSI, VOLKER BLUM, and MATTHIAS SCHEFFLER — Fritz Haber Institute, Berlin, Germany

Microsolvation studies are an important approach for analysing the influence of the solvent environment on peptides. Two small peptides have been the subject of such experimental studies in the recent years: Ac-Ala₅-LysH⁺ [1] and Ac-Phe-Ala₅-LysH⁺ [2]. The aim of this work is to theoretically identify the lowest-energy conformers of these peptides and carry out microhydration studies to find the preferred water binding sites on these conformers. We first use a molecular dynamics calculation with the OPLS-AA force-field potential in the TINKER package to scan the potential energy surface for a wide variety of candidate conformers. We then use the all-electron electronic structure code *FHI-aims* [3] to follow up these structures with van der Waals corrected density functional theory to determine the energy hierarchy, and vibrational frequencies for direct comparison with experiment. Our findings indicate that both helical and "non-helical" conformers are present among the low-energy conformers of Ac-Phe-Ala₅-LysH⁺, similar to the case of Ac-Ala₅-LysH⁺. We find that, for both Ac-Phe-Ala₅-LysH⁺ and Ac-Ala₅-LysH⁺, the water molecule binds to the protonated lysine end in the lowest energy conformer. We also address the accuracy of the pre-screening forcefield compared to DFT-*vdW*. [1] M. Kohtani and M.F. Jarrold, *JACS*, 126, 8454-8458 (2004) [2] J.A. Stearns *et al*, *PCCP*, 11, 125-132 (2009) [3] V. Blum *et al*,

Comp. Phys. Comm. 180, 2175 (2009).

BP 5.8 Mon 17:15 Poster B1

Comparison of nanomechanical properties of in vivo and in vitro keratin networks — ●ANKE LEITNER¹, TOBIAS PAUST¹, HARALD HERRMANN², MICHAEL BEIL³, and OTHMAR MARTI¹ — ¹Institute of Experimental Physics, Ulm University — ²Division of Molecular Genetics, German Cancer Research Center, Heidelberg — ³Department of Internal Medicine I, Ulm University

The mechanical properties of epithelial cells are mainly determined by the cytoskeleton. The cytoskeleton consists of three different protein networks, microtubules, the transport pathways of the cell, actin filaments, responsible for the movement, and intermediate filaments that provide the stiffness and response to mechanical stimuli. In order to find out more about the mechanical properties of the intermediate filament keratin cytoskeleton it is useful to have a look on in vitro assembled keratin filaments. In the work presented here we compare the mechanical properties of the extracted keratin cytoskeleton of pancreatic carcinoma cells with the mechanical properties of in vitro assembled keratin 8/18 networks. For this purpose we use microrheology measurements with embedded tracer beads. This method is a suitable tool, because the size of the beads compared to the meshsize of the network allows us to treat the network as a continuum. Observing the beads motion with a CCD-High-Speed-Camera then leads to the dynamic shear modulus. We draw conclusions on the network topology of the authentic isolated cellular networks and the recombinant in vitro assembled K8/18 filament systems based on the mechanical behaviour.

BP 5.9 Mon 17:15 Poster B1

Force-generation by growing microtubules — ●BJÖRN ZELINSKI¹ and JAN KIERFELD² — ¹Physics Department, TU Dortmund University, Dortmund, Germany — ²Physics Department, TU Dortmund University, Dortmund, Germany

In many cellular processes polymerization forces play an important role. We investigate force generation for growing microtubules undergoing dynamic instability using a two-state Monte-Carlo simulation. We find that the maximum force generated by a single microtubule strongly depends on the catastrophe- and rescue-dynamics. We also study cooperative effects in force generation by an ensemble of N microtubules.

BP 5.10 Mon 17:15 Poster B1

Optical tweezers to investigate receptor/ligand interactions on a single contact level — ●CAROLIN WAGNER¹, DAVID SINGER², MATHIAS SALOMO³, RALF HOFFMANN², and FRIEDRICH KREMER¹ — ¹University of Leipzig, Department for molecule Physics, Leipzig, Germany — ²University of Leipzig, Institut für bioanalytische Chemie, Leipzig, Germany — ³Fraunhofer-Institut für Zelltherapie und Immunologie, Leipzig, Germany

The extraordinary features of optical tweezers having a nm-resolution in positioning a micron-sized colloid and an accuracy of (+/-50 fN) in measuring the forces acting on it, enable one to study the interaction within a single receptor/ligand-contact. By use of dynamic force spectroscopy (DFS), the specific binding of the monoclonal antibody HPT-110 to a synthetic doubly phosphorylated tau-peptide is investigated on a single contact level. Amongst others, the massive accumulation of tangles that mainly consist of hyperphosphorylated tau-proteins is characteristic for Alzheimer's disease. Single-molecule DFS enables the investigation of the energy landscape of the bond and benefits from the fact that only minimal amounts of the sample are necessary. It is demonstrated that the rupture force depends on the loading rate. This effect is well known in the literature and the data obtained were found to be in good agreement with an already published theoretical model. By use of this model, the off-rate at zero force of 0,54 s⁻¹ is determined.

BP 5.11 Mon 17:15 Poster B1

The Nanostructure of the Tracheid Wood Cell Wall — ●MALTE OGURRECK¹, PEKKA SARANPÄÄ², MANFRED BURGHAMMER³, SEBASTIAN SCHOEDER³, CHRISTINA KRYWKA⁴, and MARTIN MÜLLER^{1,4} — ¹GKSS Research Centre Geesthacht, Germany — ²The Finnish Forest Research Institute METLA, Vantaa, Finland — ³ESRF, Grenoble, France — ⁴University of Kiel, Germany

Tracheid wood cell walls are mainly composed of cellulose nanocrystals (microfibrils) embedded in an amorphous matrix. These microfibrils

are helically wound around the cell axis and are arranged in several layers.

While the structure of tracheid wood cells has been a research topic for many decades now and the structure on the biological and molecular level are well known, the detailed structure on intermediate length scales is still largely unknown.

Here, we present results of nanodiffraction experiments carried out at the nano-/microfocus beamline ID13, ESRF. Tracheid cross sections have been scanned with a position resolution of down to 200 nm. These detailed diffraction data allows us to map the local structure in the cell wall with a very high resolution.

The comparison of wood grown under normal conditions with wood grown using special treatments (irrigation, fertilizers) allows to reach conclusions about how environmental influences affect the structure of wood.

BP 5.12 Mon 17:15 Poster B1

Entropy assists cell's contraction — ●CARSTEN SCHULDT and JOSEF KÄS — Universität Leipzig, Germany

Cell migration is an inherent quality of life. Considering the motility of cells the current model is based on three constitutive processes: first, cytoskeletal extension at the leading edge; second, adhesion to the environment to convey traction; and third, retraction at the rear. Polymerization of the cytoskeletal scaffold accounts for the extension and transmembrane proteins facilitate traction. The process of retraction is still debated.

Muscle-like actomyosin contractions were supposed to accomplish back retraction, originally. But myosin knock-out cells were still capable to migrate [1]. Alternatively, the depolymerization of cytoskeleton was proposed to cause contractile forces only by a gain in entropy in the absence of molecular motors. This concept was demonstrated on polymer meshworks of nematode's major sperm protein [2].

We intend to probe these forces in bundles of actin, which is one of the principal components of cytoskeletal biopolymer networks using optical tweezers.

[1]De Lozanne et. al., Science 236(4805)

[2]Wolgemuth et. al., Biophys. J. 88(4)

BP 5.13 Mon 17:15 Poster B1

Feeling for Cells with Light: Illuminating the Role of Biomechanics for Tumor Progression — ANATOL FRITSCH, FRANZISKA WETZEL, DAVID NNETU, TOBIAS KIESSLING, MAREIKE ZINK, and ●JOSEF A. KÄS — Division of Soft Matter Physics, Institute for Experimental Physics I, University of Leipzig

Light has been used to observe cells since Leeuwenhoek's times; however, we use the forces caused by light described by Maxwell's surface tensor to feel for the cellular cytoskeleton. The cytoskeleton, a compound of highly dynamic polymers and active nano-elements inside biological cells, is responsible for a cell's stability and organization. The optical stretcher exploits the nonlinear, thus amplified response of a cell's mechanical strength to small changes between different cytoskeletal proteomic compositions as a high precision cell marker that uniquely characterizes different cell types. Consequentially, the optical stretcher detects tumors and their stages with accuracy unparalleled by molecular biology. As implied by developmental biology the compartmentalization of cells and the epithelial-mesenchymal transition that allows cells to overcome compartmental boundaries strongly depend on cell stiffness and adhesiveness. Consequentially, biomechanical changes are key when metastatic cells become able to leave the boundaries of the primary tumor.

BP 5.14 Mon 17:15 Poster B1

Volume imaging of collagen fibrils within cortical bone — ●STEPHANIE RÖPER¹, NADINE DRECHSEL¹, ANKE BERNSTEIN², and ROBERT MAGERLE¹ — ¹Chemische Physik, TU Chemnitz, D-09107 Chemnitz — ²Experimentelle Orthopädie, Martin-Luther-Universität Halle-Wittenberg, D-06097 Halle/Saale

Biological materials such as bone and teeth are nanocomposites of a soft organic matrix (mainly type I collagen) that is reinforced by a stiff inorganic component (hydroxylapatite). Scanning probe microscopy (SPM) based nanotomography is a novel approach to image these materials on the sub-micrometer scale. For SPM based nanotomography the specimen is ablated layer-by-layer by stepwise wet chemical etching and imaged with tapping mode SPM after each etching step. Here, we focus on human cortical bone which was first mechanically grinded and polished, then stepwise etched with formic acid and sodium hypochlorite and finally flushed to stop the etching process. In the resulting

series of SFM images we mapped the position and orientation of the collagen fibrils with the typical D-band periodicity of 67 nm and reconstructed a volume image of natural collagen fibrils embedded in cortical human bone. These results are compared with reassembled collagen fibrils deposited on a solid substrate.

BP 5.15 Mon 17:15 Poster B1

Dynamical stretching response of a biopolymer held by an optical trap — ●SEBASTIAN STURM and KLAUS KROY — Institut für theoretische Physik, Universität Leipzig, Vor dem Hospitaltore 1, 04103 Leipzig

The dynamical nonequilibrium response of stiff and semiflexible polymers to external stimuli has been a subject of intense theoretical research during the last decade. Whereas pioneering works on the subject catered to very specific experimental scenarios, a subsequently developed multiple-scale (MSPT) analysis unified the previous approaches under a systematic and rigorous mathematical framework. Building on this MSPT theory, a large number of different external perturbations have found theoretical treatment, with BD simulation data corroborating the analytical results [1]. To allow for direct experimental verification of the abovementioned MSPT theory, we extend it to the practically relevant case of a semiflexible polymer held by means of an optical trap.

[1] B. Obermayer, W. Möbius, O. Hallatschek, E. Frey and K. Kroy, Freely relaxing polymers remember how they were straightened, Phys. Rev. E (2009)

BP 5.16 Mon 17:15 Poster B1

Elasticity of Fiber Networks as Function of Crosslink Density — ●SUSAN SPORER¹, MAHYAR MADADI², CHRISTOPH ARNS³, KLAUS MECKE¹, and GERD E. SCHRÖDER-TURK¹ — ¹Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — ²Applied Mathematics, The Australian National University, Canberra, Australia — ³School of Petroleum Engineering, The University of New South Wales, Sydney, Australia

Crosslinkers determine the architecture of polymer networks and thus are of great importance for the resulting mechanical properties. A morphological model is proposed for investigating the change of the linear elastic response of 3D fiber networks when randomly disconnecting network nodes. The networks have a given volume fraction regulated by the radius of the fibers and are modeled as one body consisting of a homogeneous, locally isotropic, linear elastic material. The network nodes rigidly crosslinking fibers are randomly split into two locally unconnected fibers which causes a morphology change of the network. The effective shear modulus is studied using a voxel-based finite element method. Our results show an exponential decay of the shear modulus with decreasing number of crosslinking nodes without any signs of a percolation transition. By associating the fibers with polymer chains and all network nodes with junctions connected by a crosslinking molecule, this approach is a model for elasticity of biological networks with varying crosslinker density.

BP 5.17 Mon 17:15 Poster B1

Elastic and Morphological Properties of Porous Biomaterials — ●SEBASTIAN KAPPER, SUSAN SPORER, KLAUS MECKE, and GERD E. SCHRÖDER-TURK — Friedrich-Alexander-Universität, Erlangen, Germany

The relationship between effective elastic moduli and morphological properties of microstructured porous biomaterials including bone, wood, biomineralised skeletons of crustaceans, biopolymer networks and cubic lipid mesophases remains an open question. We compute effective elastic moduli and morphological properties of ordered porous media models based on triply-periodic minimal and constant-mean-curvature surfaces of cubic symmetry.

Bulk and shear moduli are computed using voxel-based finite-element method considering the solid fraction to be a homogeneous linear elastic solid. For fixed volume fraction of 50%, we find that within classes of geometrically similar media the effective bulk modulus decreases with increasing heterogeneity of the domain thickness of the solid fraction which is quantified by using euclidean distance maps and percolation critical radii. On the other hand, we find significant differences between the elastic moduli of topologically distinct classes of media. In particular, a porous medium where the solid fraction comprises a thick warped sheet separating two hollow labyrinthine network domains has larger bulk modulus than a medium where both the solid and the void fraction are represented by congruent labyrinthine domains.

BP 5.18 Mon 17:15 Poster B1

Cartilage Proteoglycan Aggrecan Self-Adhesion at the Single Molecule Level — ●ALEXANDER HARDER¹, THOMAS DIERKS², XAVIER FERNANDEZ-BUSQUETS³, and DARIO ANSELMETTI¹ — ¹Department of Physics, Experimental Biophysics and Applied Nanoscience, Bielefeld University, D-33615 Bielefeld, Germany — ²Department of Chemistry, Biochemistry I, Bielefeld University, D-33615 Bielefeld, Germany — ³Biomolecular Interactions Team, Nanobioengineering Group, Institute for Bioengineering of Catalonia, and Nanoscience and Nanotechnology Institute, Barcelona Science Park-University of Barcelona, E-08028 Barcelona, Spain

Self-adhesion processes based on glycan-glycan interaction play an important role in cellular systems. A more detailed understanding of such a cation-mediated glycan-glycan interaction is important for aspects in embryogenesis, metastases, and other cellular proliferation processes that are mediated by glycan self-recognition. Proteoglycans which consist of a core protein with attached glycosaminoglycans are model systems for investigations of glycan-glycan interaction. The biological roles of proteoglycans are highly diversified, ranging from relatively straightforward mechanical functions to effects on more dynamic processes such as cell adhesion and motility, to more complex and still poorly understood roles in cell differentiation and development. Here, we investigated the self adhesion between highly negatively charged proteoglycan aggrecan from cartilage extracellular matrix in the presence of Ca²⁺ with atomic force microscopy (AFM) and single molecule force spectroscopy.

BP 5.19 Mon 17:15 Poster B1

PEG-Pillars as Force-Sensor-Arrays — ●SABRI RAHMOUNI^{1,2}, AARON LINDNER¹, TAMAS HARASZTI¹, and JOACHIM SPATZ^{1,2} — ¹Institut für Biophysikalische Chemie, Heidelberg, Germany — ²Max-Planck-Institut für Metallforschung, Stuttgart, Germany

The measurement of forces in biological systems is a very wide field of activity that led to a large variety of experimental approaches, e.g. optical and magnetic tweezers, atomic force microscopy, deformation of hydrogels and the bending of micropillars. All these techniques have their specific range of application, force sensitivity and resolution. In this work we present PEG (polyethylenglykol) based micropillar-force-sensor-systems for measurements in the sub nanonewton regime. When compared to silica- or PDMS-pillars the softer PEG-pillars provide a notably higher and easily tunable force sensibility. Our novel way of construction allows a direct variation of the separation, diameter, stiffness and functionalisation of the PEG-pillars. We show first applications of different PEG-pillar-arrays for analysis of the acting forces in actin-networks.

BP 5.20 Mon 17:15 Poster B1

Active growth of actin filaments can lead to a non-exponential length distribution — ●CHRISTOPH ERLenkÄMPER and KARSTEN KRUSE — Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany

Important properties of the actin cytoskeleton depend on the distribution of actin filament lengths. Here, we study the growth dynamics of actin filaments, taking into account addition and removal of monomers at both ends, the different phosphorylation states of the monomers and a stochastic dephosphorylation of monomers within the filaments [1,2]. The assembly of actin is active: While energy-rich ATP-bound actin monomers are readily integrated into filaments, the dephosphorylated ADP-actin monomers only have a low affinity for the filament and easily detach from it. In contrast to unregulated filament growth, we find that the active growth can lead to non-exponential length distributions. We show that they result from a stability gradient of monomers within a treadmill filament. This is similar to a possible mechanism of length regulation by destabilizing proteins [3].

- [1] Bindschadler et al, *Biophys. J.* **86** (2004) 2720.
- [2] Stukalin and Kolomeisky, *Biophys. J.* **90** (2006) 2673.
- [3] Erlenkämper and Kruse, *Phys. Biol.* **6** (2009) 046016.

BP 5.21 Mon 17:15 Poster B1

Microrheology: On the comparison of the pancreatic carcinoma cytoskeleton and the in vitro assembled keratin network — ●TOBIAS PAUST¹, ANKE LEITNER¹, ULLA NOLTE¹, MICHAEL BEIL², and OTTHMAR MARTI¹ — ¹Institute of Experimental Physics, Ulm University — ²Institute of Internal Medicine I, Ulm University

The intermediate filament cytoskeleton of pancreatic carcinoma cells is responsible for elasticity and stiffness of the cell and furthermore

for shielding its nucleus. Therefore the mechanical properties of the cytoskeleton have to be determined. After polymerization the in vitro assembled keratin 8/18 networks should show similar mechanical properties depending on the ratio of components. By using microrheology methods both the intermediate and the assembled networks were analyzed and then the mechanical properties, the structure and the behaviour under stress were compared.

For this purpose Microrheology with embedded tracer beads is a suitable tool, because the size of the beads compared to the mesh size of the network allows to treat the network as a continuum and to use an analytical model. Observing the beads motion with a CCD-High-Speed-Camera with a time resolution better than 0.25ms leads to the dynamic shear modulus of the networks.

The measurements show storage moduli and the dissipative loss in the extracted cytoskeleton compared to the in vitro assembled network. This is related to differences in the structure of the network and the polymerization process. The results of this experiments will be discussed.

BP 5.22 Mon 17:15 Poster B1

Single molecule force measurements of single-stranded RNA-molecules with optical tweezers — ●TANJA PLÖTZ¹, FABIAN EBER², ANNA MÜLLER², CHRISTINA WEGE², ANDY SISCHKA¹, and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University — ²Department of Molecular Biology and Plant Virology, Institute of Biology, Stuttgart University

The formation of RNA secondary structures is fundamental for systems biology, because of their regulatory functions on different levels. For understanding protein interactions with single-stranded RNA secondary structures it is of special interest to gain quantitative insights into the binding mechanisms and the interplay at the single molecule scale.

Therefore, we investigated the force extension curves of single-stranded RNA for the breakup of secondary structure, in experiments using a compact single beam optical tweezers platform [1,2] with a custom-made hybridization chamber.

We will expand our experiments to investigate protein-RNA interactions in the *Tobacco mosaic virus* (TMV) ssRNA genome with viral coat protein subunits, in order to find out whether initiation of the self-assembly of the TMV nucleoprotein tube strictly depends on protein-RNA interaction at hairpin loop structures located within the RNA's origin of assembly.

- [1] A. Sischka et al., *Rev. Sci. Instrum.* **74**, 4827, 2003
- [2] A. Sischka et al., *Rev. Sci. Instrum.* **79**, 063702, 2008

BP 5.23 Mon 17:15 Poster B1

Analysis of multivalent effects using pyridine coordination compounds in single molecule force spectroscopy (SMFS) — ●MANUEL GENSLER¹, CHRISTIAN EIDAMSHAUS², HANS-ULRICH REISSIG², and JÜRGEN P. RABE¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin — ²Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

Multivalent interactions are of great importance in supramolecular chemistry, nanotechnology or biochemistry [1]. They influence binding free energies and kinetics, which leads to strongly increased interaction strengths between partners of appropriate geometry. Thus it is important to obtain a deeper understanding of the basic factors influencing multivalent interactions.

SMFS provides a direct measurement of forces [2] and is therefore an ideal tool to study multivalency on the molecular level. We synthesized pyridine nanorods and coupled them to Au covered tips and surfaces, using thiol chemistry and PEG as spacer. Force-distance measurements at different loading rates were performed to estimate associated binding properties of mono- and multivalent coordination compounds with metal salts in aqueous solutions. Our model system can be extended to various solvents and geometries and therefore provide fundamental knowledge also for more complex biological and supramolecular systems.

- [1] M. Mammen et al. *Angew. Chem. Int. Ed.* **37** (1998) 2754-2794.
- [2] M.I. Gianotti et al. *ChemPhysChem* **8** (2007) 2290-2307.

BP 5.24 Mon 17:15 Poster B1

The conformations of a stiff polymer in random media — ●MARCEL HENNES and KLAUS KROY — Institut für Theoretische Physik, Universität Leipzig, Deutschland

Stiff polymers play a crucial role in many biophysical processes. In the eukaryotic cell, they assemble to a dense meshwork, the cytoskeleton, which confers the cell its unique mechanical properties. In this highly crowded environment the conformations and dynamic properties of the biopolymers are strongly influenced by the surrounding macromolecules. The theoretical description of the resulting complicated many body problem is usually provided by a mean field Ansatz, like the tube model or the glassy wormlike chain [1].

Little attention has been paid so far to the effect of a quenched random environment on a stiff filament. We present a study of the influence of quenched random forces and a quenched random potential on the conformations of a semiflexible chain in the weakly bending rod limit. The results are obtained with the help of the replica trick, which has proved to be a successful tool in determining the characteristics of directed polymers and flexible chains in random media.

[1] K. Kroy, J. Glaser, *New J. Phys.* **9** (2007) 416.

BP 5.25 Mon 17:15 Poster B1

Microrheology: A system for the comparison of pancreatic carcinoma cells in an optical tweezers device and an electron microscope — ●TOBIAS PAUST¹, ANKE LEITNER¹, ULLA NOLTE¹, MICHAEL BEIL², PAUL WALTHER³, and OTHMAR MARTI¹ — ¹Institute of Experimental Physics, Ulm University — ²Institute of Internal Medicine I, Ulm University Hospital — ³Central Electron Microscopy Unit, Ulm University

Nowadays the studies of pancreatic carcinoma cells are very important to get a insight into the behavior, structure and properties of these cells. Optical tweezers and microrheology methods allow to measure the mechanical properties of a selected cell. By tracing incorporated nanoparticles the trajectory of this particles and then the dynamic shear modulus of the cells or the a network can be determined. Electron microscopes can be used for resolving structures down to a nanometer level and clearly depict the pancreatic carcinoma cells to gather information about the arrangement of the network in the cell. Combining both the microrheology and the pictures of the electron microscope allow to check whether the measurement at a specific cell was meaningful and the determined mechanical properties are appropriate input parameters for numeric simulations. For this purpose a method was developed for marking the position of the analyzed cell during the microrheology measurement and find again the same position in the electron microscope to examine the structure of the network and the positions of the traced beads.

BP 5.26 Mon 17:15 Poster B1

Non-Gaussian tube width distributions in entangled solutions of filamentous actin — ●INKA LAUTER¹, MASASHI DEGAWA¹, NORBERT KIRCHGESSNER¹, BERND HOFFMANN¹, RUDOLF MERKEL¹, MARGRET GIESEN¹, JENS GLASER², DIPANJAN CHAKRABORTY², and KLAUS KROY² — ¹Institute of Bio- and Nanosystems 4: Biomechanics, Forschungszentrum Jülich GmbH, 52425 Jülich — ²Institute of Theoretical Physics, University of Leipzig, PF 100920, 04009 Leipzig, Germany

Actin is evolutionarily one of the most conserved components in eukaryotic cells. Actin filaments are interesting model systems to study the physical properties of semi-flexible polymers. One theoretical concept is the tube model which provides a simple phenomenological description of the complicated topological constraints in entangled solutions of semi-flexible polymers. Here, the tube defines the accessible space of a fluctuating filament which is topologically constrained by the presence of other filaments. Various theoretical models assume the tube width along the filament contour being constant. However, recent experiments and simulations showed substantial deviations from this assumption. We introduce a systematic extension [J. Glaser, I. Lauter et al., arXiv:0910.5864] of Morse's binary collision approximation (BCA) [D.C. Morse, PRE 63:031502 (2001)], which predicts a varying tube width along the filament contour. We measured tube width distributions of individual actin filaments as a function of filament density. Our experimental data are well described by the extended BCA model.

BP 5.27 Mon 17:15 Poster B1

Transport of a semiflexible filament in a network — ●TERESA BAUER¹, FELIX HÖFLING^{1,2}, ERWIN FREY¹, and THOMAS FRANOSCH^{1,3} — ¹Arnold Sommerfeld Center (ASC) for Theoretical Physics and Center for NanoScience (CeNS), Fakultät für Physik, Ludwig-Maximilians-Universität München, Germany — ²Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United

Kingdom — ³Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Germany

The cytoskeleton of a cell is comprised of a network of various biopolymers. A prominent example is the filamentous actin, a semiflexible polymer studied extensively also *in vitro*. The transport of a single semiflexible filament in a strongly entangled network is highly directed along the confining tube formed by the surrounding network.

We have investigated the dynamics of a semiflexible filament in a plane in the presence of immobilized obstacles mimicking the constraints of the crosslinked network. The inextensibility constraints are encoded via a bead-rod-algorithm extended by a suitable collision rule and extensive simulations are performed. In particular we measure the translational and rotational diffusion investigated for a broad density range. Furthermore we discuss the role of undulations as the filament leaves its confining tube when the persistence length is varied.

BP 5.28 Mon 17:15 Poster B1

Selecting structure prediction candidates using sequence-derived structure profiles — ●KATRIN WOLFF¹, MICHELE VENDRUSCOLO², and MARKUS PORTO¹ — ¹Institut für Festkörperphysik, TU Darmstadt, Germany — ²Department of Chemistry, University of Cambridge, UK

Selection of promising structure candidates for high-resolution refinement is a crucial step in protein structure prediction. Several prediction tools rely on the generation of very many low-resolution candidates and subsequent high-resolution refinement. Only few of the structures, however, are of sufficient quality to converge in the refinement step. Due to limited computer time it is therefore important to restrict the number of candidates and select only the few good ones. As the energy function used in the coarse-grained step is not very useful for recognizing good structures, we here discuss the use of structure profiles for this task. We show that the exact profile (derived from the native structure) is very reliable in choosing candidates with low cRMSD and TMscore to the native structure and clearly outperforms other methods such as filtering by energy or clustering. These profiles can also be predicted to good accuracy from the amino acid sequence. We therefore explore the use of sequence-derived profiles and demonstrate that for sufficiently high prediction accuracy this approach is also superior to the other methods of filtering and independent of the method used for coarse-grained structure generation [1].

[1] K. Wolff, M. Vendruscolo, and M. Porto, *Proteins*, 2009 in print, DOI 10.1002/prot.22533.

BP 5.29 Mon 17:15 Poster B1

Interaction of Boron-Clusters with liposomes : Influence on the Zeta-potential — ●ALEKSANDRE JAPARIDZE¹, MATHIAS WINTERHALTER¹, and DETLEF GABEL² — ¹School of Science and Engineering, Jacobs University Bremen, Campus Ring 1,D-28759 Bremen,Germany — ²Department of Chemistry, University Bremen, PO Box 330440, D-28334 Bremen, Germany

Boron clusters have potential for clinical use in the so-called boron neutron therapy. Therefore it is of interest to study the interaction between the clusters and the cells. In order to quantify the affinity of charged Boron cluster to lipid membranes we may use Zeta-potential measurements of liposomes. In following experiments we have been investigating the interaction of negatively charged boron-clusters with neutral POPC liposomes, focusing on the change in Zeta potential. Liposomes were used as a cell membrane model for the experiments. For example, the Zeta-potential of POPC liposomes with Na₂B₁₂I₁₂ clusters was -47mV at pH value 7.4 .

BP 5.30 Mon 17:15 Poster B1

Dynamic measurement of the persistence length of intermediate filaments — ●BERND NÖDING, SUSANNE BAUCH, and SARAH KÖSTER — Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany

The eukaryotic cytoskeleton, which is responsible for the mechanics of the cell, mainly consists of three types of fibrous proteins. While microtubules and microfilaments are highly conserved, intermediate filaments (IFs) vary from cell type to cell type. Here, we focus our study on vimentin, which occurs in cells of mesenchymal origin. Investigations of mechanical properties of individual filaments are a necessary prerequisite for a better understanding of the mechanics of biopolymer networks and eventually whole cells. The mechanical rigidity of a polymer is characterized by its persistence length L_p . In the case of vimentin, L_p was found to be on the order of one μm using atomic

force and electron microscopy. However, in both cases the filaments need to be adhered to a substrate. Our aim is to perform dynamic measurements of filaments in solution without any interaction with a substrate whatsoever. To this end we fluorescently label the filaments and confine them in microchannels with a width of about one μm , thereby realizing the Odijk confinement regime. The contour of the filaments is imaged by epi-fluorescence microscopy. The purpose of the channels is twofold: the filaments are prevented from coiling and they are restrained to a single focal plane. Since IFs can be classified as semiflexible polymers we assume the worm-like-chain model for our fluctuation analysis. The channel walls are included as parabolic potential in our model.

BP 5.31 Mon 17:15 Poster B1

Microfluidic Drops as Tuneable Bio-Environments — ●CHRISTIAN DAMMANN, BERND NÖDING, SUSANNE BAUCH, and SARAH KÖSTER — Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany

The structure and function of biological systems depends sensitively on their bio-environmental context. Here, we present a novel microfluidic device that offers the possibility to monitor the behavior of biological systems over time while tuning external parameters. We produce monodisperse aqueous emulsion drops that act as picoliter bio-compartments in a continuous oil phase. A series of drops is created and the content compositions are varied from drop to drop. The drops are then stored in the device and thus long-time observations are possible while the information about the composition of each drop is known. Possible applications for such microfluidic platforms are manifold. Here, we show the utility of the device by investigating assembly and network formation of vimentin intermediate filaments in confined geometry by imaging fluorescently tagged proteins. Vimentin assembly and network formation depends on ionic strength. Therefore, we define the salt concentration for each drop. These drop series are stored and observed over time by means of fluorescence microscopy. This study is an important step towards a better understanding of the assembly dynamics of vimentin and the final structure of the networks and demonstrates the well-defined conditions which can be established in microfluidic devices.

BP 5.32 Mon 17:15 Poster B1

Biomimetic Modelling of Cellular Morphogenesis — ●BJÖRN STUHRMANN, FENG-CHING TSAI, and GJJSJE KOENDERINK — FOM Institute AMOLF, Amsterdam, The Netherlands

Migration and division of living cells are ultimately generated by the coupled morphogenesis of the cell cytoskeleton and the plasma membrane. Despite impressive advances in the identification of the cell molecular inventory, the underlying processes are still poorly understood. We strive to discern biophysical principles of cytoskeletal and cell morphogenesis. To this end, we construct a biomimetic model system of the cytoskeleton by confining to liposomes cross-linked actin biopolymers driven by the active processes of polymerization and motor sliding. The key innovation of this project lies in its systematic biomimetic approach alongside quantitative morphological and mechanical examination and theoretical modelling.

BP 5.33 Mon 17:15 Poster B1

A strong structural instability in the microtubule lattice revealed by imaging and molecularly reconstructing the inside of flattened microtubules — ●JAN KLEEBLATT, FLORIAN HAGEN, IWAN A.T. SCHAAP, and CHRISTOPH F. SCHMIDT — Drittes Physikalisches Institut, Fakultät für Physik, Georg-August-Universität Göttingen

Microtubules (MT) are an important part of the cytoskeleton. In the living cell microtubules are non-equilibrium polymers with complex chemical and mechanical properties. These properties are likely to be strongly influenced by microtubule-associated proteins (MAPs). We have here used atomic force microscopy to image MAPs (Clip 170) and the MT fine structure. We found evidence for an intriguing structural instability in microtubules which leads to a zig-zag pattern of protofilaments in MTs that are flattened inside-out against the substrate surface. We performed molecular reconstructions based on the tubulin atomic structure to model our results in terms of the local arrangement of tubulin monomers in neighboring protofilaments.

BP 5.34 Mon 17:15 Poster B1

Self-assembled 3-dimensional DNA structures investigated with fluorescence microscopy — ●ALEXANDER BENKSTEIN¹, ZHAO

WANG¹, CHRISTOPH ERBEN², IWAN A. T. SCHAAP¹, ANDREW J. TURBERFIELD², and CHRISTOPH F. SCHMIDT¹ — ¹Drittes Physikalisches Institut, Fakultät für Physik, Georg-August Universität, 37077 Göttingen — ²Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU, UK

Well established synthesis procedures and the "programmability" of DNA binding via base pairing makes DNA ideal for the design of nanostructures.

We here investigate the characteristics of self-assembled tetrahedra from DNA oligomers with dimensions smaller than 10 nm. We labeled tetrahedra with the intercalating dye YOYO-1 and imaged using total internal reflection fluorescence microscopy. We investigate the photobleaching of the dye bound to the DNA tetrahedron and estimate the number of dyes on the single structure.

BP 5.35 Mon 17:15 Poster B1

Multivariate analysis for surface-enhanced Raman scattering (SERS) probe multiplexing and imaging in biological matrices — ●ANDREA MATSCHULAT^{1,2}, DANIELA DRESCHER^{1,2}, and JANINA KNEIPP^{1,2} — ¹Institut für Chemie, HU, Brook-Taylor-Str. 2, 12489 — ²Bundesanstalt für Materialforschung und -prüfung (BAM), Richard-Willstätter-Str.11, 12489 Berlin

Raman Spectroscopy as a non-destructive spectroscopic technique allows the study of vibrational fingerprints by which chemical and biological compounds can be identified. An improvement of the spatial resolution on the nm-scale is provided by local optical fields surrounding plasmonic nanostructures which are excited by the incident electromagnetic field. Such so-called surface-enhancement provides more sensitive detection. SERS has therefore attracted considerable interest for its application in bioanalytical chemistry. SERS offers numerous opportunities in the study of spectral changes during molecular interactions in complex biosystems. We demonstrate a multivariate approach for SERS hybrid probe multiplexing and imaging implementing principal component analysis and cluster algorithms. As a first application, we introduced two biocompatible Raman reporter molecules attached to Au nanoaggregates into living 3T3-cells. Such a hybrid probe approach enables the identification of different SERS probes in multiplexed experiments. We present results of hyperspectral mapping analysis providing us information about the cellular uptake, localization and amount of both reporter molecules inside the biosystem.

BP 5.36 Mon 17:15 Poster B1

In situ actin bundling and network formation using microfluidics — SIDDHARTH DESHPANDE¹, DAGMAR STEINHAUSER², and ●THOMAS PFOHL^{1,2} — ¹Chemistry Department, University of Basel, Basel, Switzerland — ²Max Planck Institute for Dynamics and Self-Organization, Göttingen

The approach is to use microflow devices consisting of microchambers connected to a main channel through narrow connecting channels. High flow conditions can be achieved in the main channel to control the concentration and composition of aqueous solution while the transport within the microchambers and connecting channels is governed by diffusion. Rhodamine labeled actin monomers are used to form filamentous actin under appropriate conditions (KCl concentration). Once polymerized, the actin filaments formed inside the chamber will remain confined within it. The network formation can be induced in presence of cross-linking proteins. Fluorescence microscopy is used to study these phenomena. This *in situ* study will help us in understanding the mechanisms of bundle and network formation with increasing hierarchy and complexity.

BP 5.37 Mon 17:15 Poster B1

Testing the elastic anisotropy of microtubules by leveraged bending experiments — ●FABIAN STIEWE and CHRISTOPH F. SCHMIDT — Drittes Physikalisches Institut, Georg-August-Universität Göttingen

Microtubules are cylindrical protein shells with a distinct structural anisotropy, stemming from their construction from straight protofilaments that are connected more weakly laterally. This could lead to a length-dependence of the flexural rigidity and the persistence length of microtubules as reported recently. The effect is the stronger the "weaker" the connection between the protofilaments gets. We present here a method for sensitively testing this model. Two optical traps are used to suspend a microtubule with the help of two micron-sized beads. A force developed by pulling the traps apart leads to bending of the microtubule. A large difference between Young's and shear

modulus should lead to a significant back-bending of the free ends of a bent microtubule, minimizing its free energy. We have used finite-element simulations to check the expected magnitude of this relaxation effect and compare the simulation results with data obtained in bending experiments using optical traps. To date we have not observed any back-bending in our experiments. Therefore we conclude that the difference in Young's and shear modulus might be too small to cause some of the reported effects.

BP 5.38 Mon 17:15 Poster B1

Structural organization and mineral distribution in load-bearing exoskeleton parts of the edible crab *Cancer pagurus* — KATJA HUEMER¹, SIMONE KARSTEN², KEERTHIKA BALASUNDARAM², DIERK RAABE², SABINE HILD¹, and HELGE-OTTO FABRITIUS² — ¹Department of Polymer Science, Johannes Kepler University Linz, Altenbergerstraße 69, 4040 Linz, Austria — ²Department Microstructure Physics and Metal Forming, Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40237 Düsseldorf, Germany

The exoskeleton of crustaceans is a structural entity formed by the cuticle. It is a hierarchically organized chitin-protein fiber based nanocomposite, organized in form of a twisted plywood that can be reinforced in the load-bearing parts with both crystalline and amorphous biominerals. During evolution, all parts of the exoskeleton were optimized to fulfill different functions according to the different ecophysiological strains faced by the animals. This is mainly achieved by modifications in microstructure and chemical composition. To understand the relationship between structure, composition, mechanical properties and function we characterized the carapace cuticle of the edible crab *Cancer pagurus* with light and scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), confocal mikro-Raman spectroscopy and nanoindentation tests. The results show local differences in structure and mineralization on the fiber level as well as the twisted plywood level resulting in a pronounced gradient of the reduced elastic modulus throughout the carapace cuticle of *C. pagurus*.

BP 5.39 Mon 17:15 Poster B1

Flax or Nettle? Using X-ray Microdiffraction to Identify Ancient Textile Fibres — STJEPAN HRKAC¹, BRIDGET MURPHY¹, MARTIN MUELLER¹, MARGARITA GLEBA², ULLA MANNING², MARIE-LOUISE NOSCH², GIANANGELO BRACCO³, MANFRED BURGHAMMER⁴, HANS GEORG GEBEL⁵, BODIL HOLST⁶, and CHRISTIAN BERGFJORD⁶ — ¹Laboratory Institut fuer Exp. und Angewandte Physik Universitaet Kiel Leibnizstrasse 19 D-24118 Kiel Germany — ²Laboratory Centre for Textile Research The SAXO Institute University of Copenhagen Njalsgade 106 2300 KØbenhavn Denmark — ³Laboratory Dipartimento di Fisica Università di Genova INFN and CFSBT of CNR Via Dodecaneso 33 I-16146 Genova Italy — ⁴Laboratory E.S.R.F. 6 rue Jules Horowitz B.P 220 F-38043 Grenoble Cedex France — ⁵Laboratory Freie Universitaet Berlin Institut fuer Vorderasiatische Altertumskunde Huttenweg 7 D-14195 Berlin Germany — ⁶Laboratory Department of Physics and Technology, University of Bergen N-5007 Bergen Norway

Remains of cloth from one of the most famous Danish bog bodies, the Huldremose Woman (55 AD), believed to stem from a hitherto unknown garment, were investigated by a combined approach using microscopy (optical and SEM) X-ray microbeam diffraction, X-ray microbeam fluorescence and micro Raman. For identification purposes samples were compared to modern fibers. We present our preliminary results in this poster

BP 5.40 Mon 17:15 Poster B1

Network properties of an aggregate of perylene bisimide based molecules — CARLO DI GIAMBATTISTA¹, ANKE LEITNER¹, MASOUD AMIRKHANI¹, ANNE-MARIE SAIER¹, SUHRIT GHOSH³, FRANK WÜRTHNER³, MICHAEL BEIL², and OTHMAR MARTI¹ — ¹Institute of Experimental Physics, Ulm University, Germany — ²Institute of Internal Medicine I, Ulm University Hospital, Germany — ³Institute of Organic Chemistry, Würzburg University, Germany

Due to non-covalent binding the perylene bisimide based molecules form a network able to bind a solvent. This combination of network and solvent is a so called organogel. Organogels are excellent examples of the construction of higher order self-assembled structures from properly designed small-molecule building blocks*. Because of the type of binding we are interested in the resulting network properties. We want to compare those properties to the ones of intermediate filaments. These filaments are as well assembled by small building blocks. To gain an idea of the microscopic structure of the organogels we use atomic force microscopy. Furthermore we do rheological measurement on the phase transition as well as on the final gel.

*S. Ghosh et al. Chem. Eur. J. 2008, 14, 11343-11357

BP 5.41 Mon 17:15 Poster B1

Investigation of the nanomechanical properties of the cytoskeleton protein Keratin 8/18: Force microscopy measurements and simulations — ANDREAS HÄUSSLER¹, TOBIAS PAUST¹, ANKE LEITNER¹, MICHAEL BEIL², HARALD HERRMANN³, and OTHMAR MARTI¹ — ¹Institute of Experimental Physics, Ulm University — ²Institute of Internal Medicine I, Ulm University Hospital — ³Division of Molecular Genetics, German Cancer Research Center, Heidelberg

The protein Keratin 8/18 is one of the major components of the cytoskeleton of pancreatic cancer cells. Assembling into intermediate filaments, the protein forms a network in the cell that is responsible for the cell stiffness. As the network is determined by its building blocks, it seems to be interesting to investigate the nanomechanical properties of single intermediate filaments. By etching we create a topographic surface lattice with a length scale of about 1 micrometer. The filaments can be suspended between two mesas and be deflected by mechanical stimuli. The force measured, related to the elongation, gives us information on the elasticity of the filaments. Moreover we simulate the filaments with a finite element model. In a first approach, we assume the filaments to be a homogeneous material and adjust our calculation to our measurement results. This should give us a hint on the averaged Young's modulus. Preliminary results will be presented.

BP 6: Posters: DNA and DNA Enzymes

Time: Monday 17:15–20:00

Location: Poster B1

BP 6.1 Mon 17:15 Poster B1

Electrostatic effects in DNA cyclization and DNA looping by proteins — ANDREY CHERSTVY — IFF-2, FZ Jülich, Germany

We calculate analytically the electrostatic energy of ring formation for highly charged DNA-like polyelectrolyte chain in the ground state [1]. We study how the degree of counterion condensation differs on small DNA rings as compared to Manning prediction for straight polyelectrolytes. We apply the model to analyze how cyclization factors of short DNAs are modified, as compared to Shimada-Yamakawa theory for neutral polymers. We also perform simple computer simulations to assess the free energy of end joining of fluctuating DNA at different salinities. We study also the looping of thin charged elastic filaments under applied torque and forces, using the elasticity theory equations [2]. We predict that larger twist rates are needed to create loops in charged cables as compared to neutral ones. We determine optimal shapes of charged loops at different salinities showing that at low salts more open loops are favored due to enhanced mutual repulsion of charges. This loop opening is consistent with results of recent

computer simulations on formation of DNA loops by lac repressor.

[1] A. G. Cherstvy and R. Everaers, in preparation. [2] A. G. Cherstvy, submitted to JPCB.

BP 6.2 Mon 17:15 Poster B1

Information transfer and DNA microarrays — CHRISTIAN TRAPP and ALBRECHT OTT — Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken

DNA microarrays take advantage of the molecular recognition of DNA hybridization. They consist of surface bound probe ssDNA, which will selectively bind to complementary target strands in solution. They are widely employed in biotechnological applications such as genome expression profiling in order to assess complex mixtures of DNA. In spite of their importance DNA hybridization on microarrays remains poorly understood. We have shown that the binding to DNA microarrays can be modeled well in simple cases, where the length of probe and targets match. Here we investigate the binding of longer targets to microarrays, which may hybridize to the probes forming loops. We sys-

tematically vary loop position and loop size and check, if the result can be reproduced with simple theoretical models at thermal equilibrium. We discuss the influence of loops in terms of competitive binding. The ultimate goal is to explore the physical limits of information that can be conveyed through complex mixtures of DNA.

BP 6.3 Mon 17:15 Poster B1

High resolution optical tweezers for study of eukaryotic transcription — ●NOEMI MARIA PORCELLATO, ADAM MUSCHIELOK, and JENS MICHAELIS — Dep. für Chemie und Biochemie LMU München, Munich, Germany

For the single-molecule analysis of enzymes moving on DNA, for instance eukaryotic RNA polymerase II (Pol II), we have built a high resolution dual-trap optical tweezers apparatus. The main aim is to achieve very high spatial resolution (down to the level of single base-pairs) and low drift. Since both traps are created by the same laser and the optical path where the beams are separated is minimized, drift is essentially eliminated. Together with sound isolation and enclosure of the instrument we achieve high spatial resolution shown in test experiments with DNA tethers. In order to efficiently load beads into the traps and to control buffer conditions during the experiments we use a custom built 5 channel microfluidic flow system. We discuss general design considerations, show calibration of the trap stiffness, first test measurements and preliminary Pol II transcription data.

BP 6.4 Mon 17:15 Poster B1

single-molecule force spectroscopy on phoB-DNA complexes — ●MICHAEL BIRLO¹, KATRIN WOLLSCHLÄGER², RAINER ECKEL³, NORBERT SEWALD⁴, and DARIO ANSELMETTI⁵ — ¹Department of Physics Bielefeld University 33615 Bielefeld (Germany) — ²Department of Chemistry Bielefeld University 33615 Bielefeld (Germany) — ³Department of Physics Bielefeld University 33615 Bielefeld (Germany) — ⁴Department of Chemistry Bielefeld University 33615 Bielefeld (Germany) — ⁵Department of Physics Bielefeld University 33615 Bielefeld (Germany)

Interactions between proteins and DNA are essential for the regulation of cellular processes in all living organisms. In this context, it is of special interest to investigate the sequence-specific molecular recognition between transcription factors and their cognate DNA sequences. As a model system, peptide and protein epitopes of the DNA-binding domain (DBD) of the transcription factor PhoB from *Escherichia coli* are analyzed with respect to DNA binding at the single-molecule level. Quantitative AFM-DFS analysis proves the specificity of the interaction and yields force-related properties and kinetic data, such as thermal dissociation rate constants. An alanine scan for strategic residues in both peptide and protein sequences is performed to reveal the contributions of single amino acid residues to the molecular-recognition process.

BP 6.5 Mon 17:15 Poster B1

Binding Kinetics of Bisintercalator Triostin A Measurements with Optical Tweezers — ●ANDY SISCHKA¹, CHRISTOPH KLEIMANN², ANDRÉ SPIERING¹, KATJA TÖNSING¹, NORBERT SEWALD³, ULF DIEDRICHSEN⁴, and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanosciences, Bielefeld University, 33615 Bielefeld, Germany — ²Institut für Bio- und Nanosysteme (IBN-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ³Organic and Bioorganic Chemistry, Bielefeld University, 33615 Bielefeld, Germany — ⁴Organic and Biomolecular Chemistry, Göttingen University, 37077 Göttingen, Germany

We present single molecule binding studies where the intercalative binding kinetics of Triostin A to λ -DNA was investigated by measuring the force/extension response with our optical tweezers system [1]. These curves were analyzed based on a method for monointercalators that was extended to bisintercalators. Our measurements with Triostin A showed non-equilibrium phenomena, resulting in large hysteresis effects during a fast stretching/relaxation cycle, whereas at slow velocities, the system reaches an equilibrium state and the hysteresis vanishes. Subsequent binding analysis reveals an exponential dependence of the association constant on the external force as well as a decreasing binding site size. To explain the high-force binding site size, a new model for bisintercalation of Triostin A is proposed, where the deformation of the Triostin A binding site could thereby repeal the neighbor exclusion principle, leading to closer packaging of Triostin A.

[1] Ch. Kleimann, A. Sischka et al., *Biophys. J* 97, 2780-2784 (2009)

BP 6.6 Mon 17:15 Poster B1

Optical Tweezers Measurements of Threading Individual DNA and DNA-Ligand-Complexes through Solid-State Nanopores — ●ANDRE SPIERING¹, ANDY SISCHKA¹, TANJA PLÖTZ¹, CHRISTOPH KLEIMANN², KATJA TÖNSING¹, INA SEUFFERT³, and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanosciences, Bielefeld University, 33615 Bielefeld, Germany — ²Institut für Bio- und Nanosysteme (IBN-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ³Bioenergetics, Institute of Chemistry, Technische Universität Berlin, 10623 Berlin, Germany

We present a high precision 3D optical tweezers setup, which is incorporated in an optical inverted microscope and uses the detection of backscattered light to measure forces in the sub-pN regime and to manipulate single DNA molecules. With this novel setup, single dsDNA-molecules were threaded into a solid-state nanopore and the electrostatic forces and the ionic currents through the pore were measured simultaneously. In the force-distance diagrams, individual force steps could be observed for each DNA-molecule entering the nanopore and distinct force signals could be identified upon actively withdrawing the single DNA-molecule out of the nanopore. We found that binding of dedicated protein ligands (peroxiredoxin, *E. coli* RNA-polymerase, and RecA) to dsDNA caused a significant change in the apparent electrostatic forces that are required to thread and unthread the DNA-ligand-complex through the nanopore. Furthermore, we were able to detect the exact position of the binding ligand along the DNA strand with nanometer precision.

BP 6.7 Mon 17:15 Poster B1

Visualisation of PCNA monoubiquitination in vivo by single pass spectral imaging FRET microscopy — ●CHRISTOPHER BATTERS¹, HANNAH ZHU², and JULIAN SALE² — ¹Institute of Physiology, Ludwig-Maximilians-Universität, Pettenkofenstr. 12, 80336 München, Germany — ²Medical Research Council Laboratory of Molecular Biology, Division of Protein & Nucleic Acid Chemistry, Hills Road, Cambridge, CB2 0QH, U.K.

Monoubiquitination of the DNA sliding clamp, PCNA, plays a central role in the control of damage bypass during replication. By combining a widely-spaced FRET donor/acceptor pair (CFP and mRFP) with spectral imaging, we have developed a simple method for the visualisation of PCNA monoubiquitination in both fixed and live cells with a single imaging pass. We validate the method with genetic controls in the avian cell line DT40 and examine the intracellular dynamics of PCNA ubiquitination following subnuclear UV irradiation. This general approach is likely to be of utility for live imaging of monoubiquitination and sumoylation of a wide range of substrates in vivo.

BP 6.8 Mon 17:15 Poster B1

Stretching of DNA/TmHU-protein complexes in SMD simulations — ●CARSTEN OLBRICH and ULRICH KLEINEKATHÖFER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

The protein HU is a member of a family of prokaryotic proteins that interacts with the DNA in a non-specific way [1]. Its major function is the binding, compaction and stabilization of DNA. Steered molecular dynamic (SMD) simulations are applied to DNA which is bound to the HU protein of the bacteria *Thermotoga maritima* (TmHU). Using these all-atom simulations including explicit water and about 80,000 atoms in total, we are able to gain insight into the discrete disruptions events which occur when the DNA releases from the protein body. These disruptions were first observed in experiments performed with optical tweezers [2]. We will present a detailed view of those events on the atomistic scale.

[1] R. Dame and N. Goosen, *FEBS Lett.* **529**, 151 (2006).

[2] M. Salomo, F. Kremer et al., *J. Mol. Biol.* **359**, 769 (2006).

BP 6.9 Mon 17:15 Poster B1

Unfolding mechanisms and the free energy landscape of the DNA i-motif — ●JENS SMIAITEK and ANDREAS HEUER — Westfälische Wilhelms-Universität Münster, Institut für Physikalische Chemie, 48149 Münster, Germany

Since the discovery of the DNA i-motif, the formation and function of this specific structure has attracted broad interest. Even the pH-dependent reversible folding/unfolding mechanism has been nowadays used in technological applications like in the construction of nanocontainers. The unfolding mechanism has been investigated in high temperature simulations and is characterized in terms of the eigenvectors. Furthermore we present the results of Molecular Dynamics simulations for the free energy landscape which has been computed by a recently

developed method for several collective variables.

BP 6.10 Mon 17:15 Poster B1

Towards sub second imaging of DNA compaction by AFM — ●JAN KNAPPE¹, SEBASTIAN HANKE¹, SZABOLCS SÖRÖS², CHRISTOPH F. SCHMIDT¹, WOLFGANG FISCHLE², and IWAN A. T. SCHAAP¹ — ¹III. Physikalisches Institut, Georg-August-Universität, 37077 Göttingen — ²Max Planck Institute for Biophysical Chemistry, 37077 Göttingen

To compact and organize DNA the eukaryotic cell has developed several packaging steps. DNA is wrapped around histones to form nucleosomes, which in turn can be linked by other proteins to form larger aggregates. To study this system on a single molecule level we have set out to use atomic force microscopy (AFM) in liquid to image the binding and unbinding of DNA to the histone octamer. However to be able to study the dynamics of nucleosomal DNA on a biological relevant time scale, we need techniques that permit image acquisition in a second or faster. We will present our first results that combine imaging at low forces (~ 100 pN) with a high temporal resolution.

BP 6.11 Mon 17:15 Poster B1

BP 7: Posters: Biological Machines, Motor Proteins

Time: Monday 17:15–20:00

Location: Poster B1

BP 7.1 Mon 17:15 Poster B1

Modeling on the hydrodynamic interaction between microswimmers — ●JOHANNES GREBER and RUDOLF FRIEDRICH — Institut für Theoretische Physik, WWU Münster, Wilhelm-Klemm-Str. 9, 48149 Münster

We are interested in swimming bacteria consisting of a head and a couple of flagella. Generally it shows two states of motion: On the one hand by bundling the counterclockwise rotating flagella the bacterium translates. On the other hand the bacterium tumbles or rotates, when one flagellum rotates clockwise. Using the velocity field created in the surrounding fluid by these movements bacteria can interact with each other, which leads to the question, if there are collective effects among several bacteria.

Assuming that the velocity field of one bacterium consists of two rigidly coupled point vortices in some given distance, we derive the equations of motion for the case of interaction between two swimming objects. Moreover, we make some predictions for the trajectories of the swimmers with the help of a linear stability analysis.

BP 7.2 Mon 17:15 Poster B1

Monitoring a single Sec translocase complex in an anti-Brownian electrokinetic (ABEL) trap — ●TORSTEN RENDLER¹, STEFAN ERNST¹, KARIN SEYFERT¹, ANDREAS KUHN², and MICHAEL BÖRSCH¹ — ¹3. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Institut für Mikrobiologie und Molekularbiologie, Universität Hohenheim, Germany

Translocation of polypeptides in *E. coli* cells is catalysed by the membrane protein complex SecAYEG. This process is powered by ATP (adenosine triphosphate) hydrolysis of the SecA motor component. To investigate the translocation process, SecAYEG is reconstituted into lipid vesicles and the conformational changes during polypeptide transport are monitored by internal fluorescence resonance energy transfer (FRET). Therefore, the different SecAYEG subunits were labeled with various fluorescent markers. Previous confocal measurements of single translocases in solution suffered from the limited observation time due to Brownian motion. To increase the observation time we combined a confocal setup for FRET measurements with an anti-Brownian electrokinetic (ABEL) trap. The ABEL-trap was developed by A.E. Cohen (Harvard) and W.E. Moerner (Stanford) and is based on an active feedback mechanism consisting of a EMCCD camera to locate the complex and electrodes to apply an electrical field across the trapping region. We present preliminary FRET data of a single translocases held in solution by the ABEL-trap.

BP 7.3 Mon 17:15 Poster B1

Cooperative effects in the inhibition of a Kinesin-5-head/Kinesin-1-stalk chimera by monastrol — STEFAN LAKÄMPER^{1,2,3}, CHRISTINA THIEDE¹, ●ANDRÉ DÜSELDER¹, STEFANIE REITER^{1,3}, LUKAS C. KAPITEIN^{2,4}, ERWIN J.G. PETERMAN²,

Bayesian inference based evaluation of DNA hairpin dynamics — ●WOLFGANG KÜGEL, ADAM MUSCHIELOK, and JENS MICHAELIS — Ludwig-Maximilians-Universität, Munich, Germany

Fluorescence-correlation-spectroscopy (FCS) combined with FRET is a powerful tool to analyze dynamics in biological systems. In comparison to other approaches this technique is not limited to a narrow range of rates and can detect dynamics from the ns to s time-scale. However, the key problem is to extract the rates hidden in the correlation curve by fitting a set of parameters. Several different fitting approaches have been described in recent years but the extraction of relevant information is still limited by the fact that the set of starting values chosen predefines the result. This happens as reasonably different sets of parameters result in fitting curves that describe the data equally well. To evaluate and weigh all possible fit results for our data we have used a Bayesian inference approach and globally evaluated all information available. A first application of this approach is shown based on a representative selection of different FRET pairs bound to a hairpin DNA. We discuss how dye selection can influence the rates of hairpin opening and closing.

and CHRISTOPH F. SCHMIDT^{1,2,3} — ¹Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany — ²Department of Physics and Astronomy and Laser Centre, VU University Amsterdam, The Netherlands — ³DFG-Research Centre for Molecular Physiology of the Brain, CMPB, Göttingen, Germany — ⁴Current address: Erasmus University Medical Centre, Rotterdam, The Netherlands

Several kinesin motors are required for proper assembly of the mitotic spindle. The homo-tetrameric bipolar Kinesin-5 can cross-link and slide antiparallel microtubules apart by a motility mechanism comprising diffusional and directional motility. In order to explore the basic kinesin-5 motor activity, we generated a stably dimeric Kinesin-5 construct, Eg5Kin, consisting of motor domain and neck-linker of *Xenopus laevis* Kinesin-5 and neck coiled-coil of *Drosophila melanogaster* Kinesin-1. This chimera is highly processive. We studied the effect of the Kinesin-5-specific inhibitor monastrol in single-molecule fluorescence assays. In order to find out if one or two monastrol molecules terminate a run, we analyzed the monastrol concentration dependence of the motor run length. We found a Hill coefficient of about 2. We discuss in how far this means that two monastrols need to be bound to create an effect and what kind of cooperativity this implies for binding of monastrol to the two heads of a motor dimer.

BP 7.4 Mon 17:15 Poster B1

An in vivo approach to probing mechanotransduction apparatus function — ●BJÖRN NADROWSKI, THOMAS EFFERTZ, and MARTIN GÖPFERT — Abt. Zelluläre Neurobiologie, Universität Göttingen, MPI für Experimentelle Medizin, Hermann-Rein-Str. 3, 37075 Göttingen

The opening and closing of ion channels are mechanical events. These gating movements can be monitored in mechanosensitive ion channels provided that these channels are directly gated by force via macroscopic structures that thereby reflect the movements of the channels' gates. When coupled to molecular adaptation motors, these mechanosensitive ion channels form a transduction machinery that allows for active amplification while translating mechanical into electrical stimuli. Profiting from this experimental advantage, we have probed ion channel mechanics inside an intact *Drosophila* mechanosensory system. A physical model of this system is presented that quantitatively links ion channel mechanics, movements of molecular adaptation motors, and macroscopic mechanical events. Using this model, molecular parameters such as the gating energy required to open a single ion channel can be deduced. These energies have been determined for two force-gated ion channels. We also present evidence that these two channels are arranged in parallel in the transduction apparatus and may serve the detection of different stimuli amplitudes.

BP 7.5 Mon 17:15 Poster B1

A fast tetrameric Kinesin-5/Kinesin-1 chimera - a tool to study mechanisms of Kinesin-5 regulation — ●CHRISTINA

THIEDE^{1,2}, STEFAN LAKÄMPER^{1,2}, ALOK D. WESSEL¹, STEFANIE REITER¹, and CHRISTOPH F. SCHMIDT¹ — ¹Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany — ²these authors contributed equally to this work

The homo-tetrameric Kinesin-5 motor protein Eg5 from *X. laevis* drives relative sliding of anti-parallel microtubules (MT) by the processive action of its two opposing sets of dimeric motors. On a single MT, individual tetrameric motors move slowly (≈ 20 nm/s), but processively, alternating between a diffusional and a directional mode, while motors moving between two MTs move in a highly directional and processive fashion. In order to obtain a tetrameric model system with more easily discernible properties and motile phases, we have constructed a tetrameric chimera by replacing Eg5 motor domain and neck linker by the homologous regions of *D. melanogaster* Kinesin-1 (DK4mer). In surface-gliding assays, Dk4mer showed fast motility (553 ± 31 nm/s). Single GFP-tagged DK4mer motors moved processively along MT at comparable speeds (499 ± 3 nm/s). We observe clearly distinguished directional and diffusional episodes and an overall run length of $\approx 9 \mu\text{m}$. The DK4mer is thus an excellent model system to study regulatory aspects of Kinesin-5 due to its high speed, its long processivity and its clear separation of diffusive and directional motility.

BP 7.6 Mon 17:15 Poster B1

Direct observation of the myosin-V power stroke and its reversal — ●JAMES R. SELLERS³ and CLAUDIA VEIGEL^{1,2} — ¹Abteilung Zelluläre Physiologie, Institut fuer Physiologie, Ludwig Maximilians Universität München, Pettenkoferstrasse 12, München, Germany — ²Physical Biochemistry, National Institute for Medical Research, The Ridgeway Mill Hill, London NW7 1AA, UK — ³Laboratory of Molecular Physiology, National Heart, Lung and Blood Institute, NIH, Bethesda, MD USA 20892

Complex forms of cellular motility, including cell division, organelle trafficking or signal amplification in the auditory system, require strong coordination of the myosin motors involved. The most basic mechanism of coordination is direct mechanical interactions of individual motors that modifies their mechano-chemical cycles. Here, we used an optical tweezers-based single molecule assay to investigate the reversibility of the force generating conformational change (power stroke) of single myosin-V motor heads. By applying load to the head shortly after binding to actin, we found that at a certain load, the power stroke could be reversed. At this load the motor fluctuated between an actin-bound pre- and a post-power stroke conformation. This dramatic, load-dependent mechanical instability of a single motor head might be critical to coordinate the heads of processive, dimeric myosin-V. Interestingly, highly non-linear response to load, such as power stroke reversal, can lead to coordination, synchronisation or even oscillations already amongst motors alone. These phenomena are critical for many cellular functions.

BP 7.7 Mon 17:15 Poster B1

A tetrameric Kinesin-1/Kinesin-5 chimera promotes fast relative sliding of microtubules — ●ALOK D. WESSEL, CHRISTINA THIEDE, STEFAN LAKÄMPER, STEFANIE REITER, and CHRISTOPH F. SCHMIDT — Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany

The Eg5 protein from *Xenopus laevis* is a homo-tetrameric motor protein which moves on microtubules (MT) in a processive manner and is capable of sliding two MT apart. Single motors show a directional motility with low velocity (≈ 20 nm/s) as well as a diffusive behavior on MTs. The balance between directional and diffusive behavior is altered by cargo binding, i.e. crosslinking of MTs, or by a change of the ionic strength. In order to obtain a tetrameric model system with more clearly defined properties and motile phases, we constructed a chimera, DK4mer, by replacing Eg5-motor domain and neck-linker by the homologous regions of Kinesin-1 (*D. melanogaster*). Here we show that this tetramer, just like Eg5, promotes relative sliding when binding between two microtubules. DK4mer, however, slides two antiparallel MTs apart with a ~ 40 fold higher velocity than Eg5, between 700 and 1100 nm/s. In multi-motor relative gliding assays, different binding geometries and velocities could be observed depending on the relative MT polarity and on residual motors on the substrate surface. We further measured the dependence of relative sliding on the ionic strength. Whereas surface gliding velocity remained unchanged, the relative velocity of two MT increased by ~ 400 nm/s when increasing salt concentration from 0 to 70 mM KCl in 30 mM Pipes buffer.

BP 7.8 Mon 17:15 Poster B1

Functional Rotation of the Transporter AcrB: The Essentials of Peristaltic Motion and Subsequent Substrate Extrusion — ●ROBERT SCHULZ¹, ATTILIO VITTORIO VARGIU², MICHAEL SCHREIBER³, PAOLO RUGGERONE², and ULRICH KLEINEKATHÖFER¹ — ¹School of Engineering and Science, Jacobs University Bremen, Germany — ²SLACS & Department of Physics, University of Cagliari, Italy — ³Institut für Physik, Technische Universität Chemnitz, Germany

The RND transporter of *E. coli*'s multidrug efflux pump AcrAB-TolC is able to export structurally and chemically different, toxic substrates, including antibiotics, via a functional rotation. The three major states of this rotation cycle were found in several asymmetric crystal structures. After initially analyzing the basic mechanisms of opening of the TolC channel [1] and of substrate extrusion by AcrB [2] separately, we have continued the analysis of the latter one. Thereby, we have focused both on the local interactions between substrate and protein, the properties of the extrusion pathway, as well as the principal sub-domain movements which lead to the peristaltic motion. Furthermore, we have investigated the possibility to pull the substrate from the final state of the previous simulations out of the exit gate to estimate whether the substrate is already free to leave the protein via diffusion, which is usually beyond the time scale of computer simulations.

[1] R. Schulz, U. Kleinekathöfer, Biophys. J. 96, 3116 (2009)

[2] R. Schulz, A.V. Vargiu, F. Collu, U. Kleinekathöfer, P. Ruggerone, submitted

BP 7.9 Mon 17:15 Poster B1

Synchronisation in a Chain of Rowers with Hydrodynamic Interaction — ●CHRISTOPHER WOLLIN and HOLGER STARK — TU-Berlin, Sekr. EW 7-1, Inst. f. Theo. Physik, Hardenbergstr. 36, D-10623 BERLIN-Charlottenburg

The ciliary beat, for example of paramecium and opalina, is coordinated such that metachronal waves move along the cell surface. There is strong evidence that hydrodynamic interactions cause these waves.

In order to study the origin of metachronal waves, we investigate the collective dynamics of a chain of periodically moving beads, called rowers, which are to abstract the ciliary beat. The beads move on line segments situated close to an infinitely extended planar wall. They are driven by a force that possesses a quadratic potential and that is reversed when the bead reaches a given amplitude in each direction. We assume the beads to be pointlike and describe their hydrodynamic interaction by the Blake tensor. Varying the distance of the segments from the wall, we can tune the range of the hydrodynamic interaction.

We find that two rowers synchronize in phase or in anti-phase depending on the respective negative or positive curvature of the driving quadratic potential. Chains with more rowers display a wealth of self-organized pattern formation. In particular, in the case where two rowers would synchronize in phase, we observe stable metachronal waves when the chain is located close to the wall, i.e., when the hydrodynamic interaction predominantly acts between nearest neighbours. Moving the chain away from the wall, the metachronal waves disappear and only transient structures form.

BP 7.10 Mon 17:15 Poster B1

Dynamic length regulation of microtubules — ●LOUIS REESE, ANNA MELBINGER, and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Microtubules are highly dynamic filaments that perform a variety of tasks in living cells. They serve as intracellular highways for molecular motors, which are transported along those tracks or diffuse in the cytosol. Here we examine mechanisms to regulate microtubule-length through the concentration of motors in the cell [1]. It is analyzed how the interplay between density-dependent transport on the tracks, and filament polymerization affects the dynamics of filament length. Employing stochastic simulations complemented by analytic calculus we identify distinct dynamic regimes. The model presented is conform with recent experiments studying in vitro microtubule depolymerization [2]. Our findings show that molecular motors can specifically control MT length fluctuations.

[1] A. Parmeggiani, T. Franosch, E. Frey, Phys. Rev. Lett. 90, 086601 (2003).

[2] V. Varga, J. Helenius, K. Tanaka, A.A. Hyman, T.U. Tanaka and J. Howard, Nat. Cell Biol. 8, 957 (2006)

BP 7.11 Mon 17:15 Poster B1

Study of H/D substitution effects on the function of the cytochrome bc_1 complex of *Rhodobacter capsulatus* — ●KATRIN JAHNS¹, NATALIA VOSKOBOYNIKOVA¹, MARIA KOZLOVA^{1,2}, and ARMEN MULKIDJANIAN^{1,2} — ¹School of Physics, University of Osnabrück, D-49069 Osnabrück, Germany — ²A.N.Belozersky Institute of Physico-Chemical Biology, Moscow State University, Moscow, 119991, Russia

The cytochrome bc_1 complex is a voltage-generating membrane ubiquinol:cytochrome c oxidoreductase [1]. We have studied the effect of the H₂O/D₂O substitution on the flash-induced turnovers of the cytochrome bc_1 complexes in the vesicular preparations of the inner cellular membranes (chromatophores) of phototrophic α -proteobacteria

Rhodobacter capsulatus. We traced the kinetics of flash-induced generation of membrane voltage by the cytochrome bc_1 complex via the spectral shifts of native carotenoid pigments and correlated them with the kinetics of electron transfer as measured in the same samples. At neutral pH, the kH/kD ratio was ca. 2.3, it dropped below 2 at acidic and alkaline pH. On contrast, the rates of flash-induced cytochrome b reduction were only ca. 1.5 times slower in D₂O than in H₂O. We conclude that, at physiological pH values, the rate of proton translocation in the cytochrome bc_1 complex is limited by the breakage or formation of hydrogen bonds and not by the transmembrane electron transfer in cytochrome b .

[1] A.Y. Mulkidjanian, Photochem Photobiol Sci 6 (2007) 19-34

BP 8: SYMR: Nuclear Magnetic Resonance: From Applications in Condensed Matter Physics to New Frontiers

Time: Tuesday 9:30–12:45

Location: H1

Invited Talk BP 8.1 Tue 9:30 H1
NMR with a Magnetic Resonance Force Microscope — ●BEAT H. MEIER, KAI EBERHARDT, JOSS ROSMARIE, and TOMKA IVAN — Physical Chemistry, ETH Zurich

Magnetic Resonance Force Microscopy (MRFM) is a sensitive method to detect magnetic resonance in small volume elements and has the potential to be used for magnetic resonance imaging (MRI) on the nanoscale. As with MRI, MRFM is not limited to the three spatial dimensions. Spectroscopic dimensions can be added, providing detailed chemical and structural information at the atomic level. The talk will introduce the basic principles of imaging with the microscope and discuss the available spectral information, e.g. from dipolar and quadrupolar interactions and - most demanding but most useful - from chemical shift.

Invited Talk BP 8.2 Tue 10:00 H1
Probing Novel Electronic States in Strongly Correlated Electron Materials Using NMR and NQR — ●NICHOLAS CURRO — Department of Physics, University of California, Davis CA 95616, USA

In the last two decades several new materials have been discovered which exhibit strong electron-electron interactions that lead to novel ground states such as superconductivity, coexisting antiferromagnetism and superconductivity, and "hidden" order. NMR/NQR are ideal probe of these new states, several of which only emerge under extreme conditions in high magnetic fields, low temperatures and high pressures. By taking advantage of the hyperfine interaction, NMR/NQR can provide detailed information about order parameters and their dynamics throughout the phase diagram of these systems. Furthermore, NMR provides a local spectroscopy of the response of these systems to impurity doping. Several heavy fermion and iron pnictide materials will be discussed.

Invited Talk BP 8.3 Tue 10:30 H1
Interplay of Structure and Dynamics in Macromolecular and Supramolecular Systems as Revealed by NMR Spectroscopy — ●HANS WOLFGANG SPIESS — Max-Planck-Institute for Polymer Research, Mainz, Germany

Traditionally, the determination of structure and the elucidation of dynamics of matter are considered separately. With the advancement of characterization techniques, however, this separation becomes more and more artificial. For instance, advanced solid state NMR spectroscopy provides information on the geometry and the time scale of molecular motions independently. This site selective and specific information is highly valuable, as in soft matter function of complex synthetic as well as natural systems is often achieved by separating regions of order and disorder. Incompatibility of building blocks, e.g., backbone and side groups in macromolecules, or non-covalent interactions, such as hydrogen bonds, ionic forces or pi-pi interactions lead to self organization, in which the different units are spatially separated and may display different dynamics. Solid state NMR techniques combining fast magic angle spinning (MAS) and double quantum (DQ) NMR spectroscopy provide site-specific information about these aspects and their relation to processing and function of the materials, e.g., proton- and photoconductivity.

15 min. break

Invited Talk BP 8.4 Tue 11:15 H1
Big times for small NMR — ●BERNHARD BLÜMICH — RWTH Aachen University, ITMC, Worringerweg 1, D-52056 Aachen, Germany

NMR is most widely known for diagnostic imaging in medicine and molecular analysis in chemistry. The measurement procedure requires magnetic fields and radio-frequency waves. The largest component of an NMR machine is the magnet. While the electronics are shrinking noticeably over the years, the magnets become bigger as higher field strength is realized. Small magnets can be built from permanent magnet material at field strengths common four decades ago. Recent advances in magnet design have led to desktop magnets and miniature magnets that surround the sample in the conventional way and in magnets that accommodate the object in the stray field for relaxation analysis, imaging, and high-resolution spectroscopy. Such magnets are inexpensive and portable. Their availability makes a diversity of studies possible, which are out of question for high-field superconducting magnets. These are high-throughput analysis by parallel operation of many spectrometers, in-line monitoring with long-time use of an NMR machine in one application, NMR analysis at the site of the object, and NMR analysis in dangerous environments. The advances in building small NMR magnets are summarized, and the use of small-scale NMR devices is demonstrated with applications to chemical engineering, medicine, and materials testing.

Invited Talk BP 8.5 Tue 11:45 H1
Traveling-Wave MRI — ●KLAAS PRÜSSMANN — Institute for Biomedical Engineering, ETH and University of Zurich, Switzerland

High-field magnets of sufficient inner diameter permit the formation of axially traveling RF waves at NMR frequencies. Such traveling waves can be exploited to excite and detect NMR across large distances. This principle has been demonstrated in a wide-bore 7T magnet with an inner RF screen of 58 cm in diameter, using a patch antenna for RF transmission and reception. Proton NMR spectra of an ethanol solution have been obtained at antenna distances up to more than 3 m. In high-field MRI of humans the traveling-wave approach has the potential to improve RF uniformity, as illustrated by initial in-vivo results. The presentation will also include brief discussions of the reciprocity and efficiency of traveling-wave probes, wave impedance matching, and propagation-related phase delays. Finally it will address the feasibility of using multiple waveguide modes for establishing spatial diversity of RF fields, which underlies the practically important concepts of RF shimming and parallel MRI.

Invited Talk BP 8.6 Tue 12:15 H1
Life on the Edge: The Origins and Proliferation of Protein Misfolding Diseases — ●CHRISTOPHER M. DOBSON — University of Cambridge, Department of Chemistry, Lensfield Road, Cambridge CB2 1EW, UK

The failure of proteins to fold, or to remain correctly folded, can give rise to serious cellular malfunctions that frequently lead to disease. One particularly important group of such diseases is associated with the aggregation of misfolded proteins into thread-like structures known as amyloid fibrils, and includes disorders ranging from Alzheimer's disease to late-onset diabetes. The manner in which the normal soluble

forms of peptides and proteins can convert into these pathogenic amyloid structures is being uncovered by a wide variety of in vitro experimental studies along with theoretical simulations and bioinformatics studies [Dobson and Chiti, *Annu. Rev. Biochem.* 75, 333-366 (2006)]. As with folding, these studies are increasingly being linked to events occurring in vivo using a variety of strategies. Of particular interest are experiments designed to link the principles of misfolding and aggregation to the effects of such processes in model organisms such as

Drosophila (the fruit fly). This talk will try to draw together some of the ideas that are emerging from recent in our laboratory based on NMR spectroscopy, including evidence for the extremely narrow boundary between normal and aberrant behaviour [Tartaglia et al., *Trends Biochem. Soc.* 32, 204-206 (2007)], and how this concept sheds light on the origin, current proliferation and potential means of prevention of the associated diseases.

BP 9: Physics of Cells I

Time: Tuesday 9:30–12:45

Location: H43

Invited Talk

BP 9.1 Tue 9:30 H43

Mechanics of Cellular Aggregates — ●FRANÇOISE BROCHARD-WYART¹, CHRISTOPHE CLANET², DAMIEN CUVELIER¹, SYLVIE DUFOUR¹, DAVID GONZALEZ-RODRIGUEZ¹, and KARINE GUEVORKIAN¹ — ¹Physical Chemistry Curie, Institut Curie, Paris, France — ²Laboratoire d'Hydrodynamique, Ecole Polytechnique, Palaiseau, France

Embryonic morphogenesis, wound healing, cancer growth, and metastasis are all examples where the mechanical properties play an important role in the functioning of a tissue. It has been suggested that certain embryonic tissues mimic the behavior of viscous fluids. However, due to the immense variety of tissues ranging from very soft (brain) to very hard (bone), such an analogy between tissues and fluids remains not well understood. We shall describe aspiration and compression experiments performed on cell aggregates, which provide a convenient laboratory model to characterize the mechanical properties of tissue. Using this characterization, we study the spreading of cell aggregates on a coated substrate, as well as their deformation and detachment under flow. In addition, we perform analogous experiments on viscous pastes, which provide a comparison with an inert system. Our results should yield insights in the understanding of pathologies related to artery obstruction, such as atherosclerosis or thrombosis.

BP 9.2 Tue 10:00 H43

Centering of dynamic microtubule asters by cortical pulling forces — LIEDEWIJ LAAN¹, ●NENAD PAVIN^{2,3}, GUILLAUME ROMET-LEMONNE¹, FRANK JULICHER², and MARILEEN DOGTEROM¹ — ¹FOM Institute for Atomic and Molecular Physics (AMOLF), Amsterdam, The Netherlands — ²Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ³Department of Physics, Faculty of Science, Zagreb, Croatia

Dynamic microtubules (MTs) interact with the cortex to generate pushing and/or pulling forces that position organelles correctly with respect to the confining geometry of living cells. In particular, pulling forces mediated by dynein linked to the cortex, provide a versatile mechanism to properly position MT organizing centers in systems ranging from small yeast cells to large embryonic cells. Nevertheless, the respective roles of pushing and pulling forces, and especially the mechanism by which pulling forces may contribute to centering processes, remain poorly understood. We address this question in an in vitro experiment, where MT asters are grown in microfabricated chambers. Pushing forces arise from MT polymerization and buckling forces, and pulling forces arise from interactions between MT ends and dynein motor proteins attached to the chamber walls. Surprisingly, we find that MT asters center more reliably by a combination of pulling and pushing forces than by pushing forces alone. Our theoretical results obtained for various geometries, imply distinct positioning strategies employed in different cell types.

BP 9.3 Tue 10:15 H43

Structure formation of the bacterial cytoskeletal protein FtsZ - a theoretical study — ●ELISABETH FISCHER-FRIEDRICH, ROIE SHLOMOVITZ, and NIR GOV — Department of Chemical Physics, The Weizmann Institute of Science, P.O.B. 26, Rehovot 76100, Israel

The bacterial protein FtsZ polymerizes and attaches to the inner site of the bacterial membrane in a ring-shaped structure. This FtsZ ring marks the future site of the septum of bacterial cell division. Membrane located FtsZ structures have also been reported to occur in a helical shape, neighboring the FtsZ ring in a normally dividing cell, or during the process of sporulation in *Bacillus subtilis*. The mechanism behind FtsZ assembly and structure formation as well as switching

between ring and helix structures remains obscure. Here, we examine the process of structure formation theoretically using a coarse-grained model to describe FtsZ densities on the membrane and taking into account a spontaneous curvature of FtsZ polymers.

BP 9.4 Tue 10:30 H43

Photonic force based investigations of intracellular molecular motor dynamics during phagocytic filopodia retraction — ●FELIX KOHLER and ALEXANDER ROHRBACH — Albert-Ludwigs-Universität, Freiburg, Germany

Phagocytes use intelligent mechanisms to efficiently uptake bacteria and other particles. A fascinating method of the cell is to extract and retract lamellopodia or thin filopodia to withdraw and uptake the particles. Besides actin polymerization and depolymerization, coordinated transport of molecular motors seems to control filopodia mechanics. We use photonic force microscopy to investigate different mechanical concepts of the cell to take up $1\mu\text{m}$ beads, which serve as synthetic bacteria. The motion of an optically trapped bead is tracked interferometrically in 3D with nanometer precision at microsecond timescale. The measurement of e.g. the beads mean displacement allows determining the retraction forces of filopodia at various retraction speeds. We have measured F-actin dependent 36-nanometer steps inside living cells during filopodia retraction likely belonging to actin-based molecular motors [1]. Steps remain clearly visible even at force regimes clearly beyond the stall force of a single myosin motor. This indicates a kind of inter-motor coupling, a phenomenon which will be presented in this talk and which we try to explain by a stochastic multi-state model.

[1] Kress, Stelzer, Holzer, Buss, Griffiths, and Rohrbach: "Filopodia act as phagocytic tentacles and pull with discrete steps and a load-dependent velocity", *PNAS*, Vol.104, 2007, 11633-11638

BP 9.5 Tue 10:45 H43

Structural transitions in growing actin networks — ●JULIAN WEICHSEL and ULRICH SCHWARZ — University of Heidelberg, Institute for Theoretical Physics

The directed polymerization of a branched actin network is a universal propulsion system used in many different contexts of biological relevance, including the migration of animal cells and the motility of intracellular pathogens like *Listeria*. It also can be reconstituted in cell-free assays, for example to propel plastic beads or vesicles. Despite the universal nature of the underlying mechanisms of filament growth, branching and capping, conflicting results have been reported for the force-velocity relation of growing actin networks. Using a relatively simple theoretical model, we show that the interplay between filament and network growth leads to structural transitions in the network which can explain the experimental observations. Using a rate equation approach, we analytically calculate a phase diagram which is in excellent agreement with stochastic simulations of network growth.

15 min. break

BP 9.6 Tue 11:15 H43

Shell-String Model of Global Cell Motions, Intracellular Trafficking and Phagocytosis — ●ERICH SACKMANN¹, FELIX KEBER², and DORIS HEINRICH² — ¹Biophysik E22, Physik Department, TU München, Germany — ²Fakultät für Physik und CeNS, LMU München, Germany

The survival of cells depends on the ongoing intracellular motions and the rapid reorganisation of intracellular macromolecular scaffolds. Thus, the cytoplasmic space is explored by superpositions of directed

transport along and by random walks between microtubules. Further, cell locomotion and phagocytosis are driven by actin gelation waves. This requires cells to combine a high degree of plasticity of the intracellular space with mechanical robustness. We first provide evidence that this astonishing mechanical robustness can be explained in terms of dynamic coupling of the microtubule aster to the actin cortex. Large forces in the nN range are balanced by coupling of the microtubules to actin gelation waves rather than cellular micromuscles. Second, we show that rapid global shape changes, associated with locomotion and phagocytosis, are driven by solitary actin gelation waves acting as travelling force fields. We finally present a model explaining the travelling force field in terms of the synchronous motion of signalling lipids with adhesion domains spreading on surfaces.

BP 9.7 Tue 11:30 H43

Probing mechanical characteristics of differentiating pluripotent mouse stem cells — •LENA A. LAUTSCHAM¹, THOMAS SCHULZ², AHMED MANSOURI², CHRISTOPH F. SCHMIDT¹, and FLORIAN REHFELDT¹ — ¹Drittes Physikalisches Institut, Georg-August-Universität, Göttingen, Germany — ²Molecular Cell Differentiation Group, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

In the last decade it has become increasingly evident that local micro-environments of living cells differ significantly, not only in biochemical composition, but also in their mechanical properties. The physical characteristics of different tissue and cell types (e.g. muscle, neurons, osteoblasts) correlate with the function of the various differentiated phenotypes.

It remains a challenge to accurately determine mechanical properties of cells such as their viscoelasticity, and to quantify their own active mechanical output, e.g. contractile forces generated by the cells. Our approach uses a dual optical trap by which cells are suspended between two trapped micron-sized beads. Using a combination of active and passive microrheology allows us to precisely determine physical parameters at high resolution and bandwidth and to simultaneously quantify the fluctuating forces that the cells produce.

We here present data showing distinct changes of the mechanical properties of differentiating pluripotent mouse stem cells after well-defined biochemical stimulation was applied to differentiate the cells to either muscle cells or neuronal cells.

BP 9.8 Tue 11:45 H43

The mechanical characteristics of embryonic stem cells influence their first fate decisions — •KEVIN CHALUT¹, PENELOPE HAYWARD², FRANZISKA LAUTENSCHLAGER¹, CHEA LIM², ALFONSO MARTINEZ-ARIAS², and JOCHEN GUCK¹ — ¹Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge, UK — ²Department of Genetics, University of Cambridge, Cambridge, UK

The level of expression of the gene *Nanog* in embryonic stem (ES) cells defines their pluripotency: ES cells with a high expression of *Nanog* (HN) remain pluripotent while ES cells with a low expression of *Nanog* (LN) tend to differentiate. We used optical stretching and atomic force microscopy to explore the differences in mechanical phenotype between HN and LN embryonic stem cells. We found that LN cells are softer and more elastic than HN cells, while HN cells are highly plastic and maintain a high level of active response to forces in the environment. We will show that the highly active response of the HN cells is very robust, and has significant implications for sorting of ES cells in the embryo. Moreover, the high level of compliance of the LN cells compared to HN cells implies a susceptibility to physical cues in the environment that can steer the fate decisions of the ES cells. Finally, we present evidence that the actomyosin cytoskeleton network, which mediates the cells' active responses to their environment, fulfils an extremely important role in the fate decisions of ES cells, and in fact may define whether they maintain their pluripotent state or shift to lineage commitment.

BP 9.9 Tue 12:00 H43

Measuring cell mechanics and cell membrane properties by vertical pulling — •SCHANILA NAWAZ¹, SAI LI², MIKAEL SIMONS¹, and IWAN A.T. SCHAAP² — ¹Max Planck Institute for Experimental

Medicine, 37077 Göttingen, Germany — ²III. Physikalisches Institut, Georg-August-Universität, 37077 Göttingen, Germany

Based on optical tweezers we have developed a portable (and affordable) trapping instrument that is able to work at the surface vicinity up to 50 μm away from the surface and can exert and measure vertical forces up to 0.1 nN. We have used our method to investigate the mechanical forces driving morphological changes during the development of myelin-forming cells. Such measurements heavily rely on the vertical pulling geometry because of the flatness of myelin cells (as thin as 50 nm). A trapped bead was automatically brought down to the cell and bead-cell contact was detected via a force feedback loop. The trapped bead was then pulled in vertical direction, away from the contact point. From the force-extension curves we can detect cell deformation, from which we can calculate the elastic response. At higher forces we pulled membrane tubes (tethers) out of the cell membrane. From the measured forces required to form these tethers we estimated the membrane tension in different stages of cell development.

BP 9.10 Tue 12:15 H43

Force transduction in blood platelets — •SARAH SCHWARZ G. HENRIQUES¹, HANSJÖRG SCHWERTZ², ALEXANDER STRATE³, and SARAH KÖSTER¹ — ¹Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, Universität Göttingen, Germany — ²Division of Vascular Surgery, University of Utah, Salt Lake City, United States of America — ³Transfusion Department, University Clinic, Universität Göttingen, Germany

Blood platelets (thrombocytes) are essential for the repair of damaged blood vessels. When they become activated to form a blood clot they change their shape within minutes by dramatically rebuilding their cytoskeleton. This highly dynamic non-equilibrium process is known to be triggered by external cues and driven by cellular forces, but the basic mechanical principles are not yet understood. In our experiments we investigate the physics underlying platelet activation by measuring the forces, which platelets impose on their environment. To this end, we use traction force microscopy, a well-established technique, in which the cells are placed on thin PAA (polyacrylamide) gels of a known elastic modulus. Fluorescent tracer beads are embedded into the PAA to visualize gel deformations, which are then translated into traction force fields. In addition to measuring traction force fields, we take fluorescence microscopy images of the platelets at different activation stages. Both vinculin as well as actin are previously stained in order to map focal adhesion sites and conclude upon cytoskeletal reorganization steps. Our experimental findings are finally gathered into a mechanical model for the early stages of platelet activation.

BP 9.11 Tue 12:30 H43

Strain Energy and its Density Distribution around Invasive and Non-Invasive Carcinoma Cells in 3D Collagen Gels — •THORSTEN KOCH¹, STEFAN MÜNSTER¹, CLAUDIA MIERKE¹, JAMES BUTLER², and BEN FABRY¹ — ¹Department of Physics, University of Erlangen-Nuremberg, Germany — ²Physiology Program, Harvard School of Public Health, Boston, MA, USA

Cell invasion through a 3D matrix is believed to depend on the ability of cells to generate traction forces. To quantify the role of cell tractions during invasion in a collagen gel (shear modulus 118 Pa, 500 μm thickness, mesh size 1.6 μm), we measured the strain energy of invasive MDA-MB-231 breast and A-125 lung carcinoma cells, as well as non-invasive MCF-7 breast and A-431 lung carcinoma cells for comparison. In all cases, cells locally contracted the gel, quantified by tracking 3D positions of embedded fluorescent beads. These positions served as nodes in a finite element mesh used to compute the strain energy. The strain energy of invasive breast carcinoma cells (1.4 ± 0.2 pJ, $n=31$) was significantly higher than that of non-invasive breast carcinoma cells (0.8 ± 0.1 pJ, $n=28$). Surprisingly, the strain energy of non-invasive lung carcinoma cells (4.2 ± 0.7 pJ, $n=31$) was similar to that of invasive lung carcinoma cells (3.5 ± 0.4 pJ, $n=34$). Invasive cells assumed an elongated morphology as opposed to the round shape of non-invasive cells. Accordingly, the distribution of strain energy density around invasive cells followed patterns of increased anisotropy. These results suggest that magnitude and directionality of traction generation are important for cell invasion in 3D collagen gels.

BP 10: Evolutionary Game Theory I (joint SOE, BP)

Time: Tuesday 9:30–11:00

Location: H44

Invited Talk

BP 10.1 Tue 9:30 H44

Humans playing spatial games — ●ARNE TRAUlsen — Max-Planck-Institute for Evolutionary Biology, 24306 Plön, Germany

Probably the most thoroughly studied mechanism that can explain the evolution and maintenance of costly cooperation among selfish individual is population structure. In the past years, hundreds of papers have mathematically modeled how cooperation can emerge under various dynamical rules and in more and more complex population structures [1]. However, so far there is a significant lack of experimental data in this field. We have conducted an experimental test to address how humans are playing a particularly simple spatial game on a regular lattice [2]. The data shows that the way humans choose strategies is different from the usual assumptions of theoretical models. Most importantly, spontaneous strategy changes corresponding to mutations or exploration behavior is more frequent than assumed in many models. This can decrease the influence of some spatial structures. This experimental approach to measure properties of the update mechanisms used in theoretical models may be useful for mathematical models of evolutionary games in structured populations.

[1] Szabó and Fáth, Evolutionary games on graphs, Physics Reports 446:97-216 (2007)

[2] Traulsen, Semmann, Sommerfeld, Krambeck, and Milinski, submitted

BP 10.2 Tue 10:00 H44

Coordination with switching costs: A case for percolation in socioeconomic networks — ●CARLOS P. ROCA¹, MOEZ DRAIEF², and DIRK HELBING^{1,3} — ¹Chair of Sociology, in particular of Modeling and Simulation, ETH Zurich, Switzerland — ²Intelligent Systems and Networks Group, Imperial College London, UK — ³Santa Fe Institute, USA

Coordination is ubiquitous in social and economic interactions [1,2]. An important but not much studied issue is the influence of the costs involved in the switching of strategy, which however can be very relevant to important situations such as inefficient norms [3] or competition in technological markets [4]. We propose an extension of a binary coordination game to investigate this problem. We study it on degree-homogeneous random networks, observing that the outcome is greatly influenced by the underlying network. The dependence on the network degree is highly non-trivial and extremely large degrees are needed to recover the mean field results. The explanation of this unexpected behavior resides in a particular kind of percolation process that takes place in the networked population. These results strongly suggest that percolation phenomena may be crucial in social and economic networks when coordination interactions are in play.

[1] Lewis, Convention: A Philosophical Study, Harvard University Press, 1969 [2] Harsanyi and Selten, A General Theory of Equilibrium Selection in Games, MIT Press, 1988 [3] Mahoney, Theory and Society 29, 507-548, 2000 [4] Klemperer, The Review of Economic Studies, 62, 515-539, 1995

BP 10.3 Tue 10:15 H44

Rock-papers-scissors dynamics on complex networks — MARKUS SCHÜTT and ●JENS CHRISTIAN CLAUSSEN — Inst. f. Neuro- und Bioinformatik, Universität zu Lübeck

Cyclic coevolutionary dynamics of three cyclically dominating strategies have been found in Prisoner's Dilemma conflicts (with ALLD and TFT) as well as in bacteria (*E.coli*) and the lizards (*Uta stansburiana*). The simplest payoff matrix resembling this cyclicity is that of the rock-papers-scissors (RPS) game. The meanfield dynamics of such cyclic coevolutionary dynamics in finite population has been analyzed in previous work for the RPS game [1] as well as for a bimatrix game played between two populations [2]. Here we investigate the fixation time for the RPS game on different types of regular, random, small-world and scale-free graphs [2].

[1] JC Claussen and A Traulsen, Phys. Rev. Lett (2008)

[2] JC Claussen, Eur. Phys. J. (2007)

[3] M Schütt and JC Claussen (in preparation)

BP 10.4 Tue 10:30 H44

Evolutionary games in the multiverse — ●CHAITANYA S. GOKHALE and ARNE TRAUlsen — Max-Planck-Institute for Evolutionary Biology, August-Thienemann-Straße 2, 24306 Plön, Germany

Evolutionary game dynamics of two players with two strategies has been studied in great detail. These games have been used to model many biologically relevant scenarios, ranging from social dilemmas in mammals to microbial diversity. Some of these games may in fact take place between a number of individuals and not just between two. Here, we address one-shot games with multiple players. As long as we have only two strategies, many results from two player games can be generalized to multiple players. For games with multiple players and more than two strategies, we show that statements derived for pairwise interactions do no longer hold. For two player games with any number of strategies there can be at most one isolated internal equilibrium. We show that for any number of players d with any number of strategies n , there can be at most $(d-1)^{n-1}$ isolated internal equilibria. Thus, multiplayer games show a great dynamical complexity that cannot be captured based on pairwise interactions. Our results hold for any game and can easily be applied for specific cases, e.g. public goods games or multiplayer stag hunts.

BP 10.5 Tue 10:45 H44

Social Dilemmas for Players with Complex Personality Profiles — TADEUSZ PLATKOWSKI and ●JAN ZAKRZEWSKI — Department of Mathematics, Informatics and Mechanics, University of Warsaw

We develop a theory of evolution of social systems based on the imitation rule which generalizes the standard proportional fitness rule of the evolutionary game theory. The formalism is applied to describe the dynamics of various types of social dilemma games played in infinite populations. In particular the theory predicts the non-zero level of cooperation in the long run for the Public Good games, the existence of the nonunique stable polymorphism for particular classes of the Prisoner's Dilemma games, and stable asymptotic cooperation level for coordination games in the N-person setting, for which the standard replicator dynamics approach predicted the instable polymorphism.

BP 11: Evolutionary Game Theory II (joint SOE, BP)

Time: Tuesday 11:15–12:30

Location: H44

BP 11.1 Tue 11:15 H44

Evolutionary dynamics, intrinsic noise and cycles of cooperation — ●ALEX BLADON, TOBIAS GALLA, and ALAN J MCKANE — Theoretical Physics, School of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, United Kingdom

The puzzle of how co-operation emerges in evolving populations subject to natural selection is unsolved, and the dynamic interaction of co-operation and defection is a current topic of wide interest in game theory. Periodic cycles between co-operation, defection and retaliation have been reported in numerical simulations of the iterated prisoner's dilemma in small populations of evolving agents [PNAS, 102, 31, 10797-10800, 2005]. Using tools from statistical mechanics and non-

linear dynamics we here provide an analytical underpinning of these numerical observations and show that such cycles are the signature of amplified coherent oscillations sustained by demographic noise. We derive effective Langevin equations describing these oscillations and compute their power spectra analytically in the limit of large, but finite populations and in excellent agreement with numerical simulations. Our analytical theory reveals that the amplitude of these stochastic oscillations is, to a large degree, set by the inverse real part of the relevant eigenvalue of the deterministic dynamics, and that it can hence become singular near a Hopf bifurcation. Macroscopic oscillations are then observed even at large system sizes. Our analysis extends to cases in which errors of the 'trembling hand' type are considered, and where

the strategy space includes a win-stay, lose-shift action.

BP 11.2 Tue 11:30 H44

Evolutionary adaptation of a social norm optimizes node degree and investments on an adaptive network — ●JOHANNES HOEFENER and THILO GROSS — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

Humans established complex networks of cooperation, which are essential for our modern society. Cooperating with just a single person is not efficient and cooperating with everyone is not even possible. Thus every individual has to decide if and how much it should invest into a certain cooperation. Because the payoff provided by a cooperation is usually not known when the investments have to be done, individuals may base their decision on heuristics or social norms. These, for instance may follow the statement: "Get more. Give more." Here we study a continuous prisoner's dilemma game on an adaptive network, where the investment into cooperation is determined by a social norm function. We assume that the general form of the function is fixed, but allow the function to be modified by evolutionary adaptation of its parameters. We show that this adaptation not only establishes stable cooperation but also optimizes the node degree as well as the investments in the remaining cooperations.

BP 11.3 Tue 11:45 H44

A Homoclinic Route to Full Cooperation in the Snowdrift Game on Adaptive Networks — ●GERD ZSCHALER¹, ARNE TRAUlsen², and THILO GROSS¹ — ¹Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — ²Max-Planck-Institut für Evolutionsbiologie, Plön, Germany

We consider the evolutionary dynamics of a cooperative game on an adaptive network, where the strategies of agents, cooperation or defection, feed back on their local interaction topology. While mutual cooperation is the social optimum, unilateral defection yields a higher payoff and undermines the evolution of cooperation. Although no a priori advantage is given to cooperators, an intrinsic dynamical mechanism can lead asymptotically to a state of almost full cooperation. In finite systems, this state is characterized by long periods of strong cooperation interrupted by sudden episodes of predominant defection, suggesting a possible mechanism for the systemic failure of cooperation in real-world systems.

BP 11.4 Tue 12:00 H44

Deterministic evolutionary game dynamics in finite populations — ●PHILIPP M. ALTROCK and ARNE TRAUlsen — MPI f. Evo-

lutionary Biology, Plön, Germany

Evolutionary game dynamics describes the spreading of successful strategies in a population of reproducing individuals. Typically, the microscopic definition of strategy spreading is stochastic, such that the dynamics becomes deterministic only in infinitely large populations. Here, we introduce a new microscopic birth-death process that has a fully deterministic strong selection limit in well-mixed populations of any size. Additionally, under weak selection, from this new process the frequency dependent Moran process is recovered. This makes it a natural extension of the usual evolutionary dynamics under weak selection. We analytically find simple expressions for the fixation probabilities and average fixation times of the new process in evolutionary games with two players and two strategies. For cyclic games with two players and three strategies, we show that the resulting deterministic dynamics crucially depends on the initial condition in a non-trivial way.

[1] Goel & Richter-Dyn, *Stochastic Models in Biology*, Academic Press, NY, (1974).

[2] Altrock & Traulsen, *Phys. Rev. E* **80**, 011909 (2009).

BP 11.5 Tue 12:15 H44

Evolutionary Quantum Game Theory — ●MATTHIAS HANAUSKE¹ and JENNIFER KUNZ² — ¹Institute of Information Systems — ²Chair of Controlling and Auditing, Goethe-University, Frankfurt/M.

Quantum game theory is a mathematical and conceptual amplification of classical game theory. The space of all conceivable decision paths is extended from the purely rational, measurable space in the Hilbertspace of complex numbers. Through the concept of a potential entanglement of the imaginary quantum strategy parts, it is possible to include corporate decision path, caused by cultural or moral standards. If this strategy entanglement is large enough, then, additional Nash-equilibria can occur and previously present dominant strategies could become nonexistent. The main equation of evolutionary game theory, the Replicator equation, gets a more complex structure and other evolutionary stable strategies can appear. In addition to a detailed introduction in evolutionary quantum game theory several examples of applications will be presented during this talk. The current financial crisis will be discussed using a quantum extension of an anti-coordination game, the different publication patterns of scientist will be studied and the evolution of social norms in firms will be explained using a quantum coordination game.

(<http://evolution.wiwi.uni-frankfurt.de/Lyon2009/>, ArXiv: 0904.2113, arXiv: physics/0612234)

BP 12: Nuclear Magnetic Resonance: Frontiers and Applications (joint CPP, BP)

Time: Tuesday 13:45–16:15

Location: H48

BP 12.1 Tue 13:45 H48

Probing the Assembly and Dynamics of Graphene-Inspired Molecular Wires by Solid-State NMR Spectroscopy — ●MICHAEL RYAN HANSEN, ROBERT GRAF, DANIEL SEBASTIANI, and HANS-WOLFGANG SPIESS — Max Planck Institute for Polymer Research

Molecular wires based on polycyclic aromatic hydrocarbons (PAHs) are a promising class of materials for future applications in nano-scale electronic devices. Critical for the performance of such wires are their molecular assembly, which on the NMR length and time scales translates into the local packing arrangement, molecular dynamics, and pitch angle(s) between successive molecules. Here, we show that solid-state NMR in combination with MD and ab-initio calculations can provide unique information with respect to these structural features. To illustrate this we examine two perylene tetracarboxydiimides (PDIs) with different side chains attached and a larger triangular-shaped PAH. Specifically, we measure ¹H chemical shifts using fast MAS and their spatial connectivities through 2D 1H-1H DQ-SQ correlation spectra and probe the molecular dynamics via 1H-13C heteronuclear dipolar couplings. To support the experimental findings we have performed CPMD-NMR calculations to reveal the effects of packing on the ¹H chemical shifts for the PDIs, including an estimate of the line broadening due to local disorder. This provides a series of finger prints for different pitch angles between neighboring molecules, that are closely related to the electronic conduction properties of the supramolecular

stacks.

BP 12.2 Tue 14:00 H48

NMR studies of benzene mobility in microporous metal-organic framework MOF-5 — ●STEFAN HERTEL¹, SAEED AMIRJALAYER², MARKUS WEHRING¹, ROCHUS SCHMID², and FRANK STALLMACH¹ — ¹Universität Leipzig, Fakultät für Physik und Geowissenschaften, Deutschland — ²Ruhr-Universität Bochum, Fakultät für Chemie und Biochemie, Deutschland

Microporous metal-organic frameworks (MOF) are crystalline coordination polymers with regular three dimensional pore networks. These pore networks enable adsorption and diffusion of guest molecules. Molecular Dynamics (MD) simulations show that benzene has a liquid-like mobility inside the pores of MOF-5. Nuclear Magnetic Resonance (NMR) methods allow experimental access to guest mobilities inside such pore networks. This report presents the results of pulsed field gradient NMR (PFG NMR) self-diffusion measurements of benzene adsorbed in MOF-5. In these experiments multi-exponential spin echo decays were observed, which are usually caused by different phases of self-diffusion. These different phases of benzene mobility were unexpected for diffusion of molecules inside an isotropic framework and have to originate in the host-guest and guest-guest interaction. By modern diffusion-relaxation correlation spectroscopy (DRCOSY) translational self-diffusion and microscopic relaxation behavior were correlated. Together with magic angle spinning (MAS) NMR spectroscopy these in-

vestigations reveal that the faster component of the diffusion coefficients can be assigned to diffusion inside the porous crystal structure of MOF-5.

BP 12.3 Tue 14:15 H48

Exploring the limits to spatially resolved NMR — ACHIM GÄDKE^{1,2} and ●NIKOLAUS NESTLE^{1,3} — ¹TU Darmstadt, Institute of condensed matter physics, Germany — ²Present address: Victoria University of Wellington, New Zealand — ³Present address: BASF SE, GKC/R, Ludwigshafen, Germany

Recent advances in MRI have demonstrated resolutions down to 1 μm . Magnetic resonance force microscopy has the potential to reach sensitivity for single nuclear spins. Given these numbers, in vivo imaging of single cells or even biomacromolecules may seem possible. However, for in vivo applications, there are fundamental differences in the contrast mechanisms compared to MRI at macroscopic scales as the length scale of molecular self-diffusion exceeds that of the spatial resolution on the NMR time scale. Those effects - which are fundamentally different from the echo attenuation in field gradient NMR - even may lead to general limitations on the spatial resolution achievable in aqueous systems with high water content. In our contribution, we explore those effects on a model system in a high-resolution stray-field imaging setup. In addition to experimental results, simulations based on the Bloch-Torrey equation will be presented.

BP 12.4 Tue 14:30 H48

Polymers under mechanical stress- an NMR investigation — ●UTE BÖHME¹, BO XU², JOHANNES LEISEN², HASKELL W. BECKHAM², and ULRICH SCHELER¹ — ¹Leibniz Institute of Polymer Research Dresden — ²Georgia Institute of Technology, Atlanta, Georgia

Low-field NMR using permanent magnets in Halbach arrangements permit NMR investigation without the limits present in high-field NMR. The lower field in conjunction with confined stray field permit the application of NMR, in particular relaxation NMR in a stretching apparatus and a rheometer [1,2]. Crystalline and amorphous fraction of semi-crystalline polymers are distinguished by their transverse relaxation times. Upon mechanical load the relaxation times of the amorphous fraction changes as seen in in-situ measurements on polypropylene rods. During the formation of a neck the crystalline fraction becomes more prominent.

[1] S. Kahle et.al., K GK- Kautschuk Gummi Kunststoffe 61 (2008), 92.

[2] G. Mazzanti et.al., J. Am. Oil Chem. Soc. 85 (2008), 405.

BP 12.5 Tue 14:45 H48

Segmental Order in Polymer Networks — ●JENS-UWE SOMMER — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany

Polymer networks are structurally and topologically disordered soft solids. We consider orientation order of chain segments in polymer networks to relate NMR-experiments with molecular models of polymer networks [1,2]. We derive a general relation between segmental order and local forces acting on a chain under external constraints. Using this result, we consider good solvent conditions and we show that the solvent plays a crucial role for the tensor order parameter. In particular, we show that the tensor order parameter decreases due to excluded volume interactions. Using analytical results and scaling arguments we derive a universal behavior for the order parameter with respect to the equilibrium degree of swelling which can be experimentally verified [2]. In the light of these observation we discuss several microscopic models of network swelling. Using the general relation between local forces on chain bonds and the tensor order parameter we further discuss possible observations on structurally regular networks such as obtained recently in experiments based on force-balance arguments, as well as the role of entanglements.

[1] J.-U. Sommer and K. Saalwächter, European Phys. J. E 18 (2005) 167-182

[2] J.-U. Sommer, Walter Chassé, Juan López Valentín, and Kay Saalwächter, Phys. Rev. E 78, 051803 (2008)

BP 12.6 Tue 15:00 H48

Ultrafast velocity-mapping in microfluidic setups — ●EVA PACIOK, ANDREA AMAR, FEDERICO CASANOVA, and BERNHARD BLÜMICH — ITMC, RWTH Aachen University, Germany

NMR in combination with designated rf coils has proven to be a power-

ful tool for the investigation of microfluidic setups, e.g. microreactors, micromixers and fluid drops, since it has the potential to reveal both spectroscopic, spatial and velocity information non-invasively. Despite the high spatial resolution NMR offers, the temporal resolution of NMR imaging and velocity mapping experiments in microfluidics has been low so far, because the application of ultrafast NMR velocity mapping methods to microfluidics has failed. These methods are based on multi-echo generation give rise to problems concerning magnetic field inhomogeneities (EPI), rf field inhomogeneities (PGSE-RARE) and velocity/acceleration limitations (EPI and PGSE-RARE).

In this work, we exploit the advantages of the FLIESSEN (Flow Imaging Employing a Single Shot ENcoding) pulse sequence, a new ultrafast RARE-based imaging and velocity mapping method. An adjusted phase encoding strategy and a frequent update of velocity encoding during the multi-echo train makes FLIESSEN highly resilient to field inhomogeneities and velocity/acceleration effects. The performance of this technique is demonstrated on acetone flow in a microstructured phantom. Using FLIESSEN and a surface rf coil, high-fidelity 2D velocity maps were acquired within seconds.

BP 12.7 Tue 15:15 H48

Structural characterization of lyotropic lamellar phases by NMR spectroscopy — BRUNO MEDRONHO^{1,2}, MARIA G. MIGUEL¹, ULF OLSSON², and ●CLAUDIA SCHMIDT³ — ¹Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal — ²Physical Chemistry, Center of Chemistry and Chemical Engineering, Lund University, Box 124, 221 00 Lund, Sweden — ³Department of Chemistry, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

The lyotropic lamellar L_α phase is usually considered to consist of stacks of extended parallel layers. However, the application of shear may lead to defect structures consisting of close-packed multilamellar vesicles, also known as onions. Furthermore, it has been suggested that an intermediate structure of multilamellar cylinders occurs during the transformation from layers to vesicles. In this contribution we will give an overview on what kind of structural information can be obtained by deuterium NMR spectroscopy applied in situ under shear. It will be shown how different structures can be distinguished, how onions can be formed and destroyed by the application of shear and how the onion size can be measured on the basis of an NMR line shape analysis.

BP 12.8 Tue 15:30 H48

Complete NMR spectral assignment in gibbsite by first-principle calculations — ●ANASTASIA VYALIKH and ULRICH SCHELER — IPF Dresden, Hohe Str. 6, D-01069 Dresden, Germany

The structure of the mineral gibbsite is often considered as a representative of many alumino-silicate clay minerals, and therefore we use it in the present study as a model compound to establish the suitability of the computational method. Here we apply a gradient-corrected DFT method with a plane-wave basis set to assign the crystallographically distinct Al sites in gibbsite and to relate them to the hydroxide network. The experimental observation is based on high-resolution solid-state ²⁷Al NMR and ¹H CRAMPS (combined rotation and multipulse spectroscopy) data. On the basis of DFT calculations, the ¹H CRAMPS signals have been attributed to six symmetry independent hydrogen atoms and ascribed to two distinct types associated with intralayer and interlayer hydrogen bonds. The ²⁷Al NMR spectrum shows signals for octahedral aluminium only, however with two distinguished signals. The correlation between experimental and theoretical NMR parameters demonstrates that the character of the hydrogen bonds formed by the hydroxide ions is responsible for the structural differentiation of Al sites. That is, the Al-I site (CQ=4.2 MHz) is surrounded by the OH-groups participating in 4 intralayer and 2 interlayer hydrogen bonds, while the Al-II site (CQ=2.4 MHz) is coordinated by the hydroxides, 2 of which point towards the intralayer cavities and 4 OH-bonds are aligned towards the interlayer gallery.

BP 12.9 Tue 15:45 H48

Heparin-polynitroxide derivatives: biocompatible polarizing agents for dynamic nuclear polarization (DNP) — ●BJÖRN C. DOLLMANN¹, ANDREI L. KLESCHYOV², VASILY SEN³, VALERY GOLUBEV³, LAURA SCHREIBER⁴, KERSTIN MÜNNEMANN¹, and DARIUSH HINDERBERGER¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Second Department of Medicine, Johannes Gutenberg University, Mainz, Germany — ³Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, Russia — ⁴Johannes Gutenberg University Medical Center, Mainz, Ger-

many

A versatile and biocompatible class of spin-labeled macromolecules was investigated by electron spin echo-detected (ESE) electron paramagnetic resonance (EPR), continuous-wave (CW) EPR, double electron-electron resonance (DEER) and dynamic nuclear polarization (DNP). These heparin macromolecules could be utilized for *in vivo* magnetic resonance imaging (MRI DNP enhanced) and EPR imaging (EPRI). The distance distributions of the spin labels were measured and compared with the crystallographic structure of heparin. All presented heparin-polyoxides show reasonably high 1H DNP enhancement factors up to $E = -108$. The heparin-polyoxides intrinsically feature high dipolar electron spin-electron spin coupling frequencies ν_{dd} . Together with the finding that the best 1H -signal enhancements are found in the low concentration region, this proves the influence of the anisotropic electron spin distribution on DNP in liquids at room temperature.

BP 12.10 Tue 16:00 H48

Structure of Phage SPP1 Head-to-Tail Connector Reveals Gating Mechanism for DNA Ejection: an EM and NMR study — MATTHIEU GALLOPIN¹, SOPHIE LHULLIER², BERNARD

GILQUIN¹, SANDRINE BRASLÈS², ELENA ORLOVA³, JOËL COUPRIE¹, PAULO TAVARES², and SOPHIE ZINN-JUSTIN¹ — ¹Laboratoire de Biologie Structurale et Radiobiologie, iBiTec-S, CEA Saclay, Gif-sur-Yvette, France — ²Unité de Virologie Moléculaire et Structurale, UMR CNRS 2472, UMR INRA 1157 and IFR 115, Gif-sur-Yvette, France — ³Department of Crystallography, Birkbeck College, University of London, London, UK

Understanding the principles that govern macromolecular assembly is a current challenge for biochemists, molecular biologists, and structural biologists. Assembly of bacterial virus (bacteriophages) particles is a highly suitable system to investigate the molecular mechanisms that support efficient formation of a complex macromolecular machine and its function. A large number of phages and eukaryotic viruses use a portal system to control genome entry and exit from their capsids. The portal and head completion proteins form the viral head-to-tail connector. The pseudo-atomic structure of the complete closed connector of tailed bacteriophage SPP1 was determined (Lhuillier et al., PNAS 2009). Opening of the connector and DNA ejection from virions was reproduced *in vitro* by adding the host purified receptor YueB. These achievements recommend SPP1 as an excellent system to investigate the structural organization and dynamics of the viral DNA gatekeeper.

BP 13: Nanoparticles and Viruses

Time: Tuesday 14:00–16:30

Location: H45

Invited Talk

BP 13.1 Tue 14:00 H45

Carbon nanotubes fluids: simple or complex? — ●MATTEO PASQUALI — Department of Chemical & Biomolecular Engineering, Department of Chemistry, Smalley Institute for Nanoscale Science and Technology, Rice University, Houston Texas, USA

At the single-molecule level, Single-Walled Carbon Nanotubes (SWNTs) have remarkable electrical and mechanical properties, more so than previously known polymer molecules or colloidal particles. Realizing these properties in applications requires understanding and controlling the behavior of SWNTs in dilute as well as concentrated fluid phases. Yet, SWNT liquids are almost considered an oxymoron because dispersing or dissolving SWNTs into fluid phases is exceedingly difficult.

In this talk, I will discuss how SWNTs can and should be viewed as hybrids between polymer molecules and colloidal particles. Even at low concentrations (few parts per million), SWNTs form complex fluid phases with intriguing properties. When stabilized properly, dilute SWNTs behave as Brownian rods. Their interaction can be mediated by polymers and surfactants to produce complex individual architectures, or to devise ways of making transparent conductive coatings. In superacids, SWNTs dissolve spontaneously. At high concentration, they form liquid crystals that can be spun into well-aligned, macroscopic fibers. Intriguingly, the self-assembly of SWNTs into liquid crystalline phases can be understood by hybridizing Onsager's theory for colloidal rods with Flory's theory for rod-like polymers.

BP 13.2 Tue 14:30 H45

Interactions of nanoparticles with serum albumin — ●LENNART TREUEL, MARCELINA MALISSEK, JULIA S. GEBAUER, and REINHARD ZELLNER — Universität Duisburg-Essen, Essen, Germany

As nanoparticles (NPs) are of the same size scale as typical cellular components and proteins, such particles are suspected to evade the natural defences of the human organism and may lead to permanent cell damages. One major factor that may strongly influence the toxicity is the interaction of these NPs with proteins in body fluids and cells.

Circular dichroism (CD) spectroscopy is used to determine the interactions of serum albumin with a wide variety of NPs (Ag, Au, Polystyrene, ZnO etc.) in a size range between 5 nm and 100 nm. A multitude of different surface coatings (Citrate, TPPT, PVP etc.) has been used in these experiments in order to identify the key factors driving the NP / protein interaction process. From these measurements dissociation constants for different NP / protein systems have been derived. The results show a strong dependence of the interaction process on both NP material and surface coating. They further suggest a fundamental impact of the nature and persistence of the surface coating on the biological fate of the NP under consideration.

BP 13.3 Tue 14:45 H45

Electron microscopic analysis of particle uptake by lung macrophages in a murine allergic asthma model — ●CHRISTOPH WIGGE¹, MELANIE CONRAD², HOLGER GARN², HARALD RENZ², and MARIANNE GEISER¹ — ¹Institute of Anatomy, University of Bern, Switzerland — ²Department of Clinical Chemistry and Molecular Diagnostics, Philipps University of Marburg, Germany

Efficient particle uptake by lung surface macrophages is essential for the clearance of particles deposited in the peripheral lungs. Thereby, uptake of nanoparticles is of special interest, since there is evidence from epidemiology for a toxicological role of such particles. We investigated particle uptake by cells obtained from bronchoalveolar lavage of mice with induced allergic inflammation in comparison to cells obtained from healthy animals. Cells cultured on porous filter inserts were exposed to microparticles (3- μ m fungal spores) and to nanoparticles (20-nm gold) for 2 and 4 hours, respectively, and then processed for conventional transmission electron microscopy and electron tomography. We found phagocytic uptake of microparticles by macrophages in all animals, as the vesicular membrane was tightly apposed to the particles. There was evidence for rather unintentional uptake of nanoparticles, which were found in large vesicles containing other material. Electron tomography allowed detailed spatial resolution of nanoparticles in vesicles. In allergic animals, nanoparticles were also found in eosinophils. Uptake of nanoparticles by other leukocytes may contribute to nanoparticle clearance from the inner surface of lungs in inflammation.

BP 13.4 Tue 15:00 H45

Single gold nanoparticles as optothermal tools in phospholipid membranes — TOM PFEIFFER, ●ALEXANDER S. URBAN, MICHAEL FEDORUK, FERNANDO STEFANI, and JOCHEN FELDMANN — Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Amalienstr. 54, 80799 Munich, Germany

Metallic nanoparticles (NPs) can be efficiently heated by illuminating them at their plasmon resonances. In recent years, optical (plasmonic) heating of ensembles of NPs has found a number of applications including remote release [1], DNA-melting analysis [2] and even as a prospect for cancer therapy [3]. Recently, we have started the investigation and application of plasmonic heating of individual NPs, which enables unprecedented nanoscale thermal investigations. In particular, we have used the NPs to remotely (optically) induce and characterize reversible phase (gel-fluid) transitions of nanometric regions of a phospholipid membrane [4]. Furthermore, the control over the phase transition allowed us to guide the nanoparticles to specific locations on the membrane. Currently, we are investigating the possibility of manipulating transport across the membrane with optically heated NPs. It has been postulated that during the gel-fluid transition pores may

open in the membrane due to phospholipid reordering. We test this possibility by studying the penetration of the membrane by nanoparticles and molecules of different sizes as a function of the optical heating of NPs bound to the membrane.

15 min. break

BP 13.5 Tue 15:30 H45

Excited state energy transfer between CdSe nanocrystals and the isolated phycobiliprotein antenna of *A. marina* — ●FRANZ-JOSEF SCHMITT¹, VITHIYA JEYASANGAR¹, HEINRICH SÜDMAYER¹, MAX SCHOENGEN¹, VLADIMIR PASCHENKO³, HANS JOACHIM EICHLER¹, and GERNOT RENGER² — ¹Institute of Optics and Atomic Physics, Berlin Institute of Technology — ²Max-Vollmer Laboratory for Biophysical Chemistry, Berlin Institute of Technology — ³Lomonosov Moscow State University

A quantitative analysis of the interaction between semiconductor nanocrystals and isolated light harvesting complexes from photosynthetic organisms is of relevance for the development of biosensors with enhanced sensitivity. The present work describes results obtained on a hybrid system consisting of CdSe nanoparticles and rod shaped phycobiliproteins (PBP) antenna complexes from the cyanobacterium *Acaryochloris marina*. The CdSe core of the nanocrystals is covered with a ZnS shell and the surface is functionalised with anions of dihydrolipeic acid leading to electrostatic coupling to the PBPs. The measured time resolved and time integrated fluorescence spectra can be explained by a highly efficient excitation energy transfer from the nanocrystals to the PBP antenna with a time constant of about 200 ps at room temperature. At 0°C a decoupling of about 80 % of the CdSe crystals from the PBP antennae was observed. These results could be relevant for the design of switchable light harvesting systems or controlled fluorescence enhancement.

BP 13.6 Tue 15:45 H45

Nanostructured gold microelectrodes for extracellular recording — ●DOROTHEA BRÜGGEMANN, BERNHARD WOLFRUM, VANESSA MAYBECK, and ANDREAS OFFENHÄUSSER — CNi Center of Nanoelectronic Systems for Information Technology and Institute of Bio- and Nanosystems 2, Forschungszentrum Jülich

Electrophysiological activity of electrogenic cells is currently recorded with planar bioelectronic interfaces such as microelectrode arrays (MEAs). In this work, a novel concept of biocompatible nanostructured gold MEAs for extracellular signal recording is presented. MEAs were fabricated using clean room technologies, e.g. photolithography and metallization. Subsequently, they were modified with gold nanopillars of approximately 300 to 400 nm in height and 60 nm width. The nanostructuring process was carried out with a template-assisted approach using nanoporous aluminium oxide. Impedance spectroscopy of the resulting nanostructures showed higher capacitances compared to planar gold. This confirmed the expected increase of the surface area via nanostructuring.

We used the nanostructured microelectrodes to record extracellular potentials from heart muscle cells (HL1), which were plated onto the chips. Good coupling between the HL1 cells and the nanostructured electrodes was observed. The resulting signal-to-noise ratio of

nanopillar-MEAs was increased by a factor of 2 compared to planar MEAs. In future applications this nanopillar concept can be adopted for distinct interface materials and coupling to cellular and molecular sensing components.

BP 13.7 Tue 16:00 H45

Nsp7-Nsp8 Supercomplex Building of Fe-CoV — ●HENNING SEIDEL¹, YIBEI XIAO², RAJESH PONNUSAMY², ROLF HILGENFELD², and CHRISTIAN G. HÜBNER¹ — ¹Institute of Physics, Ratzeburger Allee 160, 23538 Lübeck, Germany — ²Institute of Biochemistry, Ratzeburger Allee 160, 23538 Lübeck, Germany

Coronaviruses are enveloped positive-stranded RNA viruses. They possess the largest known RNA genome. Their RNA-dependent RNA-polymerase (RdRp) activity is supplied by the non-structural protein 12 (nsp12) [1]. For SARS-CoV, it was shown that coronaviruses also encode a second RdRp build from nsp7 and nsp8. This hexadecameric nsp7-nsp8 supercomplex is a hollow, cylinder-like structure assembled from eight copies of nsp8 and held together by eight nsp7 molecules [2]. We are aiming at understanding the assembly process and related conformational changes of the supercomplex for the related Feline Coronavirus. The structural and functional examination of the nsp7-nsp8 supercomplex building should help in understanding the replication and transcription mechanisms of Fe-CoV and other coronaviruses like SARS-CoV. In order to gain knowledge of the complex building, we apply methods of single molecule fluorescence, namely fluorescence correlation spectroscopy (FCS) and fluorescence resonance energy transfer (FRET).

[1] Imbert I. et al., The EMBO Journal, Vol 25, 4933-4942 (2006)

[2] Zhai Y. et al., Nature Structural and Molecular Biology, Vol 12, No 11, 980-986 (2005)

BP 13.8 Tue 16:15 H45

Swelling and softening of the CCMV plant virus capsid in response to pH shifts — ●BODO D. WILTS¹, IWAN A.T. SCHAAP¹, CHRIS C. BROOMELL², CHARLES M. KNOBLER³, and CHRISTOPH F. SCHMIDT¹ — ¹III. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — ²Center for Bio-Inspired Nanomaterials, Montana State University, Bozeman, MT, USA — ³Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA, USA

Previous research on cowpea chlorotic mottle viruses (CCMV) has revealed a swelling transition and a softening of the protein capsid in response to a pH increase. In this study, we have performed nano-indentation experiments using an atomic force microscope and tested the shell response from low (4.8) up to high pH (7.5) in the absence of divalent ions. We could, for the first time, study the elastic behavior of the swollen virions. Indentations were performed in the reversible linear regime with indentation forces up to 200 pN. The results show a gradual swelling transition of the RNA-filled capsids preceded by a softening of the shell as a function of pH. Control measurements with the empty capsid and a salt-stable mutant revealed that the softening is not directly coupled to the swelling of the protein shells. Instead we hypothesize that the softening of the CCMV virions is triggered by pH-dependent opening of bonds within the protein shell which may be necessary, but not sufficient for swelling.

BP 14: Evolutionary Game Theory III (joint SOE, BP)

Time: Tuesday 14:00–16:00

Location: H44

Invited Talk

BP 14.1 Tue 14:00 H44

Stochasticity and specificity in DNA repair — ●THOMAS HÖFER¹, MARTIJN LUIJSTERBURG², GESA VON BORNSTAEDT¹, and ROEL VAN DRIEL³ — ¹Deutsches Krebsforschungszentrum, Heidelberg, Germany — ²Karolinska Institute, Stockholm, Sweden — ³University of Amsterdam, The Netherlands

To understand how multi-protein complexes assemble and function on chromatin, we have combined quantitative analysis of a mammalian DNA repair machinery in living cells with mathematical modeling. We found that the individual components exchange rapidly at the repair sites whereas their net accumulation evolved on a much slower timescale. Based on the experimental data, we developed a predictive kinetic model of how multi-protein repair complexes assemble. Complex formation is orchestrated by progressive enzymatic modifications

of the chromatin substrate, leaving considerable freedom for the binding mode of individual proteins. We demonstrate that the faithful recognition of DNA lesions is a time-consuming process, while subsequently repair complexes form rapidly through random and reversible assembly. Our analysis reveals a fundamental conflict between specificity and efficiency of chromatin-associated protein machineries and shows how a trade-off is negotiated through reversibility of protein binding.

BP 14.2 Tue 14:30 H44

Predicting correlated mutations of amino acids from protein structure — ●JONAS MINNING¹, UGO BASTOLLA², and MARKUS PORTO¹ — ¹Technische Universität, Darmstadt, Germany — ²Centro di Biología Molecular, 'Severo Ochoa', CSIC-UAM, Madrid, Spain

Even though the average sequence similarity for homologous proteins sharing the same fold can reach the threshold of randomness, amino acid sequences maintain the fingerprint of selective pressures on structure and function. We have previously developed an analytical method for computing the probability to observe a given amino acid at a given site in a protein with known native structure, based on an independent site approximation of protein evolution subject to selective constraints on unfolding and misfolding stabilities [1]. However, substitutions at different sites are known to be correlated, and these correlated mutations may give important information for reconstructing native contacts, protein interaction interfaces, or clusters of functionally important residues. Here, we present a model which allows to quantitatively predict the correlated mutations that arise from selective constraints on unfolding and misfolding stabilities. Our model is verified against simulated data of protein sequence evolution and statistical data of proteins in the Protein Databank.

[1] U. Bastolla *et al.*, *Proteins* **73**, 872 (2008).

BP 14.3 Tue 14:45 H44

Stability of an underdominant polymorphism in the presence of migration — ●PHILIPP M. ALTROCK, ARNE TRAUlsen, R. GUY REEVES, and FLOYD A. REED — MPI f. Evolutionary Biology, Plön, Germany

In population genetics, underdominance refers to natural selection against individuals with a heterozygous genotype [1]. Here, we analyse a single-locus underdominant system of two large local populations that exchange individuals at a certain migration rate and can be characterized by fixed points in the joint allele frequency space. We specifically address the conditions under which underdominance can be applied to stably and reversibly transform a local population that is receiving untransformed migrants, where an exact relationship between the rate of migration and the degree of selection against heterozygotes, that allows stable local transformations, exists [2]. We also approximate the critical minimum frequency required to result in a stable population transformation. For doubly asymmetric configurations, i.e. different homozygote fitness and unequal migration rates, there is a regime where a stable transformation is only possible in one of the two populations. The stability of the system is robust to the migration of gravid females. We also address the relative influence of various forms of stochasticity (migration versus genetic drift).

[1] Hartl & Clark, *Principles of Population Genetics*, 2nd Edition. Sinauer Associates, Inc., Sunderland, MA. (1989).

[2] Karlin & McGregor, *Theor. Pop. Biol.* **3**, 186 (1972).

BP 14.4 Tue 15:00 H44

Recombination suppresses peak escape in rugged fitness landscapes — ●JOACHIM KRUG and SU-CHAN PARK — Institut für Theoretische Physik, Universität zu Köln, Germany

The adaptive value of recombination is at the heart of the long-standing debate about the evolutionary role of sex. Intuitively one might expect recombination to aid the escape of a population from sub-optimal fitness peaks and hence to accelerate the adaptive process. Here we show that the converse is true. For a deterministic, haploid two-locus model with two fitness peaks of unequal height, a stationary low-fitness solution concentrated at the lower peak emerges beyond a critical value of the recombination rate. The bifurcation giving rise to this solution is formally equivalent to an Ising-like phase transition. Numerical simulations show that the phenomenon persists in more complex multi-locus landscapes derived from experimental fitness measurements for the asexual fungus *Aspergillus niger*.

BP 14.5 Tue 15:15 H44

Chemical Evolution in Simulating Experiments — ●EVA

WOLLRAB and ALBRECHT OTT — Biologische Experimentalphysik, Saarbrücken, Deutschland

In 1953 Stanley Miller and Harold Urey made a pioneering experiment, simulating possible primitive earth conditions. In a sealed apparatus they boiled water in an atmosphere of methane, ammonia and hydrogen circulating these compounds past an electric discharge during periods of the order of a week. The resulting samples contained several organic molecules among them also amino acids. In the following decades several experiments were made to test the spontaneous formation of the most important biomolecules under possible primitive earth conditions.

We have performed Miller's experiment. The resulting samples were analyzed by HPLC and mass spectroscopy. Our analysis performed following different run-times gives us information about the composition of the reaction products. It reveals an evolution of the emerging substances and their compositions towards increased complexity as well as a (universal?) distribution of molecular masses.

This is a first step in order to determine conditions, which ultimately allow for the birth of autocatalytic chemical cycles.

BP 14.6 Tue 15:30 H44

Evolutionarily stable demographics — ●OSKAR HALLATSCHKEK — Biological Physics and Evolutionary Dynamics, MPI DS, Goettingen

It has long been noticed that demographic stochasticity can seriously interfere with Darwin's evolutionary principles of heritable variation and selection. Advantageous genes are sometimes lost accidentally. These chance effects are considered as major retardation of Darwinian evolution. Here, we show that, in spatial systems, they can sometimes accelerate adaptive evolution. We describe a whole class of demographic parameters for which demographic stochasticity actually drives adaptive evolution. Among these traits are dispersal rates and carrying capacities, for which evolutionary optimal values (ESS's) can be given. These new class of noise driven adaptations suggests that demographic stochasticity must be considered also as an important creative Darwinian force, not only as a disrupting one.

BP 14.7 Tue 15:45 H44

Sexual and asexual reproduction in iteroparous species — ●YIXIAN SONG¹, BARBARA DROSSEL¹, and STEFAN SCHEU² — ¹Institut für Festkörperphysik, Technische Universität Darmstadt, Deutschland — ²J.F. Blumenbach Institute of Zoology and Anthropology, University of Goettingen, Germany

The evolution of sex has been discussed intensively since Charles Darwin. By considering explicitly the important fact of limited and structured resources, we explore the conditions for the maintenance of sex in spite of the cost of producing males. In this model, asexual species win over sexual species only when mortality rates are large, resources regrow quickly, many different genotypes are allowed to coexist at the same place, or when resource diversity is small. Here, we modify the limited structured resource model of Scheu and Drossel (*Proc. Roy. Soc. B.* 2007) such that it applies to iteroparous species, which reproduce more than once during their life. We therefore include age and size of individuals into the model, with the corresponding metabolic rate, mortality and fecundity. Metabolic rate per biomass and mortality decrease with increasing body weight, while the fecundity increases. Therefore, phenotypes with smaller size at maturity have a higher mass dependent metabolic rate, a higher mortality, and a lower fecundity. However, they reach maturity earlier with the same growth rate and increase thereby the chance of survival until reproduction. We determine the optimum size at reproduction and the optimum offspring size under different environmental conditions, and we evaluate the parameter range for which sexual reproduction wins over asexual reproduction.

BP 15: Physics of Cells II

Time: Tuesday 14:30–17:00

Location: H43

BP 15.1 Tue 14:30 H43

Formation of long lived local protein kinase C clusters after short Calcium puffs — ●MIKE BONNY¹, MARTIN PEGLOW¹, LARS KAESTNER², PETER LIPP², HEIKO RIEGER¹, and KARSTEN KRUSE¹ — ¹Department of Theoretical Physics, Saarland University, D-66041 Saarbrücken, Germany — ²Institute for Molecular Cell Biology, Medical Faculty of the Saarland University, D-66421 Homburg/Saar, Ger-

many

Conventional protein kinases C (cPKCs) play an important role in signal transduction and in gene regulation. PKC α , a member of the cPKC-family, translocates to the plasma membrane after activation via cytosolic Ca²⁺ ions. In particular, there exist local translocation events, when PKC α forms clusters on the membrane with limited spatial spreads ($< 4\mu\text{m}$). The lifetime of brief events is 400-1500ms,

while long lasting events have a lifetime larger than 5s, which markedly exceeds the duration of a Calcium puff [1].

We show theoretically that allosteric effects together with interactions between membrane-bound PKC α can lead to the observed behaviour. Using fluorescence resonance energy transfer (FRET) measurements we support our assumption of so far unknown interactions between PKC α molecules.

[1] Reither, G., Schaefer, M., Lipp, P. (2006). PKC α : a versatile key for decoding the cellular calcium toolkit. *JCB* 174: 521-533

BP 15.2 Tue 14:45 H43

Sensitisation waves in a bidomain fire-diffuse-fire model of intracellular Ca²⁺ dynamics — ●RÜDIGER THUL¹, STEVEN COOMBS¹, and GREG D SMITH² — ¹School of Mathematical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK — ²Department of Applied Mathematics, The College of William and Mary, Williamsburg, VA 23187, USA

We present a bidomain threshold model of intracellular calcium (Ca²⁺) dynamics in which, as suggested by recent experiments, the cytosolic threshold for Ca²⁺ liberation is modulated by the Ca²⁺ concentration in the releasing compartment. We explicitly construct stationary fronts and determine their stability using an Evans function approach. Our results show that a biologically motivated choice of a dynamic threshold, as opposed to a constant threshold, can pin stationary fronts that would otherwise be unstable. This illustrates a novel mechanism to stabilise pinned interfaces in continuous excitable systems. Our framework also allows us to compute travelling pulse solutions in closed form and systematically probe the wave speed as a function of physiologically important parameters. We find that the existence of travelling wave solutions depends on the time scale of the threshold dynamics, and that facilitating release by lowering the cytosolic threshold increases the wave speed.

BP 15.3 Tue 15:00 H43

Bifurcations and Chaos in the MAPK Signaling Cascade — ●MARTIN ZUMSANDE and THILO GROSS — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Deutschland

The mitogen-activated protein kinase (MAPK) cascade is an important signaling pathway in eukaryotic cells. It is involved in the regulation of a large number of cell functions. Many molecular details of the cascade that consists of multiple phosphorylation cycles are known today. However, many aspects of the dynamics are still unknown, most importantly how exactly the different cell functions can be triggered. We apply the method of generalized modelling [Gross, Feudel: PRE 73, 2006] to a model of the MAPK cascade. We describe how external parameters are correlated with stability of the steady states. Furthermore, we report complex oscillations and potentially chaotic behavior caused by a sequestration-based feedback mechanism. We also investigate the interplay between sequestration and external feedback loops. Our analysis thereby confirms, extends and generalizes previous results obtained by conventional modeling and points out the diversity of dynamics that sequestration can bring about.

BP 15.4 Tue 15:15 H43

Generating alternating bidirectional gradient fields for dynamic measurement of chemotactic response in living cells — ●BÖRN MEIER, CHRISTOPH WEBER, SIMON YOUSSEF, THOMAS FRANOSCH, JOACHIM RÄDLER, and DORIS HEINRICH — Fakultät für Physik und CeNS, LMU München, Germany

Chemotactic response in eucaryotic cells is inherently probabilistic and measurements of single cell responses and population distributions help to advance quantitative understanding of underlying signalling pathways. Therefore we have designed a microfluidic function generator, creating time-varying but spatially homogenous chemical gradients of opposing direction. In a first step we monitored the migratory response of Dictyostelium discoideum cells to alternating cAMP-gradients with decreasing switching frequency. At low switching rates directed cell migration according to the applied chemotactic sequence appears. At frequencies above 0.01 Hz cellular motility is stalled, leading to trapped cells. We monitored the actin reorganization, underlying the cell response, identified by the Lim-Gfp fluorescence distribution in the cell. Cell polarization, reflected by the dipolar moment of the fluorescence distribution, expresses a delayed cell response, where two phases of opposing actin polymerization are intercepted by a phase of decreased actin polymerization.

BP 15.5 Tue 15:30 H43

Does Molecular Crowding affect DNA Hybridization in vivo? — INGMAR SCHOEN, HUBERT KRAMMER, and ●DIETER BRAUN — Systems Biophysics, Center for Nanoscience, Ludwig Maximilians University, Munich, Germany

Molecules in a cell are subject to significant crowding from their sister molecules. While measurements of anomalous diffusion inside cells point towards a marked effect of molecular crowding, its impact on the rate of reactions is hard to assess.

We have developed a novel technique to image kinetics in living cells using an optical lock-in approach[1]. The reaction time constant is resolved in frequency space with optical resolution under a moderate temperature oscillation and sinusoidal illumination.

DNA hybridization kinetics in living cells is strongly length selective: 16 base pair DNA has a seven-fold faster on-rate as compared to the in vitro situation, whereas 12bp DNA has a five-fold slower on-rate in vivo as compared to in vitro. Evidence points towards a catalytic acceleration for longer DNA and a slowing down by DNA binding proteins.

Above results are not expected from molecular crowding. We assessed molecular crowding with Dextran and Ficoll at high concentrations [20% (w/v)] and find no significant changes in the hybridization kinetics, indicating a minor role of molecular crowding for bi-molecular DNA hybridization.

[1] Schoen, Kramer and Braun, PNAS, in press

15 min. break

BP 15.6 Tue 16:00 H43

Correlation of protein density with cell morphology both in motile mouse fibroblasts and slime molds — ●ERIK BERNITT, CHRISTINA OETTMEIER, SIDDHARTH DESHPANDE, and HANS-GÜNTHER DÖBEREINER — Institut für Biophysik, Universität Bremen

We have characterized cell motility as temporal sequences of distinct dynamic phases. Transitions between these phases are indicated by a number of cellular observables including adhesion area, membrane front velocity, topological markers, and special characteristics of internal density fields. In this talk, we present examples of two species from different evolutionary kingdoms. Under environmental stress, the slime mold *Physarum polycephalum* exhibits a transition from a globular phase to an extended network with an increasing number of holes. This change in topology is coupled to a pronounced variation in the frequency of area oscillations and internal density waves. We calculate multidimensional cross correlations of these phase indicators. Mouse embryonic fibroblasts show distinct phases of spreading. We correlate front velocity with actin distribution in these phases.

BP 15.7 Tue 16:15 H43

The role of the G protein-coupled receptor CXCR4 in angiogenesis - a single-molecule approach — ●SUSANNE FENZ¹, CASSANDRA VERHEUL¹, EWA SNAAR-JAGALSKA², and THOMAS SCHMIDT¹ — ¹Leiden Institute of Physics, Leiden, The Netherlands — ²Institute of Biology, Leiden, The Netherlands

Directed cell movement in a chemical gradient, chemotaxis, is a prerequisite for many vital processes like the immune response, but it is also the basis for cancer metastasis. Chemotaxis is governed by extracellular gradients of small molecules, the chemokines. While their receptors in the cell membrane are identified, it is still unknown how the cell subsequently builds up an asymmetric phenotype with defined front and rear edge, necessary for directed movement. This polarization is triggered by tiny gradients and is robust in noisy environment. Thus, we propose that universal physical mechanisms underlie the first steps towards polarity.

Two potential ordering parameters, the receptor mobility and cytoskeleton-induced membrane domains, were investigated on a molecular level in living mouse fibroblasts and human vascular endothelial cells. We applied single-molecule fluorescence microscopy to characterize the diffusion behaviour of CXCR4-eYFP upon stimulation with its chemokine SDF and to probe for potential association with CCR5. Since it is known that tumor cells expressing CXCR4 perform metastasis not only by direct migration to organs expressing SDF, but additionally promote angiogenesis towards the tumor our model system will yield insights into both mechanisms.

BP 15.8 Tue 16:30 H43

A model for thickness oscillations in protoplasmic droplets of Physarum polycephalum — MARKUS RADSZUWEIT¹, HARALD ENGEL², and MARKUS BÄR¹ — ¹Physikalisch Technische Bundesanstalt, Berlin — ²Technische Universität Berlin

A model for explaining thickness oscillations in protoplasmic droplets in true slime mold *Physarum polycephalum* is proposed and numerical simulations are presented. An autonomous Ca^{2+} -oscillator based on the regulation of myosin binding to actin is combined with a two phase mechanical model for a polymer gel. Using Darcy's law of porous media for the endoplasmic flow field and theory of active elastic gels a full description of the flow, pressure and deformation field is obtained. The nonlocal feedback of this quantities on the reaction-diffusion-advection system of the chemical oscillator leads to the formation of various dynamical patterns like targets, standing or spiral waves.

BP 15.9 Tue 16:45 H43

Impact of microscopic motility on overall swimming behaviour of parasites — SRAVANTI UPPALURI¹, JAN NAGLER¹, ERIC STELLAMANN¹, NIKO HEDDERGOTT², STEPHAN HERMINGHAUS¹,

MARKUS ENGSTLER², and THOMAS PFOHL^{1,3} — ¹Max Planck Institute for Dynamics and Self Organization, Göttingen — ²Biocenter, University of Würzburg — ³Chemistry Department, University of Basel

Trypanosomes, causative agents of sleeping sickness and Chagas disease, exhibit complex flagellum mediated motility. In trypanosomes this flagellum mediated motility has been shown to be essential for cell division, viability, and immunological escape from the host. Trypanosomes swim in one of three distinct motility modes: random walk, directional persistence, and an intermediate class in which they exhibit a combination of both. Using high-speed microscopy with a frame rate of 1000 Hz, we investigate the microscopic origin of these macroscopic motility modes. The experimentally observed motility modes correspond to distinct physical movements and can be attributed to distinct cell shape conferred mainly by flagellum dynamics. We find that directional persistence arises only with stretched cells implying that there are significant energy or stiffness differences within a single population. We report our findings on the dependence of cell shape on the cell cycle in which the flagellum plays a key role.

BP 16: SYMM: Magnetism and Medicine

Time: Wednesday 9:30–12:30

Location: H1

Invited Talk BP 16.1 Wed 9:30 H1
Magnetic resonance imaging: an ongoing success story — JENS FRAHM — Biomedizinische NMR Forschungs GmbH, Am Fassberg 11, 37070 Goettingen, Germany

The fascinating development of magnetic resonance imaging (MRI) started more than 35 years ago when Paul Lauterbur published a seminal paper on an imaging method based on nuclear magnetic resonance (NMR). Since then, MRI evolved from a toy for physicists to one of the most important tools in diagnostic imaging, with almost 100 million examinations per year worldwide. In addition, noninvasive MRI studies of experimental animals (e.g., genetically modified mice) play a unique role in translational biomedical research linking advances in molecular biology to studies of human patients. The main driving force behind the large range of diverse MRI methods and applications is the quest for image quality, specificity, and speed. This presentation will illustrate some of these developments by focusing on selected examples. Specific topics include the MRI access to human brain function and the underlying axonal connectivity and fiber architecture. The talk will further address recent progress in real-time MRI yielding movies with up to 40 frames per second. Such techniques exploit non-Cartesian radial encoding schemes and iterative image reconstructions using regularized nonlinear inversion.

Invited Talk BP 16.2 Wed 10:00 H1
Biomedical nanomagnetism: A spin through new possibilities — KANNAN KRISHNAN — University of Washington, Seattle, USA

Two of the principal challenges in biomedicine are the detection of disease at the earliest possible time prior to its ability to cause damage (diagnostics and imaging) and delivering treatment at the right place, at the right time whilst minimizing unnecessary exposure (targeted therapy with a triggered release). In this context, we have been developing theranostic magnetic nanoprobe (TMN) with tailored properties for high moment or high frequency applications, optimized for localized heating, MRI contrast enhancement and triggered drug release, and individually conjugated for specific functionality. Advantages of these TMNs include (a) the flexibility and precision with which the physical properties of the nanoparticle core – size, size distribution, MRI relaxivity, magnetic relaxation dynamics and pH-sensitivity – can be tailored and optimized. (b) their functionality as ultrasmall and ultrasensitive MRI contrast agents with competitive performance suggesting lower dose and increased penetration. (c) the optimized properties of these TMNs to generate heat locally and the therapeutic potential that this feature implies. (d) their biocompatibility and very low cytotoxicity and (e) their potential for the development of a magnetic particle imaging microscope – an inexpensive, quantitative nanoimaging platform for meaningful dosimetry. Details of our current work in these areas, including translational application, primarily focused on detection and treatment of cancer, will be discussed.

Invited Talk BP 16.3 Wed 10:30 H1

Recent SQUID applications in medicine — HANS KOCH — Physikalisch-Technische Bundesanstalt (PTB), Berlin

An overview will be presented on more recent applications of SQUID sensor systems in medicine, namely in the fields of magnetoencephalography, magnetic nanoparticle probes, and low field magnetic resonance. As a particular aspect the merits of these applications will be highlighted with respect to the grand competition of magnetic resonance imaging.

Invited Talk BP 16.4 Wed 11:00 H1
Biomedical Magnetic Resonance using Hyperpolarized Gases and Liquids — LAURA SCHREIBER — Section of Medical Physics, University Medical Center, Mainz, Germany

Biomedical magnetic resonance imaging (MRI) is an inherently insensitive methodology since it requires mmol amounts of the detected nuclei. Therefore, MRI of respiratory gases (O₂, CO₂, N₂) is not feasible in-vivo. Sophisticated hyperpolarization techniques, i.e. optical pumping of nuclear states, increase the nuclear polarization of the noble gases ³He and ¹²⁹Xe by five orders of magnitude and thus permit a direct imaging of the inhaled gases as they distribute within the lung of a human subject. Therefore, assessment of human lung ventilation becomes feasible. Moreover, techniques have been developed to measure functional lung parameters like intrapulmonary oxygen concentration or the integrity of the alveoli using hyperpolarized gases.

Hyperpolarization of liquids has also become feasible recently using Dynamic Nuclear Polarization (DNP) or Parahydrogen Induced Polarization (PHIP) techniques. This is of particular interest for low sensitivity nuclei like ¹³C where measurement times are long. Now metabolic studies with DNP- or PHIP-hyperpolarized ¹³C-labeled substances have become feasible with measurement times on the order of seconds, thus permitting non-invasive assessment of reaction kinetics in-vivo.

Invited Talk BP 16.5 Wed 11:30 H1
Recent Developments in Healthcare Biomagnetics — QUENTIN PANKHURST — Director, Davy-Faraday Research Laboratory, The Royal Institution of Great Britain, 21 Albemarle Street, London W1S 4BS

Healthcare biomagnetics - the sensing, moving and heating of magnetic nanoparticles in vitro or in the human body - is a rapidly changing field that is attracting a great deal of interest worldwide. It offers the potential to develop safe and convenient alternatives for a diverse range of therapeutic and diagnostic healthcare applications, using injectable materials of proven safety and reliability. In doing so, it makes use of the three fundamental action-at-a-distance properties of magnetic materials - their ability to act as remote sensors, mechanical actuators, and heat sources. The versatility of the field is leading to the emergence of multi-modal applications, combining two or more of the sensing-moving-heating properties in the same product. Similarly, certain applications are now entering or are close to beginning Phase I/II

clinical trials, or in the case of in vitro products, are already entering the marketplace. In this lecture some recent developments in the field will be described and discussed.

Invited Talk BP 16.6 Wed 12:00 H1
SQUIDS for Noninvasive Magnetogastrography — ●ALAN BRADSHAW^{1,2}, LEO CHENG³, ANDREW PULLAN³, and WILLIAM RICHARDS⁴ — ¹Vanderbilt University, Nashville, TN — ²Lipscomb University, Nashville, TN — ³Auckland University, Auckland, NZ — ⁴University of South Alabama, Mobile, AL

The magnetogastrogram (MGG) and magnetoenterogram (MENG) have been studied over the past 20 years to assess digestive and motility issues in the stomach and small bowel. While the electrogastrogram

(EGG) is capable of measuring frequency dynamics of the stomach's electrical activity, spatiotemporal analyses afforded by multichannel magnetogastrography may prove critical to the assessment of stomach disorders such as gastroparesis. Our recent results from MGG measurements and modeling suggest differences in gastric slow wave propagation between normal controls and diabetic gastroparetics. The electroenterogram (EENG) is not readily recordable in most subjects because of the intervening fat layers, but the MENG is less susceptible to volume conduction effects because of the relative similarity of the magnetic susceptibility of tissue and air. Mesenteric ischemia is a potentially deadly disease characterized by dysrhythmias of the intestinal electrical activity. These dysrhythmias can be detected in the MENG, and our recent studies are investigating the threshold at which effects can be discerned.

BP 17: Anomalous Transport I (joint BP, DY)

Time: Wednesday 9:30–11:00

Location: H38

BP 17.1 Wed 9:30 H38
Elucidating the origin of anomalous diffusion in crowded fluids — JEDRZEJ SZYMANSKI and ●MATTHIAS WEISS — Cellular Biophysics Group, German Cancer Research Center, Heidelberg

Anomalous diffusion in crowded fluids, e.g. in the cytoplasm of living cells, is a frequent phenomenon. So far, however, the associated stochastic process, i.e. the propagator of the random walk, has not been uncovered. Here, we show by means of fluorescence correlation spectroscopy and simulations that the properties of crowding-induced subdiffusion are consistent with the predictions for fractional Brownian motion or obstructed (percolation-like) diffusion, both of which have stationary increments. In contrast, our experimental results cannot be explained by a continuous time random walk with its distinct non-Gaussian propagator.

Reference J. Szymanski & M. Weiss, Phys. Rev. Lett. 103, 038102 (2009).

BP 17.2 Wed 9:45 H38
Macromolecular crowding - probing the microscopic protein diffusion on nanosecond time scales — ●FELIX ROOSEN-RUNGE¹, MARCUS HENNIG^{1,2}, FAJUN ZHANG¹, TILO SEYDEL², and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, Germany — ²Institut Laue-Langevin, Grenoble, France

In the cellular interior, macromolecules occupy high volume fractions. This so-called macromolecular crowding affects both cellular structure and function, as reported from both simulations and kinetic measurements. From a dynamical point of view, however, protein diffusion in crowded media is far from understood. The nature of diffusion is expected to show different regimes of simple and anomalous diffusion, depending on the respective time and length scale.

Using quasi-elastic neutron scattering (QENS) at time scales of nanoseconds and length scales of several nanometers, we probe the self diffusion in crowded solutions of bovine serum albumin (BSA). The temperature dependence of the effective diffusion coefficient below thermal denaturation can be rationalised based on the Stokes Einstein relationship; addition of NaCl cause little or no changes. The concentration dependence is the most pronounced effect: the apparent diffusion coefficient, covering volume fractions ranging from 5% up to 40%, strongly decreases with increasing protein concentration. A careful deconvolution of rotational and translational contributions provides insights in the simple diffusive nature of protein motions probed by neutron backscattering. The findings are also discussed in comparison to results from colloid physics.

BP 17.3 Wed 10:00 H38
Electrostatic interactions modulate particle translocation in reconstituted mucus hydrogels — ●OLIVER LIELEG, IOANA VLADSCU, and KATHARINA RIBBECK — FAS Center for Systems Biology, Harvard University, Cambridge, USA

Biological functional entities surround themselves with selective barriers which control the passage of certain classes of macromolecules while rejecting others. A prominent example of such a selective permeability barrier is given by mucus. Mucus is a biopolymer based hydrogel which lines all wet epithelial surfaces of the human body. It regulates the uptake of nutrients from our gastrointestinal system, ad-

justs itself with the menstrual cycle to control the passage of sperm, and shields the underlying cells from pathogens such as bacteria and viruses. In the case of drug delivery, the mucus barrier needs to be overcome for successful medical treatment. Despite its importance for both physiology and medical applications, the underlying principles which regulate the permeability of mucus remain enigmatic. Here, we analyze the mobility of microscopic particles in reconstituted mucin hydrogels. We show that electrostatic interactions between diffusing particles and mucin polymers regulate the permeability properties of reconstituted mucin hydrogels. As a consequence, various parameters such as particle surface charge, mucin density, and buffer conditions such as pH and ionic strength can modulate the microscopic barrier function of the mucin hydrogel. Our findings suggest that the permeability of a single biopolymer based hydrogel such as native mucus can be tuned to a wide range of settings in different compartments of our bodies.

BP 17.4 Wed 10:15 H38
Subdiffusive Dynamics in Dense Driven Granular Media — ●MATTHIAS SPERL and ELMAR STAERK — DLR Cologne

Granular media is characterized by non-elastic collisions among particles and obstacles; collisions lead to dissipation of energy. This lost energy needs to be replenished to achieve a steady state, and such a non-equilibrium steady state is investigated in our experiments. The driving is realized in two dimensions on a vibrating table; the particles dynamics is monitored by high-speed cameras with a specially adapted long-time recording system: Several minutes of dynamics can be recorded with millisecond resolution. The dynamical window allows the identification of several decades of anomalous dynamics and respective exponents in the mean-squared displacement. We investigate two granular systems in their dense regime: (1) a granular Lorentz system, where a single particles explores an environment of quenched disorder, and (2) the glass-like dynamics of a system with many particles. In both cases, the resulting dynamics shows both remnants of their equilibrium counterparts and marked differences. E.g., results vary with differences in the rates of driving and dissipation. A comparison with results from theory and computer simulation will be performed.

BP 17.5 Wed 10:30 H38
Localization and glass formation of colloids confined in porous media — ●JAN KURZIDIM, DANIELE COSLOVICH, and GERHARD KAHL — Institut für Theoretische Physik and Center for Computational Materials Science, Technische Universität Wien, Wiedner Hauptstraße 8-10, A-1040 Wien, Austria

Using molecular dynamics simulations we study the slow dynamics of a hard-sphere fluid confined in a matrix quenched from an equilibrated hard-sphere fluid [Kurzydum *et al.*, PRL **103**, 138303 (2009)], resembling the movement of hard colloids in porous environments. We observed the presence of both discontinuous and continuous glass transitions, anomalous diffusion, and a de-coupling of the time scales for the relaxation of the single-particle and the collective correlators. Our observations are consistent with many predictions of a recent extension of mode-coupling theory for so-called “quenched-annealed” systems. Notably, however, we found no evidence of the re-entrant regime in the kinetic diagram predicted by the theory. To provide a deeper insight into the microscopic details of the underlying processes, we

calculated the quantities of interest separately for particles trapped in voids formed by the matrix and for particles that unrestrictedly move through the entire system. In order to evaluate the degree of universality of the observed phenomena, we extended our investigation to model colloids with soft interactions, employing both numerical solutions of the equations of the theory, and molecular dynamics simulations.

BP 17.6 Wed 10:45 H38

Anomalous transport in a medium subjected to phase transition — DARIA KONDRASHOVA, JÖRG KÄRGER, and •RUSTEM VALIULLIN — Department of Interface Physics, University of Leipzig, Leipzig, Germany

Diffusion in spatial structures created via invasion percolation may naturally exhibit anomalous properties. It is now becoming evident that phase transitions occurring in heterogeneous media, may also be described using the concept of invasion percolation [1]. Hence, trans-

port properties of tracer particles in media subjected to phase changes can strongly be affected by the latter process, including conditions giving rise to anomalous transport patterns. In this work, we experimentally demonstrate that such fractal-like structures are developing during freezing and melting transitions of liquids in disordered mesoporous matrices. We show that the effective self-diffusivity in the pore space, occupied by the liquid phase at a given fraction, depends on a particular configuration of the frozen phase [2]. Interestingly, by using a porous material with tubular pore morphology, we were able to relate the phase transition kinetics to the propagation of the liquid-solid interfaces in the pores. Depending on temperature, this propagation itself is found to exhibit a spectrum of behavior from diffusive to anomalous. The data obtained may have implications for understanding anomalous transport in bio-systems such as lipid membranes.

1. Page, J. H., J. Liu, B. Abeles, H. W. Deckman and D. A. Weitz, Phys. Rev. Lett., 71, 1216 (1993). 2. Dvoyashkin, M., A. Khokhlov, R. Valiullin and J. Kärgner, J. Chem. Phys., 129, 154702 (2008).

BP 18: Anomalous Transport II (joint BP, DY)

Time: Wednesday 11:15–13:15

Location: H38

BP 18.1 Wed 11:15 H38

Anomalous lateral diffusion in a layered medium — •EUGENE B. POSTNIKOV¹ and IGOR M. SOKOLOV² — ¹Staatliche Universität Kursk, Russland — ²Institut für Physik Humboldt - Universität zu Berlin, Deutschland

We consider the marker's diffusion in a layered medium, with the lateral diffusion coefficient being the function y -coordinate, i.e. the problem described by the diffusion equation for the marker density $u(x, y, t)$

$$\partial_t u = D_x(y) \partial_{xx} u + D_y \partial_{yy} u$$

with anisotropic diffusion coefficient \hat{D} . We show that the mean density averaged over the height, $U(x, t)$, follows the Bachelor's one-dimensional diffusion equation with time-dependent diffusion coefficient

$$\partial_t U = D_x(t) \partial_{xx} U$$

and obtain the expression of $D_x(t)$. As an example, we discuss the exact analytical solution in the case of a parabolic distribution $D_y \sim y^2$, leading to the anomalous (superdiffusive) behavior of a mean-square displacement $\langle x^2 \rangle \propto t^{3/2}$. This result is confirmed by the numerical solution.

The approach is applied for the continual description of experimental results on inhomogeneous molecular diffusion in layered structures of thin liquid films deposited on solid surfaces [J. Schuster, F. Cichos, C. von Borzyczkowski. Eur. Polym. J. 40 (2004) 993].

BP 18.2 Wed 11:30 H38

From Anomalous Deterministic Diffusion to the Continuous-Time Random Walk — •MARKUS NIEMANN and HOLGER KANTZ — Max-Planck-Institut für Physik komplexer Systeme, Dresden

There are several stochastic models describing anomalous diffusion. The most common are the fractional Brownian motion and the Continuous-Time Random Walk (CTRW). The question arises how to choose the correct model for a given process. Our approach is to look for deterministic foundations of these models. We present a method how to derive a CTRW as asymptotic description of a deterministic diffusion process.

We have introduced a diagrammatic method to determine the joint probability distributions of CTRWs. This method is extended to allow couplings between steps. These couplings may arise from deterministic maps, thereby allowing a unified treatment of stochastic and deterministic systems. Often, these processes converge in the scaling limit to a CTRW without coupling between steps. We apply the theory to a diffusion process driven by a deterministic map of Manneville-Pomeau type. Depending on the parameter, one gets a transition from an uncoupled to a coupled CTRW and a transition from sub- to superdiffusion. These findings are well supported by numerical simulations.

BP 18.3 Wed 11:45 H38

Random walks on d -dimensional Sierpinski gaskets: Asymptotics, DSI, and Puzzles — •SEBASTIAN WEBER¹, JOSEPH KLAFTER^{2,1}, and ALEXANDER BLUMEN³ — ¹Freiburg Institute For Advanced Studies (FRIAS), University of Freiburg, Germany — ²School of Chemistry, Tel Aviv University, Israel — ³Theoretical Polymer Physics, University of Freiburg, Germany

We study the effect of the embedding dimension d of a random walk (RW) taking place on a d -dimensional Sierpinski gasket fractal in its classical and dual versions. In the limit of large d the spectral dimension d_s approaches 2 such that the RW dynamics, which is governed by the d_s , is expected to behave similarly to a RW on a 2 dimensional lattice. In sharp contrast to that, we observe much richer characteristics for the RW. First, the time discrete scale invariance (DSI) phenomena cause log-periodic oscillations, which increase in amplitude for larger d . Second, the asymptotic approach to theoretically predicted power-laws of standard RW observables is significantly altered, depending on the variant of the Sierpinski gasket used (classical or dual) and on d . Furthermore, we address the suitability of standard RW observables to determine the spectral dimension d_s . This analysis is of great practical relevance and shows unexpected, puzzling results.

BP 18.4 Wed 12:00 H38

Front propagation in an $A+B \rightarrow 2A$ reaction-subdiffusion system — •DANIELA FROEMBERG and IGOR M. SOKOLOV — Humboldt Universität Berlin

Using the Continuous Time Random Walks approach, we derive reaction-subdiffusion equations for the irreversible autocatalytic $A+B \rightarrow 2A$ reaction, which have an integro-differential form. We show that, in contrast to the case of normal diffusion where a constant minimal velocity of the front is attained, this minimal velocity is zero in the subdiffusive case. This suggests propagation failure. Numerical simulations show that this propagation failure corresponds to a front of a stable form whose velocity decays with time. The asymptotic behavior of this velocity decay can be obtained by a crossover argument.

BP 18.5 Wed 12:15 H38

Anomalous Transport in Porous Media I: Diffusion in Carbonate Rock — •S. AFACH¹, B. BISWAL², R. HELD³, V. KHANNA¹, J. WANG¹, and R. HILFER^{1,4} — ¹Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart — ²S.V. College, University of Delhi, New Delhi 110021 Delhi, India — ³StatoilHydro ASA, N-7005 Trondheim, Norway — ⁴Institut für Physik, Universität Mainz, 55099 Mainz

We study diffusion through multiscale carbonate rocks using a continuum pore scale reconstruction technique. The method combines crystallite information from two dimensional high resolution images with sedimentary correlations from a three dimensional low resolution tomographic image to produce a rock sample with calibrated porosity, structural correlation and diffusion coefficient [1].

[1] B. Biswal, R. Held, V. Khanna, J. Wang, R. Hilfer, Phys.Rev.E 80 041301 (2009)

BP 18.6 Wed 12:30 H38

Anomalous transport in porous media II: Momentum diffusion in multiscale media — •THOMAS ZAUNER¹ and RUDOLF HILFER^{1,2} — ¹Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — ²Institute for Physics, University of Mainz, 55099 Mainz, Germany

We study viscous momentum diffusion in porous media using lattice Boltzmann simulations. A crucial transport parameter describing momentum diffusion is permeability. It is determined by the underlying stochastic geometry at the pore scale. When the geometry exhibits structure at several scales, viscous dissipation becomes scale dependent. As a consequence the permeability may become scale dependent. We use a recently introduced multiscale model for carbonate rocks [1]. Carbonate rock is known for exhibiting anomalous transport phenomena. Two methodically different lattice Boltzmann implementations, with single- and multirelaxation time collision operator, are used for numerical calculations. We find anomalous behavior in the sense of scale dependent momentum diffusion.

[1] Biswal, B. and Oren, P. E. and Held, R. J. and Bakke, S. and Hilfer, R., Phys. Rev. E, 75, 2007.

Topical Talk BP 18.7 Wed 12:45 H38
Anomalous Diffusion and Fractional Time — ●R. HILFER —

Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart
— Institut für Physik, Universität Mainz, 55099 Mainz

The intimate relation between anomalous diffusion in the sense of Montroll and fractional diffusion equations has been known for a long time [1]. Its fundamental importance for the theoretical understanding of anomalous diffusion processes is reflected in a growing number of applications to experimental observations [2]. Generalized fractional Riemann-Liouville derivatives of general type appear in these applications. Recently an operational calculus of Mikusiński type was developed for the resulting generalized fractional diffusion equations and their mathematical treatment [3].

[1] R. Hilfer and L. Anton, Phys.Rev.E **51**, R848 (1995)

[2] R. Hilfer, in: *Anomalous Transport: Foundations and Applications* Part I, Chapter 2, pages 17-75, Wiley-VCH, Weinheim (2007)

[3] R. Hilfer, Y. Luchko, Z. Tomovski, Fractional Calculus and Applied Analysis **12**, 299 (2009)

BP 19: Membranes and Vesicles

Time: Wednesday 10:00–12:45

Location: H43

BP 19.1 Wed 10:00 H43
Dynamics of endosomal population and cargo trafficking — ●JONATHAN EDWARD DAWSON¹, LIONEL FORET³, ROBERTO VILLASEN², CLAUDIO COLLINET², YANNIS KALAIKIDIS², MARINO ZERIAL², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden — ²Max Planck Institute for Molecular Cell Biology and Genetics, Dresden — ³Ecole Normale Supérieure-LPS, Paris

Endosomes are vesicular structures that transport cargo molecules that are internalized into the cell by endocytosis. Endosomes exchange material by fusion and fission and form a cellular compartment in which cargo is sorted. We present a theoretical description of a population of endosomes. In the description we capture the cargo trafficking on a population level and take cargo influx, outflux, fusion and fission into account. Experimentally the cargo distribution in the endosomal population can be determined by fluorescence microscopy. Our theory predicts scaling properties of the network which are observed experimentally. The theory also describes characteristic features of steady state distribution of cargo molecules in Rab5 positive endosomes. We compare our theory to experimental data and determine the kinetic parameters of the early endosomal network in HeLa cells.

BP 19.2 Wed 10:15 H43
Forming vesicles by different methods: the advantages of microfluidic jetting — ●SILKE KIRCHNER¹, ALEXANDER OHLINGER¹, ANDREY A. LUTICH¹, FERNANDO D. STEFANI², and JOCHEN FELDMANN¹ — ¹Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität, München, Germany — ²Departamento de Física Universidad de Buenos Aires, Buenos Aires, Argentina

Phospholipid bilayer vesicles have attracted significant attention during the last decade being a simple model system for cell membranes. The fabrication of vesicles with controlled size distribution, membrane thickness and entire vesicle filling is of particular interest. Among the widely-used methods of vesicle formation are ultrasonification and electroformation. Although these techniques were extensively used and developed they have a number of disadvantages: the low degree of control over and the broad distribution of the vesicles' sizes.

In order to overcome these difficulties the microfluidic jetting technique can be used. The microfluidic jetting method is supposed to increase the degree of control over the vesicles formation process. We will discuss the effect of changing the jet parameters (speed and volume of the jetted liquid) and the membrane properties (combination of different lipids and membrane phase controlled by temperature) on the vesicle fabrication process. Apart from the well-controlled vesicle's size distribution microfluidic jetting offers the possibility to produce vesicles filled with any required solution.

BP 19.3 Wed 10:30 H43
Effective attraction of curved inclusions in membranes — ●THORSTEN AUTH and GERHARD GOMPPER — Forschungszentrum Jülich, Institut für Festkörperforschung, 52425 Jülich, Germany

Conical inclusions in a lipid bilayer generate an overall spontaneous

curvature of the membrane that depends on concentration and geometry of the inclusions. Examples are integral and attached membrane proteins, viruses, and lipid domains. We propose an analytical model to study budding and vesiculation of the lipid bilayer membrane, which is based on the membrane bending energy and the translational entropy of the inclusions. If the inclusions are placed on a membrane with similar curvature radius, their repulsive membrane-mediated interaction is screened. Therefore, for high inclusion density the inclusions aggregate, induce bud formation, and finally vesiculation. Already with the bending energy alone our model allows the prediction of bud radii. However, in case the inclusions induce a single large vesicle to split into two smaller vesicles, bending energy alone predicts that the smaller vesicles have different sizes whereas the translational entropy favors the formation of equal-sized vesicles.

BP 19.4 Wed 10:45 H43
Free energy calculations of the main phase transition in lipid bilayers — ●MARTIN HÖMBERG and MARCUS MÜLLER — Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

In coarse-grained models of lipid bilayers one integrates out local degrees of freedom, so that the study of collective phenomena, like phase transitions, lateral phase separation in heterogeneous bilayers, and self-assembly, becomes feasible in computer simulations. However, the precise calculation of phase diagrams is still a formidable task due to hysteresis effects and metastability in the vicinity of phase transitions.

Here we employ DPD for the simulation of a coarse-grained solvent-free model for single component lipid bilayers. The non-bonded interactions between the lipids are derived from an excess free energy, which takes the form of a weighted density functional. We find a rich phase diagram, study the main phase (liquid-gel) transition, and present a method to calculate the free energy at this transition as a function of an orientational order parameter. We apply a combination of Umbrella Sampling and histogram reweighting techniques for transforming the liquid phase reversibly into a gel phase. We are able to locate the phase transition point precisely from the free energy profile and we obtain a value of the line tension between liquid and gel domains. This value is compared to the value obtained from a spectral analysis of the boundary fluctuations of gel domains in a liquid phase.

15 min. break

BP 19.5 Wed 11:15 H43
Effects of the bulk in a simple model of nonequilibrium formation of lipid domains in biomembranes — SERGIO ALONSO and ●MARKUS BÄR — Physikalisch-Technische Bundesanstalt, Berlin, Germany

Proteins inside the cell strongly interact with biological membranes depending on the lipid composition and the interaction with other proteins. We consider a simple model of membrane organization into domains based on a cyclic binding and unbinding of the MARCKS protein to acidic lipids known as myristo-electrostatic (ME) switch. The model describes the formation of membrane domains under nonequi-

librium conditions, because the ME switch consumes ATP and leads to non-vanishing currents of proteins. We study the coarsening dynamics and the effects of the coupling to a three-dimensional bulk in the domain pattern formation. The effect of the bulk is an effective decrease of reaction rates in the ME switch, for which simple expressions can be derived. The predictions are verified by comparison of numerical simulations including the bulk and analytically obtained phase diagrams.

BP 19.6 Wed 11:30 H43

Influence of Additives on the Short-Time Dynamics of the Phospholipid DMPC — ●SEBASTIAN BUSCH and TOBIAS UNRUH — Physik Department E13 and Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, Lichtenbergstraße 1, 85748 Garching bei München

In nature as well as in industrial applications, phospholipid membranes contain many components which have significant influence on the properties of the membrane. A striking example is the use of sodium glycocholate (NaGC) as co-emulsifier which enhances the stability of phospholipid-stabilized emulsions by orders of magnitude.

In pharmaceutical technology, the term "fast co-emulsifier" was coined to describe the ability of NaGC to even stabilize droplets which undergo a rapid deformation due to crystallization.

On the other hand, the status-quo of the description of phospholipid membrane dynamics, the free volume theory, predicts a decrease of mobility when additives fill up voids within the lipophilic core of the membrane.

We are able to show with quasielastic neutron scattering that the addition of NaGC indeed increases the picosecond dynamics of the phospholipid DMPC. This effect is compared to the influence of lipophilic additives, namely myristic acid, farnesol, and cholesterol.

BP 19.7 Wed 11:45 H43

Exploring the Nanoscale: Dynamics of Lipid Rafts Revealed by STED Fluorescence Fluctuation Spectroscopy — ●VERONIKA MUELLER, CHRISTIAN RINGEMANN, REBECCA MEDDA, CHRISTIAN EGGELING, and STEFAN HELL — Max-Planck-Institute for Biophysical Chemistry, Department of NanoBiophotonics, Am Fassberg 11, 37077 Goettingen, Germany

The study of molecular dynamics at the single-molecule level with fluorescence far-field optics offers new detailed insights into scientific problems, especially in living cells. Unfortunately, the resolution of common far-field techniques is limited to about 200nm in the lateral direction by diffraction. In recent years, several concepts such as stimulated emission depletion microscopy (STED) have been successfully applied to overcome the diffraction barrier. We present the combination of high resolution STED microscopy with different fluorescence fluctuation techniques providing the unique ability to study molecular dynamics with high spatial (<40nm) and temporal resolution (<1ms) in living cells. Using fluorescence correlation spectroscopy (FCS), we were able to explore single-molecule dynamics in up to 70-fold reduced focal volumes on two-dimensional samples such as lipid membranes with excellent signal-to-noise ratios. Special attention is drawn to inhomogeneous lipid diffusion on the plasma membrane of living cells. This new technique provides the possibility to non-invasively record molecular time traces and fluctuation data in continuously tuneable nanoscale focal areas and thus offers a powerful new approach to study the dynamics of biomolecules in living cell membranes.

BP 19.8 Wed 12:00 H43

Response of tethered membranes to pH, ionic strength and temperature variations studied by neutron and x-ray reflectometry — ●SAMIRA HERTRICH, JOACHIM RÄDLER, and BERT NICKEL — Ludwig-Maximilians-Universität, Department für Physik und CeNS, Geschwister-Scholl-Platz 1, 80539 München

Lipid membranes chemically grafted to a solid surface provide model systems to study membrane-protein interactions. Here, a multi-step chemical reaction is employed to fabricate tethered membranes on silicon oxide by silane chemistry. Reflectometry measurements show that the lipid bilayer is elevated from the surface through a PEG cushion

by 7nm. Fluorescent labeled lipids allow for optical characterization by microscopy confirming homogeneity and mobility of the lipid bilayer. The stability of this system has been tested in a wide pH range from 4 to 11. With x-ray reflectivity (D4, HASYLAB) we observe a reversible contraction of the PEG layer at pH > 9.5, originating from a dehydration of the PEG interlayer as is shown by neutron reflectivity (REFSANS and N-Rex, FRM-2). In contrast, temperature changes and variation of the ionic strength of the buffer did not cause significant changes of the PEG interlayer thickness. The tethered membrane system is now used to test for the binding of neural proteins to the membrane. Initial experiments indicate that the effects of protein binding are a thinning of the lipid bilayer and an increase of water in both the head and the chain region of the membrane. Assistance from Martin Haese-Seiller and Adrian Rühm with the neutron experiments is gratefully acknowledged.

BP 19.9 Wed 12:15 H43

Diffusing proteins on a fluctuating membrane: Analytical theory and simulations — ●ELLEN REISTER, STEFAN M. LEITENBERGER, and UDO SEIFERT — II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

Using both analytical calculations and computer simulations we consider the lateral diffusion of a membrane protein and the fluctuation spectrum of the membrane in which the protein is embedded. The membrane protein interacts with the membrane shape through its spontaneous curvature and bending rigidity. Using a rigorous path-integral approach we derive an analytical expression for the effective lateral diffusion coefficient of the protein in the limit of small ratios of temperature and bending rigidity, which is the biologically relevant limit. Simulation results show good quantitative agreement with our analytical result. The analysis of the correlation functions contributing to the diffusion coefficient reveals that correlations between the stochastic force of the protein and the response in the membrane shape are responsible for the reduction of the diffusion coefficient.

Our quantitative analysis of the membrane height correlation spectrum shows a non negligible influence of the protein-membrane interaction causing a distinctly altered wave-vector dependence compared to a free membrane. Furthermore, the time correlations exhibit the two relevant timescales of the system: that of membrane fluctuations and that of protein diffusion that is typically much longer than the other. We suggest that the long-time decay of height correlations may provide a means to determine effective diffusion coefficients of proteins.

BP 19.10 Wed 12:30 H43

Mesoscopic simulations of membrane protein trafficking and signal transduction across membranes — ●DIANA MOROZOVA, GERNOT GUIGAS, and MATTHIAS WEISS — DKFZ, Cellular Biophysics Group, Im Neuenheimer Feld 280, D-69120 Heidelberg

Acylation is a frequent posttranslational modification that triggers the membrane association of soluble proteins. Besides those peripheral membrane proteins (PMPs) also many transmembrane proteins are subject to lipid modifications, hence indicating that these membrane anchors may also regulate the trafficking of transmembrane proteins. Using coarse-grained membrane simulations we find that acylation indeed significantly alters the tilting of transmembrane proteins with respect to the bilayer normal. Cluster formation and partitioning behavior due to hydrophobic mismatching with the surrounding lipid bilayer is also altered, therefore allowing for ample possibilities to regulate the trafficking of transmembrane proteins via palmitoylation [1].

Using the same simulation approach, we also have studied the trafficking of peripheral membrane proteins (PMPs). In particular, we have observed a cross-leaflet oligomerization of PMPs due to membrane mediated attraction. The strength of this effect is determined by the radii and membrane anchor lengths of the involved PMPs. Since both of these might be altered, for example by ligand binding, the observed cross-leaflet oligomerization may be the fundamental process by which PMPs can trigger an intracellular signalling cascade without the need for accessory transmembrane factors.

[1] D. Morozova & M. Weiss, *Biophys. J.*, in press

BP 20: Networks: From Topology to Dynamics I (joint DY, BP, SOE)

Time: Wednesday 10:15–12:45

Location: H44

BP 20.1 Wed 10:15 H44

Stability of continuous vs. Boolean dynamics — ●ФАКНТЕН GHANBARNEJAD and KONSTANTIN KLEMM — Department of Bioinformatics, University of Leipzig, Germany

Boolean networks are time- and state-discrete models of dynamical systems with many variables and quenched disorder in the couplings. The use of such discrete models makes large systems amenable to detailed analysis. The discretization, however, may bring about “artificial” behavior not found in the continuous description with differential equations. The usual definition of Boolean attractor stability is based on flipping the state of single nodes and checking if the system returns to the attractor, similar to a damage spreading scenario. This stability concept, however, does not reflect the stability of limit cycles in the corresponding continuous system of delay differential equations. Here we have a fresh look at the correspondence of stability definitions in continuous and discrete dynamics. We run extensive numerical simulations to test stability on various system architectures (networks). We establish a criterion for assessing stability of the continuous dynamics by probing the discrete counterpart.

BP 20.2 Wed 10:30 H44

Reliable Boolean networks with threshold functions — ●MANUEL ROSS, TIAGO PEIXOTO, and BARBARA DROSSEL — Institut für Festkörperphysik, TU Darmstadt

Boolean networks are used to model biological networks, such as gene regulatory networks. The nodes of the networks are in this case interpreted as genes, and the state is taken as activity, discretised to Boolean values. An attractor trajectory of the Boolean network is equivalent to a periodic time evolution of the respective network. The usual approach to analyzing these models consists in studying the dynamics of a given network or ensemble. The reverse approach, which we take here, is to deduce the structure of a network from dynamical properties, done for instance by Lau et al. [1]. The dynamical property considered here is a robust sequence of states, i.e., the dynamical trajectory shall not change under perturbations in the update times. We consider the extreme case where the dynamics is reliable under any update sequence, so only one node can possibly change its state at any given moment in time. Such reliable networks were introduced recently in our group [2]. We now extend this work by permitting only threshold functions as update functions. This imposes severe restrictions on the possible reliable trajectories, in contrast to the original study, where all Boolean functions were permitted. We explore the consequences of this restriction for the statistical properties of the possible dynamical trajectories. These statistical properties are finally compared to microarray data. References: [1] K. Y. Lau et al. Phys. Rev. E, 75(5):051907, 2007. [2] T. Peixoto and B. Drossel. arXiv:0905.0925v1, 2009.

BP 20.3 Wed 10:45 H44

Contact networks and the spread of MRSA in hospitals — LISA BROUWERS¹, ●ANDRZEJ JARYNOWSKI^{1,2,3}, FREDRIK LILJEROS¹, and XIN LU¹ — ¹Stockholm University, S106 91 Stockholm, Sweden — ²Department of Physics, Cologne University, Zùlpicher Str. 77. 50937 Köln, Germany — ³The UNESCO Chair of interdisciplinary studies, Wrocław University, pl. M. Borna 9 50-204 Wrocław, Poland

The bacterium meticillin resistant Staphylococcus aureus(MRSA) is known to be the largest care related the infection problem. We investigated the Common Care Registry containing information about all patient visits within Stockholm County during the outbreak period with registry over diagnosed MRSA cases. Methods to analyze the contact network of persons visiting the same care unit is developed within the project as well as methods to analyze in what way network structure affects the transmission of MRSA. We study matrixes of disease transition in hospitals population (infected versus people, who could sent infection). In stationary case:(a) We have matrixes of estimators of that probabilities and other statistical properties of contact networks. In time evolution case:(b) We divided outbreak in smaller, periodical intervals and looked at how MRSA was spreading in time. Quasi-MCMC(Markov chain Monte Carlo) method and artificial networks(main parameter is number of contacts during specific time interval) help us to understand real- and simulated-paths of disease transition. Matrixes of probabilities(b) were used to find mechanism of

change states(vectors of all population 0-health or 1-ill) and we can run quasi-MCMC to get most likely paths.

BP 20.4 Wed 11:00 H44

A novel threshold mechanism for epidemics on complex networks — ●VITALY BELIK¹ and THEO GEISEL^{1,2} — ¹Max-Planck-Institut für Dynamik und Selbstorganisation — ²Georg-August-Universität Göttingen

Recently much effort was devoted to modeling of spatial spread of infectious diseases, triggered by latest pandemics, such as SARS and H1N1 influenza. Theoretical understanding of different modeling frameworks and taken assumptions are substantial factors determining reliability of predictions based on the models. We investigate on an epidemiological model explicitly taking into account such an important factor of human mobility as tendency to move frequently among several most preferred locations rarely undertaking long trips. We considered complex network topologies as an underlying mobility network and discovered new threshold behavior of the global epidemic outbreak in terms of time spent on distant location. Our results are supported by extensive stochastic numerical simulations. We believe our findings contribute to understanding of epidemiological dynamics and development of effective control and preventive measures.

BP 20.5 Wed 11:15 H44

Stochastic load-redistribution model for cascading failures in interconnected systems — ●JÖRG LEHMANN and JAKOB BERNASCONI — ABB Switzerland Ltd., Corporate Research, Segelhofstrasse 1K, CH-5405 Baden-Dättwil, Switzerland

We present a new class of stochastic models for cascading failure propagation in interconnected systems [1]. These models take into account, in a statistical sense, important physical characteristics of realistic load-redistribution mechanisms: (i) the load increments after a failure depend on the load of the failing element; (ii) the failed load is redistributed non-uniformly among the remaining elements. Within a Markov approximation, we are able to describe the cascading failure dynamics of these models in terms of a generalized branching process. This yields an analytical solution for the breakdown probability in the limit of large system sizes. The application to blackouts in power grids is discussed.

[1] J. Lehmann and J. Bernasconi, arXiv:0909.4185.

15 min. break

BP 20.6 Wed 11:45 H44

Synchronization in laser networks: From motifs to complex topologies with multiple delays. — ●THOMAS DAHMS and ECKEHARD SCHÖLL — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate networks of delay-coupled lasers. These include small network motifs, i.e. uni- and bidirectional rings and linear chains, as well as complex topologies including random and small-world networks. The nodes of the networks are described by the widely used Lang-Kobayashi model. By extending the well-known master stability function to networks with time-delay and non-vanishing coupling terms, we are able to separate the local dynamics from the topology. This way we can predict stability of synchronization for any network topology simply by calculating the eigenvalues of the corresponding adjacency matrix. Besides in-phase synchronization, we also observe alternating anti-phase synchronization, where only the next-nearest neighbors are synchronized. Our approach provides deep insight and understanding of the connection between topology and stability of synchronization. While our results are obtained for laser networks, we stress that the results are applicable to a wider range of systems, since only the local dynamics in terms of the master stability function will differ for other models.

BP 20.7 Wed 12:00 H44

Dynamics of neural networks with delay — ●JUDITH LEHNERT, THOMAS DAHMS, PHILIPP HÖVEL, and ECKEHARD SCHÖLL — Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate synchronization in networks of delay-coupled FitzHugh-

Nagumo systems. The parameter values are chosen such that an uncoupled element operates in the excitable regime. However, the coupling acts as a noninvasive control force (Pyragas control) stabilizing the unstable periodic orbit of the synchronized oscillation of all elements. We calculate the master stability function, which denotes the maximum transverse Lyapunov exponent of the synchronization manifold as a function of the eigenvalues of the coupling matrix. Hereby we are able to demonstrate that all network topologies realized by excitatory coupling terms show stable synchronization in a wide range of coupling strengths and delay times.

Furthermore, we investigate small-world-like networks: In a regular network of neurons with excitatory coupling we randomly interpose additional inhibitory links. We show that this introduces a phase transition from the synchronized state to a desynchronized one as the number of these additional inhibitory links approaches a critical value.

BP 20.8 Wed 12:15 H44

Criticality in models of evolving neural networks — ●MATTHIAS RYBARSCH and STEFAN BORNHOLDT — Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee, 28359 Bremen

We investigate self-organization mechanisms in models of evolving neural networks. Already simple spin models can exhibit self-regulated evolution towards a critical state and are used as toy models for self-tuning in biological neural networks [1]. Recent models as, for example, ref. [2] are defined closer to the biological details, resulting in more complex node dynamics and link evolution. Here, we study a correlation-dependent mechanism for self-organized connectivity evolution as introduced in ref. [1]. In particular we focus on a model that is biologically motivated, yet keeping the dynamics as simple as possible. We find that independently from initial connectivity, the network evolves to an average connectivity close to criticality in terms of damage spreading.

[1] S. Bornholdt and T. Roehl: Self-organized critical neural net-

works, Phys. Rev. E 67, 066118 (2003)

[2] A. Levina, J.M. Hermann, and T. Geisel: Dynamical Synapses Causing Self-Organized Criticality in Neural Networks, Nature Physics 3, 857-860 (2007)

BP 20.9 Wed 12:30 H44

Spreading Synchrony in Neural Networks with Non-Additive Interactions. — ●SVEN JAHNKE^{1,2,3}, RAOUL-MARTIN MEMMESHEIMER⁴, and MARC TIMME^{1,2,3} — ¹Network Dynamics Group, Max-Planck-Institute for Dynamics & Self-Organization, Germany — ²Bernstein Center for Computational Neuroscience, Germany — ³Georg-August-University, Göttingen, Germany — ⁴Center for Brain Science, Faculty of Arts and Sciences, Harvard University, USA

Recent neuro-physiological experiments [1] revealed that the response of cortical neurons to simultaneous pre-synaptic stimulation may be supra-additively enhanced. This enhancement is due to active nonlinear waves on the dendrite of a neuron (dendritic spikes) and offers a mechanism to synchronize neural spiking activity. Here we study the impact of nonlinear coupling on the dynamics of large neural circuits provide evidence that nonlinear dendritic enhancement is capable of inducing propagation of synchrony [2]. This yields the possibility to generate patterns of precisely timed spiking activity, as observed in several neuro-physiological experiments. Our results indicate that and explains why densely connected feed-forward anatomy, as so far assumed in model studies [3], is not required for synchrony propagation but much more sparser connectivity is sufficient.

[1] Polsky, A., Mel, B.W. and Schiller, J., Nature Neurosci. 7 (2004).

[2] Memmesheimer, R.M. and Timme, M., Frontiers Comput. Neurosci., doi: 10.3389/conf.neuro.10.2008.01.009 (2008).

[3] Diesmann, M., Gewaltig, M.O. and Aertsen, A., Nature 402 (1999); Kumar, A., Rotter, S., and Aertsen, A., J.Neurosci. 28 (2007).

BP 21: Neurobiophysics and Sensory Transduction

Time: Wednesday 14:00–17:00

Location: H43

Invited Talk

BP 21.1 Wed 14:00 H43

Deconstructing hearing: mechanisms and molecules — BJÖRN NADROWSKI, THOMAS EFFERTZ, and ●MARTIN GÖPFERT — Abt. Zelluläre Neurobiologie, Universität Göttingen, MPI Experimentelle Medizin, Hermann-Rein-Str. 3, 37075 Göttingen

Our ability to hear relies on dedicated mechano-electrical transduction (MET) channels in our inner ear that convert stimulus forces into electrical signals. Molecularely, these channels have not been identified yet. Work on vertebrate hair cells has provided insights into the physical workings of these channels, including their permeation characteristics and their direct gating by stimulus force. Work on *Drosophila*, in turn, has put forward channel proteins that are required for hearing, yet whether and, if so, how these channels contribute to the MET channel function remains unclear. Recent studies have shown that the gating of MET channels modulates the macroscopic performance of the fly's auditory system, setting the stage for a combined physical and genetic dissection of MET channel function in the *Drosophila* ear. This ongoing dissection will be the topic of this presentation: Firstly, physical models will be presented that allow to quantitatively characterize MET channel function; these models suggest that at least two types of MET channels coexist in the *Drosophila* ear. And secondly, mutant analyses will be presented that identify genes that are needed for MET channel function. Some of these genes seem required for the proper MET channel localization or may form MET channels themselves.

BP 21.2 Wed 14:30 H43

Coupling a sensory hair-cell bundle to cyber clones enhances nonlinear amplification — ●KAI DIERKES¹, JÉRÉMIE BARRAL², BENJAMIN LINDNER¹, FRANK JÜLICHER¹, and PASCAL MARTIN² — ¹MPIPKS, Dresden, Germany — ²Institut Curie, Paris, France

The mammalian cochlea's performance is marked by its exquisite sensitivity to weak amplitude stimuli, its sharp frequency selectivity and its wide dynamic range. It owes these abilities to a nonlinear process that actively boosts vibrations of the basilar membrane. Active hair bundle motility has been suggested to contribute to this cochlear amplifier.

Indeed, hair bundles can actively oscillate and act as tuned nonlinear amplifiers. Their responsiveness, however, is limited by intrinsic fluctuations. Hair bundles typically are elastically coupled by overlying gelatinous membranes. In a recent theoretical work we have shown that elastic coupling of small groups of hair bundles could greatly enhance hair-bundle mediated amplification by means of a noise reduction effect (Dierkes et al., PNAS, 2008). Here we report on an experimental study for which we have interfaced dynamic force clamp performed on a hair bundle from the bullfrog's sacculus with real time stochastic simulations of a biophysical description of stochastic hair bundle dynamics. By means of this setup we could couple a hair bundle to two virtual neighbours, called cyber clones. We show that elastic coupling leads to synchronization and an increased coherence of spontaneous oscillations. Also, the sensitivity to weak driving is enhanced. Our results thus demonstrate the hair bundle's ability to team-up with other hair bundles to overcome the limitations of intrinsic noise.

BP 21.3 Wed 14:45 H43

Independent components of neural activity in the auditory midbrain — ●DOMINIKA LYZWA¹, DMITRI BIBITCHKOV², HUBERT H. LIM³, and J. MICHAEL HERRMANN^{1,4} — ¹Dept. Nonlinear Dynamics, MPI for Dynamics and Self-Organization, 37073 Göttingen, Germany — ²Dept. Membrane Biophysics, MPI for Biophysical Chemistry, 37077 Göttingen — ³Dept. Otolaryngology, Medical University, 30625 Hannover, Germany — ⁴IPAB, School of Informatics, University of Edinburgh, Edinburgh EH8 9AB, U. K.

We study mechanisms of sound encoding in the inferior colliculus (IC) which recently has become a new target for auditory implants. The analysis is based on neural recordings where double-tetrodes were used in the IC in cats for acoustic stimulation at various frequencies and volumes. The multi-dimensional data is projected to independent components that are obtained by Independent Component Analysis (ICA) using the Molgedey-Schuster algorithm (MS), FastICA and JADE. The single-trial components are then classified with respect to the stimulus properties. The classification proves best for low frequencies and volumes (1-2 kHz, 10-20 dB) and depends on the localisation in the inferior colliculus, where the stimulus is applied. The results of the

data analysis are used to justify a numerical model of the encoding mechanism.

BP 21.4 Wed 15:00 H43

Local exponents of nonlinear compression in periodically driven noisy oscillators — ●BENJAMIN LINDNER, KAI DIERKES, and FRANK JÜLICHER — Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

Nonlinear compression of periodic signals is a key feature of the active amplifier in inner ear organs of all vertebrates. Different exponents $\alpha_0 \in [-0.88, -0.5]$ of the sensitivity vs forcing amplitude $|\chi| \sim f^{\alpha_0}$ have been observed. Here we calculate analytically the local exponent for a generic oscillator, the normal form of a Hopf bifurcation driven by noise and a periodic signal. For weak noise and sufficient distance from the bifurcation on the unstable side, the exponent may be close to -1 for moderate forcing amplitudes beyond linear response. Such strong compression is also found in a model of hair bundle motility. Ref.: Lindner, Dierkes, Jülicher Phys. Rev. Lett. (in print, 2010)

BP 21.5 Wed 15:15 H43

When less is more: Spike Sequence Processing in Neurons with Adaptive Synapses — ●HINRICH KIELBLOCK¹ and MARC TIMME^{1,2} — ¹Network Dynamics Group, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Bernstein Center for Computational Neuroscience Göttingen, Germany

The input-output relation of a neuron centrally underlies the computational capabilities of neural circuits. The response of a neuron to incoming spike signals strongly depends on the relative timing of the presynaptic spikes. For example, if the input's timing is highly regular, an increase in excitatory input can lead to a decrease of the neurons firing rate. This counterintuitive phenomenon occurs in various neural systems but its underlying mechanism is still unclear.

Here we investigate single neuron systems where a neuron receives precisely timed spiking input via one depressive synapse. Our analysis reveals that and how non-monotonic input-output relations are created by a spike timing-dependent transmission efficiency.

15 min. break

BP 21.6 Wed 15:45 H43

Effect of noisy adaptation on the interspike interval statistics of neurons — ●TILO SCHWALGER¹, KARIN FISCH², JAN BENDA², and BENJAMIN LINDNER¹ — ¹Max-Planck-Institut für Physik komplexer Systeme, Dresden — ²Biozentrum der LMU, Department Biologie II, Planegg-Martinsried

Adaptation and noise are key features of almost any neuron and have a profound impact on signal processing by neurons. This neural processing depends on the specific biophysical implementation of spike generation and spiking variability. In particular, different noise sources might result in markedly different statistics of neural spike trains. However, for many neurons, especially for sensory neurons, the major source of noise is hard to identify. Here, we study analytically a perfect integrate-and-fire neuron with adaptation and either white noise driving or noise resulting from fluctuations in the slow adaptation mechanism. The latter "adaptation noise" could, for instance, arise from channel noise associated to the slow adaption current. Surprisingly, we find a large difference in the statistics of interspike intervals (ISI): A stochastic adaptation current can be mapped to an effective colored noise driving giving rise to long-range positive ISI correlations and a pronounced peak of the ISI density. In contrast, when variability stems from white noise one observes anticorrelations and a less pronounced peak. These results suggest that insight into the major source of noise in certain neurons might be gained from the ISI statistics.

BP 21.7 Wed 16:00 H43

Controlling effective connectivity between cortical areas via collective dynamics transitions — ●DEMIAN BATTAGLIA^{1,3}, ANNETTE WITT^{1,2,3}, THEO GEISEL^{1,3}, and FRED WOLF^{1,3} — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen — ²German Primate Center, Göttingen — ³Bernstein Center for Computational Neuroscience, Göttingen

Anatomic connections between cortical areas constrain the spatio-temporal complexity of brain rhythmic activity. However, structural connectivity does not coincide with effective connectivity, related to the more elusive question: Which areas cause the activity of which others? Effective connectivity is directed and task-dependent. Its fast

changes are incompatible with the slow variation of anatomical connections in a mature brain.

We propose here a theory of controllable rewiring of effective connectivity based on dynamical transitions in the collective organization of neural activity. We consider small network motifs of interacting cortical areas, modeled first as mean-field rate units and then as large populations of spiking neurons. Even when the underlying structural networks are fully symmetric, we obtain chaotic dynamical configurations which spontaneously break the permutation symmetry between areas. Different dynamical configurations are shown to correspond to different causality flows when probed by tools like Granger Causality, Mutual Information or the better performing Transfer Entropy. Fully symmetric structural networks can thus give rise to multiple selectable effective connectivities with reduced symmetry.

BP 21.8 Wed 16:15 H43

Soft Brains, Signal Amplification through Noise, and Taking the Brain by its Horns — ALLEN EHRLICHER, TIMO BETZ, DANIEL KOCH, THOMAS FUHS, MELANIE KNORR, KRISTIAN FRANZE, STEVE PAWLIZAK, and ●JOSEF A. KÄS — Division of Soft Matter Physics, Institute of Experimental Physics I, University of Leipzig

For the brain's viscoelastic properties single cell measurements reveal the softness of neurons and Glial cells, which consequentially rules out the notion of Glial cells as structural support. In contrary the mechanosensitive neurons follow in their growth and development the even softer Glial cells by inverse durotaxis. The motion of growth cones, the leading motile structures of growing neurons, results from a competition of stochastic processes responsible for forward and backward movement. Noise tuning of the growth cone's stochastic fluctuations increases neuronal sensitivity to chemotaxis. The forces underlying the spatial interplay of random actin polymerization driving the forward motion and molecular motor-based retrograde flow responsible for stochastic retraction are measured either by applying conservation laws (continuity equation and force balance) to the cytoskeletal dynamics of GFP-actin transfected growth cones or by directly detecting these forces with AFM. By a simple mechanical lever arm effect weak optical gradient forces acting on the spike-like filopodia, the exploring "horns" of growth cones, are sufficient to control the direction of growth cones' stochastic forward motion.

BP 21.9 Wed 16:30 H43

Chromatin rearrangements transform mammalian photoreceptor nuclei into micro-lenses — ●MORITZ KREYSING¹, LARS BOYDE¹, KEVIN CHALUT¹, IRINA SOLOVEI², BORIS JOFFE², LEO PEICHEL³, THOMAS CREMER², and JOCHEN GUCK¹ — ¹Cavendish Laboratory, University of Cambridge, UK — ²Institute for Human Genetics, LMU Munich, Germany — ³MPI for Brain Research, Frankfurt, Germany

The vertebrate retina is inverted with respect to its optical function. This means light needs to propagate through hundreds of microns of living neuronal tissue before it can be detected by the photoreceptor cells.

In this work we focus on the optical properties of the photoreceptor nuclei that are stored in multiple layers directly before the light sensitive segments. Based on micro-interferometry we show that a unique inversion of their spatial chromatin distribution in mammals with a nocturnal lifestyle transforms these nuclei into micro-lenses. Analytical models and finite difference time domain simulations suggest that the arrangement of these nuclei in columns greatly improves transmission characteristics by a reduction of scattering and an effective channeling of light through the outer nuclear layer.

These results change our understanding of the mammalian retina as an optical system. Furthermore, our findings indicate that the standard model of a nucleus with the heterochromatin located near the nuclear envelope is not the only solution to gene expression and regulation.

BP 21.10 Wed 16:45 H43

Analytical multi-particle scattering model for the simulation of light propagation through biological tissue — ●LARS BOYDE — Biological and Soft Systems, University of Cambridge, UK

The scattering of light from an assembly of arbitrarily arranged, dielectric particles has a multitude of applications in the fields of physics, biology, and medicine. Specific examples include aerosol scattering, remote sensing, radiative transfer, and the propagation of light through biological tissue, such as the retina of the eye.

The author developed and implemented an analytical model that

can be used to compute the electromagnetic near- and far-field intensities for the incidence of a plane wave or Gaussian laser beam on an ensemble of dielectrically coated particles. The underlying theoretical basis of the model is the solution of Maxwell's equations using Mie theory and the so-called vector translation theorems which facilitate the transformation of the fields between the coordinate systems of the individual particles.

The model has been applied to simulate the propagation of light

through the outer nuclear layer of the retina in the mammalian eye – one of the crucial stages of light transmission in the process of vision. Using the established properties of the photoreceptor cell (PRC) nuclei embedded in this layer, the simulations conclusively show that the PRC nuclei of *nocturnal* animals act as strongly focusing micro-lenses. Unlike their *diurnal* counterparts, the chromatin-inverted, nocturnal PRC nuclei effectively channel light onto the light-sensitive outer segments of the rods and cones, leading to enhanced night vision.

BP 22: Networks: From Topology to Dynamics II (joint DY, BP, SOE)

Time: Thursday 9:30–10:15

Location: H44

Invited Talk

BP 22.1 Thu 9:30 H44

Wave localization in complex networks — ●JAN W. KANTELHARDT¹, LUKAS JAHNKE¹, RICHARD BERKOVITS², and SHLOMO HAVLIN² — ¹Institut für Physik, Fachgruppe Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — ²Minerva Center and Department of Physics, Bar-Ilan University, Israel

Complex networks can show transitions from phases with propagating modes to localized phases without transport. In the simplest case such a transition is caused by breaking the network, a classical percola-

tion transition. Wave-like excitations, on the other hand, can exhibit a quantum phase transition (Anderson-like transition) already when the network is still intact. We suggest that this type of localization-delocalization transition could become experimentally observable in optical networks composed of fibers and beam splitters on an optical table. We study the phase transition numerically by level statistics of the eigenvalues for coherent waves in scale-free networks. We show that a strong clustering of the links, i. e., a high probability of closed triangles in the network structure, can induce the transition to localized states. Clustering thus represents a new degree of freedom that can be used to induce and study phase transitions in complex networks.

BP 23: Biopolymers

Time: Thursday 10:00–13:00

Location: H43

Invited Talk

BP 23.1 Thu 10:00 H43

Single-molecule Fluorescence Studies of RNA Folding and Function — ●GERD ULRICH NIENHAUS — Institute of Applied Physics and Center for Functional Nanostructures, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

RNA is a versatile biopolymer involved in various key biological functions, including storage and transfer of information, structural scaffolding and gene expression and regulation. RNA folds into compact three-dimensional structures, and RNA self-assembly and dynamics within the functionally competent, folded structure can be visualized by transitions in a highly complex energy landscape. We study these dynamic processes in small RNAs by using single-molecule Förster (fluorescence) resonance energy transfer (FRET). The free energies of the folded, intermediate and unfolded states can be changed by varying the Mg²⁺ counterion concentration, which allows one to selectively enhance the population of various states in thermal equilibrium and to analyze the equilibrium energetics as well as the kinetics and structural properties of these states.

BP 23.2 Thu 10:30 H43

(Un)folded of a high-temperature stable polyalanine helix from first principles — ●VOLKER BLUM, MARIANA ROSSI, ALEX TKATCHENKO, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin

Peptides *in vacuo* offer a unique, well-defined testbed to match experiments directly against first-principles approaches that predict the intramolecular interactions that govern peptide and protein folding. In this respect, the polyalanine-based peptide Ac-Ala₁₅-LysH⁺ is particularly interesting, as it is experimentally known to form helices *in vacuo*, with stable secondary structure up to ≈ 750 K [1]. Room-temperature folding and unfolding timescales are usually not accessible by direct first-principles simulations, but this high T scale allows a rare direct first-principles view. We here use van der Waals corrected [2] density functional theory in the PBE generalized gradient approximation as implemented in the all-electron code FHI-aims [3] to show by Born-Oppenheimer *ab initio* molecular dynamics that Ac-Ala₁₅-LysH⁺ indeed unfolds rapidly (within a few ps) at $T=800$ K and 1000 K, but not at 500 K. We show that the structural stability of the α helix at 500 K is critically linked to a correct van der Waals treatment, and that the designed LysH⁺ ionic termination is essential for the observed helical secondary structure. [1] M. Kohtani *et al.*, JACS **126**, 7420 (2004). [2] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009). [3] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

BP 23.3 Thu 10:45 H43

Protein amyloid formation — ●CHIU FAN LEE — Max Planck Institute for the Physics of Complex Systems Nöthnitzer Straße 38, 01187 Dresden, Germany

Protein amyloid fibrils are a form of linear protein aggregates that are implicated in many neurodegenerative diseases. Here, we study the equilibrium and dynamical properties of amyloid fibril formation. In particular, we discuss the length distribution of amyloid fibrils in thermal equilibrium [1], the possibility of isotropic-nematic phase transition as monomer concentration is increased [2], and the dynamical processes of nucleation and fibril elongation [3,4]. Our methods of investigation consist of techniques in statistical mechanics and molecular dynamics simulations.

References: [1] C.F. Lee (2009) Self-assembly of protein amyloid: a competition between amorphous and ordered aggregation. Physical Review E **80**, 031922. [2] C.F. Lee (2009) Isotropic-nematic phase transition in amyloid fibrilization. Physical Review E **80**, 031902. [3] L. Jean, C.F. Lee, C. Lee, M. Shaw and D.J. Vaux (2010) Competing discrete interfacial effects are critical for amyloidogenesis. To appear in the FASEB Journal. [4] C.F. Lee, J. Loken, L. Jean and D.J. Vaux (2009) Elongation dynamics of amyloid fibrils: A rugged energy landscape picture. Physical Review E **80**, 041906.

BP 23.4 Thu 11:00 H43

Comparative analysis of rigidity across protein families — ●JOSE EMILIO JIMENEZ, STEPHEN WELLS, and RUDOLF RÖMER — Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry, CV4 7AL, UK

Protein rigidity analysis using the coarse graining FIRST/FRODA software package [1] has provided valuable insights in identifying the most flexible region of a protein [2]. Using the flexibility/rigidity restrictions given by FIRST/FRODA together with normal mode calculations makes it possible to simulate low frequency conformational changes in proteins at much lower computational cost than conventional molecular-dynamics methods.

Here we present a comparative study of rigidity across protein families that show two distinctive behaviors in their rigidity dilution patterns of proteins as hydrogen bonds are removed from weakest to strongest, one of sudden loss of rigidity and one of smooth transition [3]. This result highlights that choosing the energy cut off value should not be based on a numerical standard but chosen individually for each protein according to its rigidity pattern.

[1] S A Wells, et al, Constrained geometric simulation of diffusive

motion in proteins. *Physical Biology*, 2, S127-S136, 2005 [2] D J Jacobs, et al. Protein flexibility predictions using graph theory. *PROTEINS: Struct., Func. and Gen.*, 44:150*165, 2001. [3] S A Wells, J E Jimenez-Roldan and R A Römer. Comparative analysis of rigidity across protein families *Phys. Biol.* 6 046005, 2009

BP 23.5 Thu 11:15 H43

A Stevedore's Protein Knot — ●PETER VIRNAU¹, JOANNA SULKOWSKA², and DANIEL BÖLINGER³ — ¹Institut für Physik, Uni Mainz — ²Center for Theoretical Biological Physics, UC San Diego, USA — ³MPI für Neurobiologie, Martinsried

Protein knots, mostly regarded as intriguing oddities, are gradually being recognized as significant structural motifs. Seven distinctly knotted folds have already been identified. It is by and large unclear how these exceptional structures actually fold, and only recently, experiments and simulations have begun to shed some light on this issue. In checking the new protein structures submitted to the Protein Data Bank, we encountered the most complex, and the smallest, knots to date: A recently uncovered alpha-haloacid dehalogenase structure, contains a knot with six crossings, a so-called Stevedore knot, in a projection onto a plane. The smallest protein knot is present in an as yet unclassified protein fragment that consists of only 92 amino acids. The topological complexity of the Stevedore knot presents a puzzle as to how it could possibly fold. To unravel this enigma, we performed folding simulations with a structure-based coarse-grained model, and uncovered a possible mechanism by which the knot forms in a single loop flip.

15 min. break

BP 23.6 Thu 11:45 H43

Buckling and writhing of semiflexible polymer rings in confinement — ●KATJA OSTERMEIR, KAREN ALIM, and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics and CeNS, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstr. 37, D-80333 München

Cell walls or membranes impose a spatial confinement on semiflexible biopolymers such as DNA and cytoskeletal filaments. Restricting the accessible space changes a polymer's configurations and hence its properties in biological processes. Examining semiflexible polymer rings in spherical confinement we observe substantial transformations of polymers' shape and symmetry at relatively weak confinement.

While polymer rings with a small ratio of perimeter to persistence length would attain a planar, elliptical configuration in free space, we find that confinement forces them to buckle into banana-like shapes. We develop an analytical scaling argument which resolves a stiff polymer's shape for small flexibilities. Our calculation agrees with shape parameter measurements from Monte Carlo simulations over ranges of confinement.

More flexible free polymers rings tend to take on prolate configurations which are again suppressed by the confinement. We discover an increased writhing of the polymer in order to store length without sharp bending. In the semiflexible regime a bimodal distribution of writhe is found.

BP 23.7 Thu 12:00 H43

Influence of filament positioning on polymerization of filament ensembles — ●JAROSŁAW KRAWCZYK and JAN KIERFELD — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I,

Many cellular processes are driven by polymerization of filamentous proteins. Using stochastic simulations based on the Gillespie algorithm we investigate force-generation by polymerizing groups of filaments or protofilaments and study the influence of the relative starting positions of filaments on the dynamics of growing speed. We find a strong influence of the starting position on the growth velocity. While the growth velocity for different starting configurations differ, the stall force remains unchanged.

BP 23.8 Thu 12:15 H43

Tube Width Fluctuations in F-Actin Solutions — ●JENS GLASER¹, DIPANJAN CHAKRABORTY¹, KLAUS KROY¹, INKA LAUTER², MASASHI DEGAWA², NORBERT KIRCHGESSNER², BERND HOFFMANN², RUDOLF MERKEL², and MARGRET GIESEN² — ¹Institut für Theo-

retische Physik, PF 100920, 04009 Leipzig — ²Institut für Bio- und Nanosysteme, Biomechanik (IBN-4), Forschungszentrum Jülich, 52425 Jülich

Edwards' tube model provides a simple phenomenological description of the complicated topological constraints in entangled solutions of flexible polymers. Using scaling arguments, the idea was generalized to stiff polymers with a persistence length larger than the characteristic arclength between mutual collisions, which plays the role of the entanglement length in this context. Their large contour and persistence lengths have opened the possibility of direct microscopic visualizations of the tube by superimposing snapshots of a fluorescent test filament. We determine the statistics of the tube width in F-actin solutions, beyond the usually reported mean value [1]. The experimental observations are explained by a segment fluid description based on the binary collision approximation (BCA) [2]. In this systematic generalization of the standard mean-field approach, effective polymer segments ("entanglons") interact via a potential representing the topological constraints. The theory is complemented by Brownian dynamics and Monte Carlo simulations.

[1] J. Glaser et al., arXiv:0910.5864

[2] D.C. Morse, PRE 63:031502 (2001)

BP 23.9 Thu 12:30 H43

Intermediate filament assembly in micro-flow studied by X-ray scattering — ●MARTHA BRENNICH, JENS NOLTING, CHRISTIAN DAMMANN, BERND NÖDING, SUSANNE BAUCH, and SARAH KÖSTER — Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany

The cytoskeleton, which is responsible for many mechanical properties of the cell, primarily consists of three different types of fibrous proteins: actin filaments, microtubules and intermediate filaments (IFs). The latter comprise a variety of proteins that vary from cell type to cell type. Our work is focused on the hierarchical self-assembly of IF subunits into filaments. We study these processes on the example of vimentin where the assembly can be initiated in vitro by increasing the salt concentration of the solution. Microfluidic tools are used to establish precise pH and salt concentration gradients, wherein the assembly occurs and can be observed in situ. Because of the small channel dimensions and the corresponding laminar flow, the time axis for the assembly process is projected onto a spatial axis along the flow direction and we observe different assembly states by collecting data at different positions in the device. A new type of 3D microfluidic device optimized for small angle X-ray scattering experiments allows us to obtain structural information on the first steps of the vimentin assembly. From the changes in the structural composition we deduce the kinetics of the filament formation and elongation.

BP 23.10 Thu 12:45 H43

Biomolecule Binding quantified with Thermophoresis — ●CHRISTOPH J WIENKEN, PHILIPP BAASKE, DIETER BRAUN, and STEFAN DUHR — Systems Biophysics, Center for Nanoscience, LMU München, Germany

Methods to measure biomolecule interactions are essential for medicine, biology and pharmaceutical industry. We use thermophoresis, the directed movement of molecules in a temperature gradient, to quantify a wide range of interactions like protein-protein, protein-DNA and protein-small molecule.

By combining highly defined microfluidics with all-optical heating and detection, the thermophoretically induced concentration change is measured with high precision. We fluorescently label one binder and track the changes of thermophoretic depletion while titrating the binding partner. The results are quantitative binding curves allowing to measure dissociation coefficients in the picomolar to millimolar range.

Advantages of the method are low volume consumption, fast response time and surface-free detection. However the measurement in various physiological buffers is the hallmark of the approach. Affinities can be measured in highly complex biological fluids as blood serum.

Thermophoresis is performed in bulk fluid, and significant background signals from surface binding are avoided. Competing surface-based methods such as ELISA or surface plasmon resonance have to measure on non-physiological surfaces that are prone to unspecific biomolecule adsorption and do not allow measurements in undiluted biological liquids.

BP 24: Networks: From Topology to Dynamics III (joint DY, BP, SOE)

Time: Thursday 10:15–13:00

Location: H44

BP 24.1 Thu 10:15 H44

Detection of Mesoscopic Role-Structure in Complex Networks — ●JOERG REICHARDT¹, ROBERTO ALAMINO², and DAVID SAAD² — ¹UC Davis, CA — ²Aston University, Birmingham

Not all nodes are created equal in complex networks. Rather, they play diverse roles in the functioning of a network and their role is reflected in the network's link structure. Hence, structural analysis can be used to infer the latent roles and functions of nodes purely based on connectivity data. Currently, network structure is studied at three different levels. At the macro level, global network properties such as degree distributions, path-lengths, diameters or clustering coefficients are investigated. At the micro level, properties of individual nodes and edges such as centrality indices or rank functions such as page-rank are studied. The study of the meso-scale, which aims at studying joint properties of groups of nodes, so far has mainly been focussed on the detection of cohesive subgroups of nodes, so-called communities.

The talk will show that, though important, communities are only one special case of a much wider class of mesoscopic structures called "stochastic block structures". This name comes from the fact that latent classes of roles and their resultant patterns of connectivity in a network account for salient block structure in the adjacency matrix of a network when the rows and columns are ordered according to these latent roles.

We present an effective and accurate algorithm that performs this task employing a purely Bayesian approach, show that it outperforms competing approaches and present applications to real world data sets that open new frontiers of research in the study of both structure, function and evolution of complex networks from a mesoscopic perspective.

BP 24.2 Thu 10:30 H44

Structuring k-partite networks by decomposition into overlapping communities — ●FLORIAN BLÖCHL^{1,3}, MARA L. HARTSPERGER^{1,3}, VOLKER STÜMPFLEN¹, and FABIAN J. THEIS^{1,2} — ¹Institute for Bioinformatics and Systems Biology, Helmholtz Zentrum München — ²Department of Mathematics, TU München — ³Equal contributors

With increasing availability of large-scale networks we face the challenge to interpret these data in a comprehensive fashion. A common solution is a decomposition into modular building blocks, so-called communities. Prominent examples are functional modules in protein interactions. However, the integration of heterogeneous resources results in networks with nodes of multiple colors. Although existing algorithms address this issue, they identify separated, disjoint clusters by assigning each node to exactly one cluster. This is far from reality, where e.g. proteins are commonly part of many complexes or pathways.

We present a novel algorithm for detecting overlapping communities in k-partite graphs. It determines for each node a fuzzy degree-of-membership to each community. Moreover, we additionally estimate a weighted backbone graph connecting the extracted communities. The method is fast and efficient, mimicking the multiplicative update rules employed in algorithms for non-negative matrix factorization.

Results on a disease-gene-protein complex graph show significantly higher homogeneity within the complex and disease clusters than expected by chance. However, the algorithm is readily applicable to other domains with similar problems.

BP 24.3 Thu 10:45 H44

Large-deviation properties of random graphs — ●ALEXANDER K. HARTMANN — Institut of Physics, University of Oldenburg

The large-deviation properties of different types of random graphs are studied using numerical simulations. In particular the number of components and the graph diameter are considered. The distributions of these quantities are obtained down to very small probabilities like 10^{-700} using finite-temperature Monte Carlo and Wang Landau simulations. Different graphs ensembles as Erdős-Renyi, small-world and scale-free graphs are studied as a function of suitable control parameters. The parameter-dependend changes of the distributions are recorded, indicating the presence of non-standard transitions.

In particular, the distributions of the diameter are often given by Gumbel distributions, except right at a percolation transition, or are very close to Gumbel distributions.

BP 24.4 Thu 11:00 H44

Coupled Order Parameter Systems on Scale-free Networks — ●CHRISTIAN VON FERBER^{1,2}, REINHARD FOLK³, VASYL PALCHYKOV⁴, and YURIJ HOLOVATCH^{3,4} — ¹Applied Mathematics Research Centre, Coventry University, UK — ²Physikalisches Institut, Universität Freiburg — ³Institut für Theoretische Physik, Universität Linz, AT — ⁴Institute for Condensed Matter Physics, Lviv, UA

We analyse a system of two scalar order parameters on a complex scale-free network in the spirit of Landau theory. To add a microscopic background to the phenomenological approach we also study a particular spin Hamiltonian that leads to coupled scalar order behavior using the mean field approximation. This set up may describe a model of opinion formation where e.g. opinions on a party a candidate are coupled. Our results show that the system is characterised by either of two types of ordering: either one of the two order parameters is zero or both are non-zero but have the same value. While the critical exponents do not differ from those of a model with a single order parameter on a scale free network there are notable differences for the amplitude ratios and susceptibilities. Another peculiarity of the model is that the transverse susceptibility is divergent at all $T < T_c$ when $O(n)$ symmetry is present. This behavior is related to the appearance of Goldstone modes.

BP 24.5 Thu 11:15 H44

Discontinuous Phase Transitions in Random Network Percolation — ●JAN NAGLER^{1,2}, ANNA LEVINA^{1,3}, and MARC TIMME^{1,2,3} — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen — ²Institute for Nonlinear Dynamics, Faculty of Physics, University of Göttingen — ³Bernstein Center for Computational Neuroscience (BCCN) Göttingen

The transition to extensive connectedness upon gradual addition of links, known as the percolation phase transition, provides a key prerequisite for understanding networked systems [1]. Until recently, random percolation processes were thought to exhibit continuous transitions in general, but now there is numerical evidence for discontinuities changes of the order parameter in certain percolation processes [2]. Here we present the concepts of weakly and strongly discontinuous percolation transitions and explain the microscopic mechanisms underlying them. We study both numerically and analytically under which conditions the order parameter may change discontinuously and classify the type of transition in dependence on the dynamics of cluster joining [3].

[1] G. Grimmett, Percolation (Springer Verlag, Heidelberg,1999).

[2] D. Achlioptas, R. M. D'Souza, J. Spencer, Explosive Percolation in Random Networks, Science 323: 1453 (2009); R. M. Ziff, PRL 103, 045701 (2009); F. Radicchi and S. Fortunato, PRL 103, 168701 (2009); Y. Cho et al., PRL 103, 135702 (2009).

[3] J. Nagler, A. Levina, and M. Timme, unpublished (2009).

15 min. break

BP 24.6 Thu 11:45 H44

Evidence for power-law anti-correlations in complex networks — ●DIEGO RYBSKI¹, HERNÁN D. ROZENFELD², and JÜRGEN P. KRÖPP¹ — ¹Potsdam Institute for Climate Impact Research, 14412 Potsdam, Germany — ²Levich Institute, City College of New York, New York, NY 10031, USA

We propose a degree analysis to quantify spatial correlations in complex networks. The approach considers the degrees along shortest paths in the networks and quantifies the correlations. In this work, the Barabasi-Albert (BA) model, a fractal network model, and examples of real-world networks are studied. While for the BA model the correlations show exponential decay, in the case of the fractal networks the correlations show a power-law behavior indicating long-range correlations. The results suggest that the analysis provides complementary information to the fractal dimension as measured with box covering.

BP 24.7 Thu 12:00 H44

What scales in multiscale human mobility networks? — ●RAFAEL BRUNE^{1,2}, CHRISTIAN THIEMANN^{1,2}, and DIRK BROCKMANN¹ — ¹Northwestern University, Evanston, USA — ²Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen,

Deutschland

Although significant research effort is currently devoted to the understanding of complex human mobility and transportation networks, their statistical features are still poorly understood. Specifically, to what extent geographical scales impose structure on these networks is largely unknown. Statistical properties of these networks have been obtained either for large scale networks or on small scale systems, indicating significant differences between the two. We will present a systematic investigation of various single scale mobility networks extracted from a comprehensive multiscale proxy network, covering sequential length scales of a few to a few thousand kilometers. We will report that certain properties such as mobility flux distribution are universal and independent of length scale, whereas others vary systematically with scale. Furthermore we investigate the relation of a series of network characteristics as a function of scale and analyze how the different length scales interact in the embedding multiscale network.

BP 24.8 Thu 12:15 H44

The tomography of human mobility – what do shortest-path trees reveal? — ●CHRISTIAN THIEMANN^{1,2}, DANIEL GRADY¹, and DIRK BROCKMANN¹ — ¹Eng. Sci. & Appl. Math, Northwestern University, Evanston, IL, USA — ²Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Similar to illustrating the anatomy of organs using pictures of tissue slices taken at various depths, we construct shortest-path trees of different nodes to create tomograms of large-scale human mobility networks. This tomography allows us to measure global properties of the system conditioned on a reference location in the network to gain a fuller characterization of a node. It also suggests a canonical coordinate system for representing complex networks and dynamical processes thereon in a simplified way, revealing a new symmetry in the human mobility networks we investigated. Furthermore, introducing the notion of tree similarity, we devised a new technique for clustering nodes with similar topological footprint, yielding a unique and efficient method for community identification and topological backbone extraction. We applied these methods to a multi-scale human mobility network obtained from the dollar-bill-tracking site wheresgoerge.com and to the U.S. and world-wide air transportation network.

BP 24.9 Thu 12:30 H44

Fusion in complex networks — ●CARLUS DENEKE, ANGELO VALLERIANI, and REINHARD LIPOWSKY — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Department of Theory and Bio-

Systems, Potsdam, Germany

In real world networks, part of the information about the nodes and edges is often missing or inaccessible and single nodes might in reality consist of several nodes or subgraphs. Since these hidden structures may have a strong impact on the dynamical processes, it is important to investigate how the network properties change at different levels of resolution.

In this contribution, we investigate scale-free networks, in which randomly chosen couples of neighboring nodes are iteratively integrated or fused into single nodes. We introduce different fusion mechanisms and compare their effects on simple network properties such as the degree distribution and the degree correlations. By means of numerical simulations and analytical calculations, we show that the network properties change steadily under the iterated fusion steps.

We finally discuss possible connections to real world networks.

BP 24.10 Thu 12:45 H44

Properties of transport networks need to be invariant under coarse graining — ●FABIAN J. THEIS^{1,2}, FLORIAN BLÖCHL¹, and DIRK BROCKMANN³ — ¹Helmholtz Zentrum München, Germany — ²Department of Mathematics, TU Munich, Germany — ³Engineering Sciences and Applied Mathematics, Northwestern University, USA

Transport networks can rarely be observed directly, especially not across many scales. Instead, the flow between two locations can now only be estimated from proxy data. This results in the need for spatial averaging, so we commonly only observe a histogram of the actual distributions. We denote this process as coarse graining.

In this contribution we analyze which network properties are invariant under coarse graining, following the rationale that we can only infer such properties of the true underlying transport network from the proxy data. We show that shortest-path distances, which cannot take self-loops into account, are a poor distance measure in such networks. Instead we illustrate that a distance based on random walks, namely mean fast hitting time (MFHT), is much more adequate for such type of networks. Moreover, we show that community measures are coarse-graining invariant.

Taken together, we can develop a coarse graining method that leaves MFHT fully invariant: we first cluster the nodes into communities via hierarchical clustering of the mean commute time matrix. We then reconstruct a weighted graph connecting our communities, solving a distance realization problem, which we recently addressed in (Wittmann et al., TCS 2009). We illustrate the method on toy and real networks.

BP 25: Focus: Charge Effects in Soft and Biological Matter I (joint CPP, BP, ST)

Time: Thursday 11:00–12:45

Location: H45

Invited Talk

BP 25.1 Thu 11:00 H45

Charge effects in RNA folding — ●LOIS POLLACK — Cornell University, Ithaca, NY USA

Because nucleic acid backbones possess such a high negative charge, interactions with positively charged ions (or larger charged molecules) are critically important to the biophysics of both RNA and DNA. Our studies of the earliest events in RNA folding highlight the importance of electrostatic interactions to this conformational change. Complementary x-ray scattering experiments on short nucleic acid duplexes have elucidated the spatial distribution of condensed counterions, as well as ion-induced interactions between duplexes. Interactions between these helices can be tuned from repulsive to attractive by varying counterion charge and concentration. Interesting differences between RNA and DNA are revealed by these measurements.

BP 25.2 Thu 11:30 H45

Dielectrophoresis: a new tool for continuous DNA/protein interaction studies — ●MARTINA EVERWAND, DARIO ANSELMETTI, and JAN REGTMEIER — Experimental Biophysics & Applied Nanoscience, Bielefeld University, Universitätsstr. 25, 33615 Bielefeld

The investigation of DNA-protein interactions is of central interest in today's proteomic research like for the metabolic pathway analysis. Here, a novel microfluidic device is presented, which allows efficient separation of protein-complexed DNA from native DNA strands in continuous mode.

The Lab-on-chip device consists of a 3D-structured microfluidic

channel network incorporating an integrated barrier with nanometer dimension, that allows for electrodeless dielectrophoresis of DNA-protein complexes.

For the first time, we demonstrate that differently sized DNA fragments as well as DNA/protein and DNA/antibiotics complexes can be continuously separated from unbound DNA at a nano-microfluidic interface.

Invited Talk

BP 25.3 Thu 11:45 H45

Origin of the electrophoretic force on DNA in solid-state nanopores — ●SERGE G. LEMAY — MESA+ Institute for Nanotechnology, University of Twente

Despite gel electrophoresis being one of the main workhorses of molecular biology, the physics of polyelectrolyte electrophoresis in a strongly confined environment remains poorly understood. Theory indicates that forces in electrophoresis result from interplay between ionic screening and hydrodynamics, but these ideas could so far be addressed only indirectly by experiments based on macroscopic porous gels. I will present a direct experimental based on measuring the electrophoretic force on a single DNA molecule threading through a solid-state nanopore as a function of pore size. The stall force gradually decreases on increasing the nanopore diameter from 6 to 90 nm, inconsistent with expectations from simple electrostatics and strikingly demonstrating the influence of the hydrodynamic environment. We model this process by applying the coupled Poisson-Boltzmann and Stokes equations in the nanopore geometry and find good agreement with the experimental results.

BP 25.4 Thu 12:15 H45

DNA Translocation through Nanopores: What is the role of dielectric permittivity? — ●STEFAN KESSELHEIM¹, MARCELLO SEGA², MEHMET SÜZEN³, and CHRISTIAN HOLM¹ — ¹Institut für Computerphysik, Universität Stuttgart — ²Department of Physics and INFN, University of Trento — ³Institute of Photonic Sciences, Castelldefels (Barcelona), Spain

We investigate the free energy barrier of a single DNA molecule filed through a synthetic nanopore. We employ a recently developed algorithm (ICC*) that allows to take into account the dielectric contrast at the membrane/solute interface in coarse-grained molecular dynamics simulations. The investigations show the crucial contribution of dielectric mismatch to the translocation free energy barrier. We show that for low ionic strength and DNA fragments up to 100 bp the dielectric boundary forces dominate over the entropic contribution caused by DNA flexibility.

BP 25.5 Thu 12:30 H45

DNA: charge localisation and pathogenesis. — CHI-TIN SHIH¹, YUN-YIN CHENG¹, ●STEPHEN A WELLS², RUDOLF A RÖMER², and

CHING LING³ — ¹Department of Physics, Tunghai University, 40704 Taichung, Taiwan and The National Center for Theoretical Sciences, 30013 Hsinchu, Taiwan — ²Department of Physics and Centre for Scientific Computing, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, UK — ³Department of Physics, Chung-Yuan Christian University, Chung-Li, Taiwan

We present results from transfer-matrix modelling of charge localisation and transport in DNA sequences, using tight-binding models at several levels of detail. With parallel computing resources we are able to examine the variation in local charge-transport properties along sequences of hundreds of thousands of base pairs, covering entire genes. This has allowed us to survey large numbers of human genes for which databases of pathogenic mutations exist; we consider both cancer-related genes and those associated with other forms of genetic disorder.

Examining the correlations between charge transport (CT) properties and the sites where pathogenic mutations are observed, we find a statistically significant correlation between pathogenesis and below-average changes in CT properties. We discuss the interpretation of our results in the context of DNA physics and chemistry, and of possible cellular mechanisms for DNA damage avoidance, detection and repair.

BP 26: From Single-Molecule to Tissue Dynamics

Time: Thursday 14:00–17:15

Location: H43

Invited Talk

BP 26.1 Thu 14:00 H43

Molecular misfolding investigated by mechanically unzipping nucleic acids — ●FELIX RITORT — Departament de Física Fonamental, Facultat de Física, Universitat de Barcelona, Diagonal 647, 08028 Barcelona (Spain) — CIBER-BBN of Bioengineering, Biomaterials and Nanomedicine, ISCIII, Madrid (Spain)

Recent developments in micro and nano technologies allow for the controlled manipulation of individual molecules by exerting and detecting forces in the piconewton range. The possibility to detect such tiny forces together with the ability of measuring extensions with nanometer resolution allows scientists to monitor molecular reactions in real time (e.g. molecular folding) and characterize thermodynamics and kinetics of individual molecules (e.g. nucleic acids and proteins) with unprecedented energy accuracy within tenths of a kcal/mol.

Single molecule manipulation make possible to disrupt molecular bonds that hold native structures in nucleic acids and proteins. In this talk I will show experimental results on irreversibility and dissipation in nucleic acid hairpins that are mechanically unzipped using optical tweezers. Our aim is to explore complex molecular free energy landscapes and nonequilibrium behavior in small systems. For this we have designed DNA hairpins of specific sequences that exhibit molecular misfolding to investigate the role of irreversibility and dissipation during the folding process. Our results suggest the existence of a universal mechanism used by chaperones to assist molecular folding of RNAs and proteins.

BP 26.2 Thu 14:30 H43

Import of DNA by *Helicobacter pylori* is reversible by application of external force — ●STEPHANIE MÜLLER^{1,2}, KERSTIN STINGL^{1,2}, GERDA SCHEIDGEN-KLEYBOLDT², MARTIN CLAUSEN², and BERENIKE MAIER² — ¹equal contribution — ²Westfälische Wilhelms-Universität, Biological Department, 48149 Münster, Germany

Many bacterial species are capable of taking up and incorporating exogenous DNA in their genome. For the transport of DNA across the outer and inner membrane, the gram-negative gastric pathogen *Helicobacter pylori* uses a reverse type-IV-secretion-system, termed ComB. Besides this secretion-system related mechanism, further proteins are also involved in DNA uptake, among them the inner membrane channel ComEC. DNA-uptake experiments revealed that *H. pylori* cells possess multiple polar DNA-uptake complexes. In addition, knockout mutants in two motor proteins, ComB4 (an ATPase) and ComB6 (an inner membrane protein), and in the inner membrane channel ComEC were characterized revealing that the ComB-system and the inner membrane channel act at different steps of DNA uptake. The physical properties of the uptake motor were characterized in laser-trap experiments: Upon application of external force, previously imported DNA was extracted, revealing reversibility of the motor at 23pN external force. The average DNA import velocity was 2,2 kbp/sec. Taken all data together, a temporally uncoupled mechanism of DNA uptake is pro-

posed: First the fast and reversible uptake across the outer membrane mediated by the ComB-system, and secondly the ComEC-dependent inner-membrane transport.

BP 26.3 Thu 14:45 H43

Monitoring a single F_oF_1 -ATP synthase in an anti-Brownian electrokinetic (ABEL) trap — ●KARIN SEYFERT, TORSTEN RENDLER, ANDREA ZAPPE, STEFAN ERNST, NAWID ZARRABI, and MICHAEL BÖRSCH — 3. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart

ATP (adenosine triphosphate) is the energy currency of every cell. It is produced by the F_oF_1 -ATP synthase. This membrane-embedded enzyme consists of two rotary motors. To analyze the functioning of this enzyme, we measure FRET (Fluorescence Resonance Energy Transfer) with single, freely diffusing F_oF_1 -ATP synthases in a confocal microscope. The disadvantage of this method is the limited observation time up to 300 ms due to Brownian motion [1]. We aim to trap the enzyme inside the confocal volume. The ABEL (Anti Brownian Electrokinetic) trap is a microfluidic system invented by A.E. Cohen (Harvard) and W.E. Moerner (Stanford) [2]. Fluorescent lipid vesicles containing a single FRET-labeled ATP synthase are monitored by an EMCCD camera and the image is used for the electrokinetic feedback in real time to bring the vesicle back to a set point. Thereby, extended FRET measurements on a single enzyme in solution are possible.

[1] M.G. Duser, N. Zarrabi, D.J. Cipriano, S. Ernst, G.D. Glick, S.D. Dunn, and M. Borsch: 36 degrees step size of proton-driven c-ring rotation in FoF1-ATP synthase, *Embo Journal* 28, 2689 (2009). [2] A.E. Cohen and W.E. Moerner: Suppressing Brownian motion of individual biomolecules in solution, *Proc Natl Acad Sci U S A* 103, 4362 (2006).

BP 26.4 Thu 15:00 H43

Cooperative binding of kinesin motors on microtubules studied with atomic force microscopy — ●KAREN HOLLENBERG, IWAN A. T. SCHAAP, and CHRISTOPH F. SCHMIDT — Drittes Physikalisches Institut, Fakultät für Physik, Georg-August-Universität Göttingen

Kinesin motor proteins move actively along microtubules and drive intracellular transport of vesicles and organelles in cells. Since most transport processes involve smaller or larger ensembles of motors, it is an interesting question if and how motors communicate and coordinate their activity in such ensembles. One possibility is direct head-to-head interaction. An intriguing alternative is interaction via the substrate, the microtubule lattice.

We have here used atomic force microscopy in buffer to search for axial and lateral cooperativity in the binding of motors. The results show that kinesin-1 dimers and monomers cluster when immobilized on the track by AMP-PNP. For monomers this effect is less pronounced.

BP 26.5 Thu 15:15 H43

Nuclear centering in fission yeast mediated by kinesin-8 mo-

tor proteins — ●NICOLA MAGHELLI¹, VLADIMIR KRSTIĆ², NENAD PAVIN², FRANK JÜLICHER², and IVA TOLIĆ-NØRRELYKKE¹ — ¹MPI-CBG, Dresden, GERMANY — ²MPI-PKS, Dresden, GERMANY

In the fission yeast *Schizosaccharomyces pombe*, the nucleus is positioned at the cell center. Since the nucleus determines the cell division site, keeping the nucleus at the center is crucial for ensuring symmetrical cell division (1). Microtubules push against the cell ends and exert force on the nucleus (2), but how the cell regulates these forces in order to center the nucleus remains unknown. Here we tackle this problem by using a combination of live cell imaging, cell manipulations by laser ablation and optical tweezers, and a theoretical model. We show that microtubule pushing forces can center the nucleus because of a larger number of contacts between the microtubules and the proximal cell end than the distal one. Moreover, kinesin-8 motors (Klp5/6) increase the rate of microtubule catastrophe (transition from growth to shrinkage) in a microtubule length- and contact time-dependent manner. Thus, the motor behavior results in a longer contact between a microtubule and the proximal than the distal cell end. Taken together, our experimental and theoretical results provide a novel centering mechanism, where kinesin-8 motors increase the efficiency of nuclear centering.

1. I. Tolić-Nørrelykke, L. Sacconi, C. Stringari, I. Raabe, F. S. Pavone, *Curr Biol* 15, 1212 (Jun 30, 2005).

2. P. T. Tran, L. Marsh, V. Doye, S. Inoue, F. Chang, *J Cell Biol* 153, 397 (Apr 16, 2001).

BP 26.6 Thu 15:30 H43

Cargo transport by molecular motors against shear flow — ●FRIDTJOF KOWALD^{1,2}, CHRISTIAN KORN³, and ULRICH SCHWARZ^{2,3} — ¹Karlsruhe Institute of Technology, Theoretical Biophysics Group — ²University of Heidelberg, Institute for Theoretical Physics — ³University of Heidelberg, Bioquant

Processive molecular motors like kinesins transport cellular cargo like vesicles, organelles, nuclei or viruses along cytoskeletal tracks like microtubules. In a physiological context, the motors usually work in groups. This allows them to stay attached to the filament for a long time and to produce high levels of force. There are several sources for opposing forces which disrupt cargo transport, including viscous forces on the moving cargo, forces from motors pulling in other directions, forces from the interaction of the cargo with other cellular structures, and shear forces due to hydrodynamic flow in the environment. Here we address the latter case using computer simulations for adhesive motor dynamics. Our Langevin equation includes hydrodynamic interactions of the spherical cargo with the wall and the shear flow, rupture and rebinding of the motor connections to the filament, and motor stepping with a linear force-velocity relation. Our main result is the distribution of unbinding times as a function of motor number and shear rate. This allows us to predict how the critical shear flow for non-productive transport increases as a function of motor number. We comment on possible applications of our results to cellular systems and in nanobiotechnology.

15 min. break

BP 26.7 Thu 16:00 H43

Origin and Spatial Distribution of Forces in Motile Cells — CLAUDIA BRUNNER¹, MICHAEL GÖGLER¹, ALLEN EHRLICHER¹, DANIEL KOCH¹, THOMAS FUHS¹, CHARLES WOLGEMUTH², and ●JOSEF A. KÄS¹ — ¹Division of Soft Matter Physics, Department of Physics, University of Leipzig — ²Department of Cell Biology and the Center for Cell Analysis and Modeling, University of Connecticut Health Center

Inspired by ambivalent data of individual cellular forces we provide a first complete and consistent set of forces that act in a moving cell measured by a novel SFM technique. Besides contributions from blebbing and hydrodynamics flows it was generally believed that the protrusion of a migrating cell's leading edge is driven by actin polymerization. Our force measurements modulated by various cytoskeletal drugs show that hydrodynamics flows are negligible and solely actin polymerization drives the advancement of the central lamellipodium. Moreover, we measure the retrograde forces in the midst of the lamellipodium, the central missing link to understand how forces are balanced in motile cells. While the motions in the central lamellipodium, i.e. protrusion and retrograde flow, are solely driven by polymerization and depolymerization forces, the lamellipodial wings and the forces that pull the cell body along rely heavily on contractile actin-myosin interactions. The traction forces in the wings significantly contribute to the local

retrograde flow and are the origin of strong forces that advance the cell body.

BP 26.8 Thu 16:15 H43

Theoretical modelling of bacterial motor dynamics — ●EVA BARESEL and RUDOLF FRIEDRICH — Institute for Theoretical Physics, WWU Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany

The motion of self-propelled flagellated bacteria consists of two different modalities: "running" if all flagella rotate counter-clockwise or "tumbling" if at least one flagellum rotates clockwise. As a model for these bacterial motors we consider the dynamics of an ensemble of swimming objects which are composed of two rigidly connected point vortices. The single objects are able to show translation or rotation depending on the circulations of the single point vortices. We discuss the collective behaviour for several of these objects and the resulting velocity fields by means of numerical calculations.

BP 26.9 Thu 16:30 H43

Transition to clustering in bacterial colonies: myxobacteria mutants as self-propelled rods — ●FERNANDO PERUANI¹, JOERN STARRUSS², MARKUS BAER³, ANDREAS DEUTSCH², VLADIMIR JAKOVLEVIC⁴, and LOTTE SOGAARD-ANDERSEN⁴ — ¹Service de Physique de l'Etat Condense, CEA Saclay, 91191 Gif-sur-Yvette, France — ²ZIH, Technische Universität Dresden, Zellescher Weg 12, 01069, Dresden, Germany — ³Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany — ⁴Max Planck Institute for Terrestrial Microbiology, Karl-von-Frisch Str. 35043 Marburg, Germany

Myxobacteria, as many other bacteria, exhibit a transition from unicellularity to multicellularity when the level of nutrients is low. This fascinating process starts with the onset of clustering and collective motion. In contrast to *Dictyostelium discoideum* and other microorganisms, myxobacteria aggregate and coordinate their motion, in this early stage, without making use of diffusing chemical signals. We show through experiments with the mutant A+S-Frz- of *M. xanthus*, as well as through theoretical models, that is the active motion of the cells plus their rod-like shape what presumably allows cells to exhibit such collective effects. Provided the cell density is above a given threshold, a transition to clustering occurs. The cluster size statistics from experimental data can be reproduced by a simple models for self-propelled rods.

BP 26.10 Thu 16:45 H43

Compartment boundaries in developing epithelia — ●MARYAM ALIEE¹, KATHARINA LANDSBERG², JONAS RANFT¹, CHRISTIAN DAHMANN², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ²Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

During the development of tissues distinct cellular compartments are established. Straight and sharp interfaces between these compartments are maintained during development, so called compartment boundaries. A fundamental question is to identify the mechanisms by which boundaries form and remain stable. An important model system to study compartments is the wing development of the fruit fly *Drosophila*. Two different compartment boundaries are established during the development of the wing imaginal disc, the Anterior-Posterior boundary and the Dorsal-Ventral boundary. To study the role of cell mechanics and cell division we use a vertex model. We consider two dividing populations of cells and analyze the effect of local changes of cell bond tension and cell proliferation on the morphology of compartment boundaries. We find that a straight interface is maintained between two compartments if the proliferation rate of cells near the boundary is reduced. Increased bond tension at interface also leads to sharp boundaries. We quantify cell packing properties and interface roughness and study the interfacial tension associated with the compartment boundary using the stress profile in the system.

BP 26.11 Thu 17:00 H43

Antisymmetric stress and the role of angular momentum conservation in complex fluids. — ●SEBASTIAN FÜRTHAUER, STEPHAN GRILL, and FRANK JÜLICHER — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

The stress tensor of a Newtonian fluid is symmetric in the hydrodynamic limit. However, in complex fluids, such as nematic liquid crystals, the director field can exert a torque if it is locally rotated away

from its undistorted configuration. This produces a reactive antisymmetric contribution to the stress tensor. Here, we provide the derivation of a hydrodynamic theory for a complex fluid based on identifying the entropy production rate from the rate of change of the free energy. Analyzing the angular momentum balance, reveals that an additional dissipative contribution to the antisymmetric stress exists. We obtain

an expression for the antisymmetric dissipative stress by expanding thermodynamic fluxes in terms of thermodynamic forces, which is crucial in understanding the non-equilibrium dynamics of chiral complex fluids, such as the acto-myosin cytoskeleton or a fluid driven by beating cilia.

BP 27: Networks: From Topology to Dynamics IV (joint DY, BP, SOE)

Time: Thursday 14:00–16:00

Location: H44

BP 27.1 Thu 14:00 H44

A sequence-based framework for simulating the evolution of gene regulatory networks — ●THIMO ROHLF — Programme d'Épigenomique, Genopole Campus 1 - Genavenir 6, 5 rue Henri Desbruères, F-91030 Évry cedex, France — Max-Planck-Institute for Mathematics in the Sciences, Inselstr. 22, D-04103 Leipzig, Germany

An increasing amount of experimental data on global properties of genome organization across various species and phyla is becoming available, suggesting general principles as, e.g., scaling relationships or spatial regularities of gene distribution on DNA. A second level of information is accessible with gene regulatory networks, that control the space-time pattern of gene expression; here, similar (statistical) patterns of conserved regularities are observed. What can Statistical Physics contribute to tackle the question, which of these properties arose from combinatorial and architectural constraints, and which may have been shaped primarily by evolution? I will introduce and discuss a sequence-based artificial genome model that allows an integrative approach to model the emergence of genomic information at the levels of DNA sequence, regulatory networks and phenotype evolution. In particular, the following questions will be addressed: (1) Which types of network properties could be explained from combinatorial/statistical properties of genomes (random genome model), (2) how do they change in evolving genomes, in particular when (3) selective pressure is present, e.g. stabilizing selection for certain patterns of gene activity (phenotypes).

BP 27.2 Thu 14:15 H44

Evolution based on centrality: Bistability between hierarchical and deconstructed networks — ●CLAUDIO J. TESSONE¹, MATTEO MARSILI², and MICHAEL KÖNIG¹ — ¹Chair of Systems Design, D-MTEC ETH Zürich — ²International Centre for Theoretical Physics Abdus Salam

We study a model of network evolution in which agents attempt to become the most central ones in a network. Considering purely strategic interactions, when agents try to maximise their centrality in the network, the best strategy for them is to create links with the most central agent among those they are not still connected to. Conversely, for link removal, the most efficient strategy is to remove a link to the least central node, among the neighbours. This condition leads to a self-reinforcing mechanism signalled by the emergence of highly centralised networks. These networks have the property of nestedness: for any two agents i and j , if the degree of agent i is lower than that of j , the neighbourhood of i is contained within the neighbourhood of j . Moreover, this mechanism simplifies the computational effort needed by the agents to identify their best strategy.

Interestingly, such structures only can appear if all the agents have been developing it. If disturbances, –such as decay of edges, introduced by finite of link life-time– are in place, we show that ergodicity in the system disappears. Under these conditions two equilibrium states can coexist for a given set of parameters: one where such hierarchical structure emerges; another where a completely random network prevails.

BP 27.3 Thu 14:30 H44

Network evolution driven by spectral profile — ●SEBASTIAN WEBER¹ and MARKUS PORTO² — ¹Freiburg Institute For Advanced Studies (FRIAS), University of Freiburg, Germany — ²Institut für Festkörperphysik, Technische Universität Darmstadt, Germany

A large class of real world networks evolve over time, constantly changing and adapting their topology with respect to criteria imposed on the dynamics they mediate. The properties of the dynamics is ultimately determined by its spectral profile, which is the eigenvalue spectrum of the associated operator. This operator inevitably involves the network's adjacency matrix, establishing the connection between topology

and dynamics. Using the graph Laplacian or Kirchhoff matrix and its spectral profile as an example, the former being central in a wide class of physical processes (random walks, harmonic interaction networks, etc.) on networks, we show that a network evolution scheme recently developed by us is able to successfully evolve networks to display a given spectral profile's essential features [1].

[1] S. Weber and M. Porto, submitted.

15 min. break

BP 27.4 Thu 15:00 H44

Adaptive network approach to the collective motion of self-propelled agents — ●ANNE-LY DO¹, CRISTIAN HUEPE², GERD ZSCHALER¹, and THILO GROSS¹ — ¹MPI for the Physics of Complex Systems, Dresden — ²unaffiliated National Science Foundation grantee

Swarming is a showcase example of emergent behavior in complex many-particle systems. Previous modeling approaches rely on continuum theories or on individual based simulations and are difficult to study analytically as emergent-level equations are either complicated or not available at all. Here we propose an analytically tractable approach that bases on an adaptive network formulation. The nodes of this network represent individual animals while the links represent mutual awareness and therefore potential interaction between the linked individuals. Over time links are constantly created and broken as the movement of agents reshapes the network of contacts. Simultaneously the direction of movement can change as a result of the interactions with neighbors in the contact network. By means of moment closure approximation we derive an emergent-level description of the system and study it with the tools of nonlinear dynamics. We show that the system exhibits a phase transition from an unpolarized state, where no order motion occurs, to a state of collective motion, thus reproducing the results of recent swarming experiments.

BP 27.5 Thu 15:15 H44

The backbone of the climate network — ●JONATHAN FRIEDEMANN DONGES^{1,2}, YONG ZOU¹, NORBERT MARWAN¹, and JÜRGEN KURTHS^{1,2} — ¹Potsdam Institute for Climate Impact Research, P.O. Box 601203, 14412 Potsdam, Germany — ²Department of Physics, Humboldt University Berlin, Newtonstr. 15, 12489 Berlin, Germany

We propose a method to reconstruct and analyze a complex network from data generated by a spatio-temporal dynamical system, relying on the nonlinear mutual information of time series analysis and betweenness centrality of complex network theory. We show, that this approach reveals a rich internal structure in complex climate networks constructed from reanalysis and model surface air temperature data. Our novel method uncovers peculiar wave-like structures of high energy flow, that we relate to global surface ocean currents. This points to a major role of the oceanic surface circulation in coupling and stabilizing the global temperature field in the long term mean (140 years for the model run and 60 years for reanalysis data). We find that these results cannot be obtained using classical linear methods of multivariate data analysis, and have ensured their robustness by intensive significance testing.

BP 27.6 Thu 15:30 H44

Personalized recommendation in Collaborative Tagging Systems — ●ZI-KE ZHANG — chemin du musee, CH1700, Fribourg, Switzerland

Personalized recommender systems are confronting great challenges of accuracy, diversification and novelty, especially when the data set is sparse and lacks accessorial information, such as user profiles, item attributes and explicit ratings. Collaborative tags contain rich informa-

tion about personalized preferences and item contents. We are trying to find an efficient yet simple way to make use of tags to provide better recommendations.

BP 27.7 Thu 15:45 H44

What network analysis can tell us about car-scrap bonus: the linchpins of modern economy — ●FLORIAN BLÖCHL¹, FABIAN J. THEIS^{1,2}, and ERIC O'N. FISHER³ — ¹Institute for Bioinformatics and Systems Biology, Helmholtz Centre Munich — ²Department of Mathematics, TU Munich — ³California Polytechnic State University

An input-output matrix collects good flows between different economic sectors, structural units of the economy like "Agriculture" or "Pharmaceuticals". This matrix can be viewed as a directed weighted network. We analyze input-output graphs for a wide set of countries collected by the OECD. These networks contain only 40 nodes, but are almost

fully connected and have quite strong self-loops.

We apply two measures of node centrality, both relying on different properties of random walks on the graphs: random walk centrality and a new measure we called count-betweenness. The latter is similar to Newman's random walk betweenness, but allows for directed graphs and incorporates self-loops. Both measures give similar and reasonable results. For instance, we find that in Luxembourg the most central sector is "Finance and Insurance", in Brazil "Food Products", and in Germany "Motor Vehicles". Thus, car-scrap bonus really aimed at the linchpin of Germany's economy.

The sectors' rankings are quite different, however some sectors are important in most countries while others are never. We therefore additionally structure the data by hierarchically clustering countries. Thereby we achieve clusters that well coincide with geographical proximity or developmental status.

BP 28: Focus: Charge Effects in Soft and Biological Matter II (joint CPP, BP, ST)

Time: Thursday 14:00–17:45

Location: H37

Invited Talk

BP 28.1 Thu 14:00 H37

Electrostatic effects on depletion forces — ●ROBERTO PIAZZA¹, STEFANO BUZZACCARO¹, JADER COLOMBO², and ALBERTO PAROLA² — ¹Dipartimento CMIC, Politecnico di Milano, Milano (Italy) — ²Dipartimento di Fisica e Matematica, Università dell'Insubria, Como (Italy)

Short-ranged depletion forces give rise to a phase behavior which is totally foreign to simple molecular systems, allowing to investigate new scenarios of noticeable interest for condensed matter physics. Yet, so far, most experimental and theoretical efforts have concentrated on depletion effects induced by an ideal agent.

Here, conversely, we focus on systems where strong electrostatic coupling is present. After reviewing some recent results we have obtained by sedimentation measurements on a model system of "sticky" hard-spheres, where depletion forces are induced by nonionic surfactants, we shall present novel results pointing out the dramatic effects that the presence of a self-interacting depletant may bring in. In particular, we shall show that electrostatic repulsive forces between the depletant yield a strong increase of depletion effects, scaling with the Debye-Hückel screening length. Conversely, competitive electrostatic forces between the colloidal particles hinder, and may even totally quench depletion-induced phase separation. The observed effects are fairly well accounted for by a theoretical analysis, based on liquid-state theory, of the structural properties of the two-components (colloids + surfactant micelles) fluid.

BP 28.2 Thu 14:30 H37

Interaction of Proteins with Spherical Polyelectrolyte Brushes — ●KATJA HENZLER^{1,2}, ALEXANDER WITTEMAN¹, BJÖRN HAUPT^{1,2}, OLEG BORISOV³, and MATTHIAS BALLAUFF² — ¹Universität Bayreuth, Physikische Chemie I; Universitätstr. 30, 95440 Bayreuth, Germany — ²Helmholtz-Zentrum Berlin für Materialien und Energie; Hahn-Meitner-Platz 1; 14109 Berlin, Germany — ³Institut pluridisciplinaire de Recherche sur l'Environnement et les Matériaux, UMR 5254, CNRS/UPPA, 64053 Pau, France

Spherical polyelectrolyte brushes (SPB) are a novel class of carrier particles for the immobilization of proteins.[1] A high uptake of proteins can be achieved if the ionic strength is low, while both compounds carry an overall negative charge.[1] No adsorption takes place at higher ionic strength. The main driving force for the adsorption is the counterion release force. Counterions from the brush layer are released and the free energy of the system will be decreased. The thermodynamic of the described adsorption process can be investigated by isothermal titration calorimetry (ITC).[2] This method allows us to determine the adsorption isotherm together with the adsorption enthalpy and entropy. We demonstrated that the adsorption of β -lactoglobulin (BLG) onto the SPB is driven by a strong gain of entropy i.e. by the postulated uptake mechanism of the counterion release force. This is the first direct proof for the counterion release force.

Literature: [1] Wittemann, A.; Ballauff, M. *Phys. Chem. Chem. Phys.* 2006, 8, 5269. [2] Henzler, K.; Haupt, B.; Lauterbach, K.; Wittmann, A.; Borisov, O.; Ballauff, M. in preparation.

BP 28.3 Thu 14:45 H37

On the Question of Universality of Charge Induced Reentrant Condensation of Proteins — ●FAJUN ZHANG¹, BENJAMIN HECK¹, MARCELL WOLF¹, LUCA IANESELLI¹, MICHAEL ZILLER¹, MAXIMILIAN W. A. SKODA², ROBERT M. J. JACOBS³, OLIVER KOHLBACHER⁴, SOPHIE WEGGLER⁵, ANDREAS HILDBRANDT⁵, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — ²ISIS, Rutherford Appleton Laboratory, UK — ³Department of Chemistry, CRL, University of Oxford, UK — ⁴Zentrum für Bioinformatik Tübingen, Tübingen, Germany — ⁵Zentrum für Bioinformatik Saar, Saarbrücken, Germany

The effective interactions and phase behavior of protein solutions under strong electrostatic coupling conditions are a challenge to our understanding due to the complex charge pattern and irregular geometry of protein surfaces, which distinguishes them from related systems such as DNA or conventional colloids. In this work, we discuss the question of the universality of the reentrant condensation (RC) of proteins in solution induced by multivalent counterions, i.e. redissolution upon adding further salts after phase separation, as recently discovered [1]. The discussion is based on a systematic investigation of five different proteins with different charge patterns with five typical multivalent counterions. Zeta potential measurements confirm the effective charge inversion of proteins in the reentrant regime via binding of multivalent counterions. [1] F. Zhang, et al., *Phys. Rev. Lett.* 2008, 101, 148101.

BP 28.4 Thu 15:00 H37

Effective charge of globular proteins and dendrimers — UTE BÖHME and ●ULRICH SCHELER — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden

The density of charges on macromolecules is usually so high, that the thermal energy of the respective counterions is insufficient to escape the electric field generated from the charges on the macromolecule. Therefore a fraction of counterions condenses on the macromolecule, lowering the effective charge of the. The combination of diffusion and electrophoresis NMR provides an unambiguous possibility for the experimental determination of the effective charge, which is in good agreement with molecular simulations [1, 2]. This approach has been applied to linear polyelectrolytes as well as proteins and other globular molecules [3]. PAMAM dendrimers exhibit only two types of chargeable groups, therefore counterion condensation can easily be quantified, where the degree of protonation of the amino groups is inferred from proton NMR spectra. At low generations the fraction of condensed counterions increases with increasing molecular weight to level at about 70%. [1] U. Böhme, U. Scheler, *Colloids and Surfaces A*, 222, (2003), 35 [2] K. Grass, U. Böhme, U. Scheler, H. Cottet, C. Holm, *Physical Review Letters* 100, (2008) 096104 [3] Ute Böhme, Ulrich Scheler *Chemical Physics Letters* 435, (2007), 342

BP 28.5 Thu 15:15 H37

Charge effects in protein diffusion — ●MARCUS HENNIG^{1,2}, FELIX ROOSEN-RUNGE², FAJUN ZHANG², TILO SEYDEL¹, and FRANK SCHREIBER² — ¹Institut Laue-Langevin, Grenoble, France — ²Institut für Angewandte Physik, Universität Tübingen, Germany

Proteins in solution form highly monodisperse colloidal suspensions. Hence, protein solutions are of fundamental interest in a context of soft

matter science. A distinguishing feature to simple colloidal systems is the inhomogeneous surface charge distribution of proteins, which is assumed to have a fundamental biological relevance in controlling for instance aggregation phenomena and docking processes. In their native environment proteins are embedded in a crowded solution of various macromolecules and salt ions. These salt ions are crucial for the understanding of the effective interactions of proteins and the dynamics. We study the self-diffusion of the model globular protein Bovine Serum Albumin in aqueous solutions with different salt concentrations by quasi-elastic neutron scattering performed at selected temperatures and in high protein concentrations. Furthermore, by using spin-echo spectroscopy we investigate the collective diffusion behavior. We found that trivalent salts, particularly yttrium chloride, have a pronounced effect on the self and collective diffusion on a nanosecond time scale. Whereas monovalent and divalent salts, such as sodium chloride and calcium chloride, exhibit little or no effect, we observe that the diffusion decreases nearly 50% for a 19mM yttrium chloride concentration.

15 min. break

Invited Talk BP 28.6 Thu 15:45 H37

In-silico simulation of reentrant protein condensation with highly valent counterions — SOPHIE WEGGLER¹, MICHAEL ZILLER², FAJUN ZHANG², FRANK SCHREIBER², OLIVER KOHLBACHER³, and ●ANDREAS HILDEBRANDT¹ — ¹Center for Bioinformatics, Bld. E 2.1, Saarland University, 66123 Saarbrücken, Germany — ²Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — ³Zentrum für Bioinformatik Tübingen, Sand 14, 72076 Tübingen, Germany

Recently, it has been shown experimentally that negatively charged globular proteins in solution undergo a condensation upon adding trivalent counterions between two critical concentrations C^* and C^{**} , $C^* < C^{**}$. This reentrant condensation had previously been observed for DNA and suitable colloidal systems, where the phenomenon is well-understood theoretically, but not for proteins: while the former systems can be well approximated by simple geometries and constant surface charge distributions, proteins feature complex charge patterns on their surface and can occur in diverse geometrical arrangements.

Consequently, the mechanism behind reentrant protein condensation differs from that behind reentrant DNA condensation and can be explained by short-ranged electrostatic interactions between multivalent cations and acidic residues of the protein.

In my talk, I will present a theoretical model for reentrant protein condensation and will introduce a Monte Carlo technique for its numerical simulation.

BP 28.7 Thu 16:15 H37

Oligolamellar Lipid Layers Under Load: A Model For Artificial Implants — ●MARTIN KREUZER¹, REINER DAHINT¹, and ROLAND STEITZ² — ¹Universität Heidelberg, Physikalisch Chemisches Institut, 69120 Berlin, Germany — ²Helmholtz-Zentrum Berlin GmbH, 14109 Berlin, Germany

The mechanisms and physicochemical parameters to reduce friction in a natural joint are not yet clear and subject of controversial discussions. We represented the biological interface by a suitable model system and employed Neutron Reflectivity for studying the relevant structural features on the molecular scale. The model interface consisted of a lipid covered silicon disc measured against a model synovial fluid at elevated hydrostatic pressure. Measurements in a pressure cell against D₂O showed, that the as-prepared lipid coating remained stable on the substrate up to a hydrostatic pressure of 900bar when the lipid molecules were in their gel-like $P\beta^*$ phase. However, the lipid main phase transition from the gel to fluid-like $L\alpha$ phase at 450 bar and 38°C lead to a loss of most of the lipid bilayers and only one double layer remained on the substrate. Measurements against the model synovial fluid (3mg/ml hyaluronic acid in D₂O) showed that the lipid multilayer coatings remained stable on the substrate at 450 bar and 38°C, where formerly the phase transition into the fluid-like $L\alpha$ phase occurred. Beside that, a pronounced swelling of the oligo-lamellar films was observed. Therefore, we conclude that the synovial fluid not only plays an important role in the reduction of friction in the human joint, but also significantly stabilizes the lipid multilayer coating.

BP 28.8 Thu 16:30 H37

Ion specificity and the Jones-Ray effect at liquid-liquid interfaces — ●MARKUS BIER — Max-Planck-Institut f. Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany

The solvation shells around ions in solution are one of the key features which determine, e.g., the kinetics of electrochemical reactions and the charge transport across ion channels in biological membranes. Ion specificity of certain properties is, to a large extent, brought about by a variation of the structure or the stability of the solvation shell when considering different types of ions. In the present contribution the interfacial tension between two immiscible liquids as a function of the ionic strength is studied theoretically. For large ionic strengths the well-known linear behaviour is found, which is related to a finite size of the solvation shells. For small ionic strengths a decrease with the negative square root occurs due to an unequal partitioning of ions near the interface, which is induced by a difference of the solvation free energy contrasts between the two liquids. The crossover ionic strength between both regimes turns out to be strongly ion specific. A minimum of the interfacial tension can occur close to the crossover ionic strength, similar to the Jones-Ray effect of the electrolyte-air surface. The theoretical results are compared with experimental data and the relation to the limiting case of an electrolyte-air surface is discussed. It is argued that the dependence of the liquid-liquid interfacial tension on the ionic strength could serve as a sensitive probe to study solvation shells of various ions in various liquids.

BP 28.9 Thu 16:45 H37

Three-layer piezoelectrets from fluoroethylenepropylene (FEP) copolymer films: Arrangement, preparation and characterization — ●PENG FANG¹, FEIPENG WANG¹, WERNER WIRGES¹, HEITOR CURY BASSO², and REIMUND GERHARD¹ — ¹Applied Condensed-Matter Physics, Department of Physics and Astronomy, Faculty of Science, University of Potsdam, Potsdam-Golm, Germany — ²Department of Electrical Engineering, São Carlos School of Engineering, University of São Paulo, São Carlos - SP, Brazil

Piezoelectrets are very useful transducer materials for electromechanical and electroacoustical sensors and actuators. A new process for the preparation of three-layer FEP-sandwich piezoelectrets is introduced. The samples are prepared from commercial FEP films by means of simple procedures such as laser cutting, laser bonding, electrode evaporation and high-field poling. The resulting dielectric-resonance spectrum demonstrates the piezoelectricity of the FEP sandwich. A DC poling voltage of around -4 kV is sufficient to achieve piezoelectric d₃₃ coefficient as high as 40 to 50 pC/N. After a continuous dynamic measurement of d₃₃ over 5000 cycles (around 1 day), samples still retain 90% of their initial piezoelectricity. Higher measuring frequencies lead to a decrease of d₃₃. At 100 Hz, d₃₃ is 70% of the value at 2 Hz. Samples charged at elevated temperatures show much better thermal stability of d₃₃. No obvious decay of d₃₃ is found on samples charged at 130 degree C after one-hour storage at 120 degree C. Samples retain more than half of their initial piezoelectricity after a thermal treatment at 140 degree C and are still piezoelectric at 160 degree C.

BP 28.10 Thu 17:00 H37

The conformation of poly(styrene sulfonate) layers physisorbed from salt solutions of different concentration studied on two different length scales: superposition of electrostatic and steric forces — ●STEPHAN BLOCK and CHRISTIANE A. HELM — Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17489 Greifswald, Germany

AFM is used to measure the surface forces and to image sodium poly(styrene sulfonate) (PSS) layers physisorbed from NaCl solutions with an ionic strength ranging between 0 M and 1 M NaCl. Colloidal probe tapping mode imaging shows that domains of PSS brushes coexist with flatly adsorbed PSS. The brush area fraction increases with rising degree of polymerization and NaCl concentration in the adsorption solution. Colloidal probe technique reveals that the surface forces are a superposition of steric and electrostatic forces, their respective contribution is determined by the brush area fraction. Interestingly, the internal properties of the brush domains (i.e. brush thickness and average chain distance) are independent on the adsorption salt concentration and depend only on the degree of polymerization and (for the brush thickness) on the surrounding salt concentration. Using these complementary techniques we derive the scaling laws for the average chain distance and the brush thickness and area fraction. Thereby it is possible to form PSS brushes with the desired properties (brush thickness between 20 and 400 nm, brush area fraction between zero and full surface coverage) and hence to control the range and magnitude of the surface forces by choosing the appropriate preparation conditions.

BP 28.11 Thu 17:15 H37

Changes of the Molecular Structure in Supported Polyelectrolyte Multilayers under Mechanical Stress — ●JOHANNES FRÜH¹, MAREIKE KIEL^{1,2}, RALF KÖHLER^{1,3}, and RUMEN KRASTEV^{1,4} — ¹Max Plank Institut für Kolloid- und Grenzflächenforschung, 14424 Potsdam, Germany — ²Uni Potsdam, 14476 Potsdam, Germany — ³Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — ⁴NMI an der Universität Tübingen, 72770 Reutlingen, Germany

Polyelectrolyte multilayers (PEM) are extensively applied in contemporary technique. They are composed of oppositely charged polymers. The build-up process is based on the electrostatic interactions between the interface and the polymer molecules. Application of lateral stress on PEM changes the molecular conformation and the orientation of the polymers, and the electrostatic interactions between them. This leads to changes in the interfacial properties of the PEM coatings. The pyrene fluorescence is a tool to study the molecular coiling and polarity in PEM. We used this to follow the changes in the molecular structure of PEM prepared from pyrene labelled poly-styrene sulphonate and poly-(diallyldimethylammonium) chloride deposited on sheets of PDMS. We found that PEM undergo a plastic deformation under mechanical stretching. The polymer molecules organised in PEM experience a transition from coiled to decoiled state. The deformation strongly depends on the salt concentration of the solution from which the PEM are prepared, respectively on the molecular coiling and electrostatic interactions.

BP 28.12 Thu 17:30 H37

About the interfacial behaviour of PEM films of different charge density — ●RALF KÖHLER^{1,2}, INGO DÖNCH¹, PATRICK OTT³, ANDRÉ LASCHEWSKY³, ANDREAS FERY⁴, and RUMEN KRASTEV^{1,5} — ¹MPI of Colloids and Interfaces, 14424 Potsdam — ²Helmholtz Centre Berlin for Materials and Energy, 14109 Berlin — ³University of Potsdam, 14476 Potsdam — ⁴University of Bayreuth, 95440 Bayreuth — ⁵NMI at the University of Tübingen, 72770 Reutlingen, Germany

Polyelectrolyte Multilayers (PEM) consist in complexed layers of organic polyions of opposite charge build-up on solid substrate by layer-by-layer deposition. Although PEM materials are studied since more than a decade, the interplay of internal interactions and structure is still far from being understood.

We investigate the internal structure of PEM by means of swelling experiments, i.e. an internal mechanical stress is induced into PEM by uptake of solvent molecules from adjacent solvent vapour (H₂O) of varying saturation. Here neutron reflectometry proves to be a powerful tool due to its ability to test for the thickness of the sample and for its specific material content at the same time.

Three different PEM systems made from PSS/PDDA (1) are investigated; each containing a derivative of the polycation PDDA of 75, 89, or 100% charge density, also the number of adsorbed layers is varied.

It shows that the swelling characteristics changes continuously with the initial film thickness indicating internal transitions of structure and swelling. (1) poly-styrene sulphonate/ poly-diallyldimethyl ammonium

BP 29: Biomolecular Spectroscopy

Time: Thursday 14:30–17:00

Location: H45

BP 29.1 Thu 14:30 H45

Determining the structure of Ac-Ala_nLysH⁺ in vacuo: computational spectroscopy using DFT — ●MARIANA ROSSI, VOLKER BLUM, PETER KUPSER, GERT VON HELDEN, FRAUKE BIERAU, GERARD MEIJER, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut, D-14195 Berlin, Germany

Well defined secondary structure motifs (e.g., helices) in polypeptides can be systematically studied in vacuo, offering a unique "clean room" condition to quantify the stabilizing intramolecular interactions. Here we address theoretically the structure of alanine polypeptides Ac-Ala_nLysH⁺ (n=5,10,15), for which gas-phase helical structure was indicated in experiment [1]. Using van der Waals (vdW) corrected [2] Density Functional Theory (DFT), we present vibrational spectra and compare to room temperature multiple photon IR spectroscopy data obtained at the FELIX free electron laser. For the longer molecules (n=10,15) α-helical models provide good qualitative agreement (theory vs. experiment) already in the harmonic approximation. For Ac-Ala₅LysH⁺, the predicted lowest energy conformer ("g-1") in vdW corrected DFT (PBE, B3LYP, revPBE) is not a simple helix. However, the harmonic free energy suggests that g-1 and the lowest-energy α-helical conformers are energetically close at 300 K, and thus might all coexist in experiment. Consistently, their calculated vibrational spectra agree with experiment, but only if anharmonic effects are included by explicit molecular dynamics simulations. [1] R. Hudgins *et al.*, JACS **120**, 12974 (1998) [2] A. Tkatchenko and M. Scheffler, PRL **102**, 073005 (2009)

BP 29.2 Thu 14:45 H45

Multivariate analysis for surface-enhanced Raman scattering (SERS) probe multiplexing and imaging in biological matrices — ●ANDREA MATSCHULAT^{1,2}, DANIELA DRESCHER^{1,2}, and JANINA KNEIPP^{1,2} — ¹Institut für Chemie, HU, Brook-Taylor-Str. 2, 12489 Berlin — ²Bundesanstalt für Materialforschung und -prüfung (BAM), Richard-Willstätter-Str.11, 12489 Berlin

Raman Spectroscopy as a non-destructive spectroscopic technique allows the study of vibrational fingerprints by which chemical and biological compounds can be identified. An improvement of the spatial resolution on the nm-scale is provided by local optical fields surrounding plasmonic nanostructures which are excited by the incident electromagnetic field. Such so-called surface-enhancement provides more sensitive detection. SERS has therefore attracted considerable interest for its application in bioanalytical chemistry. SERS offers numerous opportunities in the study of spectral changes during molecular in-

teractions in complex biosystems. We demonstrate a multivariate approach for SERS hybrid probe multiplexing and imaging implementing principal component analysis and cluster algorithms. As a first application, we introduced two biocompatible Raman reporter molecules attached to Au nanoaggregates into living 3T3-cells. Such a hybrid probe approach enables the identification of different SERS probes in multiplexed experiments. We present results of hyperspectral mapping analysis providing us information about the cellular uptake, localization and amount of both reporter molecules inside the biosystem.

BP 29.3 Thu 15:00 H45

Characterization of artificial peptide receptors by UV resonance Raman spectroscopy and non-negative matrix factorization — ●CHRISTOPH HERRMANN¹, STEPHAN NIEBLING¹, SUNIL KUMAR SRIVASTAVA¹, CARSTEN SCHMUCK², and SEBASTIAN SCHLÜCKER¹ — ¹Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück — ²Institut für Organische Chemie, Universität Duisburg-Essen, Universitätsstr. 5, 45141 Essen

Guanidiniocarbonyl pyrroles are artificial peptide receptors which serve as model systems for investigating the principles of peptide binding. Their carboxylate binding site (CBS) can be selectively monitored by UV resonance Raman (UVR) spectroscopy. UVR spectra of guanidiniocarbonyl pyrroles we recorded at different pH values in the range of 4 to 9 in order to characterize the corresponding acid/base equilibrium. By using non-negative matrix factorization (NMF), we were able to extract the pure spectra of the neutral and protonated CBS species from the experimental UVR spectra. This allowed the quantification of their relative contributions and the site specific pKa determination of the CBS in these artificial peptide receptors.

BP 29.4 Thu 15:15 H45

Conformation studies of the gram-negative-bacteria protein TonB by pulse EPR — ●SILVIA DOMINGO KÖHLER¹, ANEMARIE WEBER², WOLFRAM WELTE², and MALTE DRESCHER¹ — ¹Department of Chemistry, University of Konstanz, 78457 Konstanz, Germany — ²Department of Biology, University of Konstanz, 78457 Konstanz, Germany

To transport Iron complexed in ferric siderophores through the outer membrane of gram-negative bacteria energy is required. It is proposed that a complex composed in particular by the TonB protein and anchored in the inner membrane opens channels in the outer membrane. The energy needed is only available in the inner membrane, in form of the proton motive force. Structure and dynamics of the protein

TonB plays a key role in unraveling how the energy is transferred to the outer membrane, in order to induce a conformational change in the outer membrane receptors. However, the structure of TonB is not completely determined and the mechanism of energy transduction remains still unclear.

To unravel structure and functionality of TonB site-directed spin-labeling in combination with pulsed electron paramagnetic resonance (EPR) techniques is an outstandingly suitable tool. Determining conformation and conformational changes of TonB helps to elucidate a mechanism which has general implications for signal transduction within and between proteins.

BP 29.5 Thu 15:30 H45

Motional effects on coherent exciton transport in a chain — ●MARKUS TIERSCH^{1,2}, ALI ASADIAN^{1,2}, GIAN GIACOMO GUERRESCHI^{1,2}, JIANMING CAI^{1,2}, SANDU POPESCU³, and HANS BRIEGEL^{1,2} — ¹Institut für Quantenoptik und Quanteninformation der Österreichischen Akademie der Wissenschaften, Innsbruck, Austria — ²Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria — ³H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol, BS8 1TL, United Kingdom

In a reduced model of coherent excitation transport in α -helical polypeptides, individual amide units in a chain carry the excitation, and are coupled through dipole-dipole interactions. Vibrations of the chain cause a modulation of the distance dependent dipolar coupling between the individual sites, and thereby influence the transport efficiency through the chain. In this setting, we report on the motion-induced, effective locking and guiding of excitations, and investigate control mechanisms to enhance the transport through the chain.

15 min. break

BP 29.6 Thu 16:00 H45

Pigment fluorescence in protein environment — ●FRANZ-JOSEF SCHMITT¹, HEINRICH SÜDMEYER², KAI REINEKE¹, INSA KAHLEN¹, JOACHIM BÖRNER¹, MAX SCHOENGEN¹, PATRICK HÄTTI¹, HANS JOACHIM EICHLER¹, and HANS-JOACHIM CAPPIUS² — ¹Berlin Institute of Technology, Berlin — ²Laser- und Medizintechnologie GmbH, Berlin

The electronic properties of organic molecules strongly depend on the local environment. Therefore it is difficult to detect specific molecules if the environment of the molecules is not clearly defined. On the other hand the fine tuning of the local protein environment leads to specific pathways for excitation energy migration between pigments in e.g. photosynthetic plant complexes and the influence of the environment is essential for the light harvesting functionality. In this study we compare the time resolved fluorescence of pigments (e.g. fluorescein, chlorophyll) and pigment protein complexes (e.g. Bovine serum albumin, water soluble chlorophyll binding protein and photosynthetic light harvesting complexes). The protein matrix has an own characteristic influence onto the chromophores and strongly diminishes the environmental influence onto the chromophores. The fluorescence of fluorescein and chlorophyll molecules on glass surface is strongly quenched while the pigments bound to protein complexes show only slight changes of the fluorescence dynamics due to the surface contact.

Financial support by DFG project Sfb 429 and Federal Ministry of Education and Research (BMBF) is gratefully acknowledged.

BP 29.7 Thu 16:15 H45

Excitation energy transfer in the Phycobiliprotein Antenna of the cyanobacterium *Acaryochloris marina* investigated by transient fs absorption spectroscopy. — ●COLLINS NGANOU¹, MORITZ GREHN¹, CHRISTOPH THEISS¹, MARCO VITALI², FRANZ-JOSEPH SCHMITT¹, HANS JOACHIM EICHLER¹, and HANN-JÖRG ECKERT² — ¹Institute of Optics, Technical University Berlin, Straße des 17. Juni 135, Berlin-Germany — ²Max-Volmer-Laboratory for Bio-

physical Chemistry, Technical University Berlin, Straße des 17. Juni 135, Berlin-Germany

The investigation of excitation energy transfer (EET) in the antenna system of *Acaryochloris marina* containing both chlorophyll (Chl) d and phycobiliprotein (PBP) as light harvesting pigments continue to be a case of debate in the scientific community. The PBP-antenna is a rod-shaped antenna of three homo-hexamers containing phycocyanin (PC) and one hetero-hexamer of PC and allophycocyanine (APC). In the present work we discuss the EET in isolated PBP-antennae by transient fs absorption spectroscopy measurements and show that the presence of phosphate in the buffering medium is an important requirement to preserve the EET between the PBP pigments.

BP 29.8 Thu 16:30 H45

Describing transient Fluorescence induction curves by modelling the electron transfer of photosystem II — ●JOACHIM BÖRNER¹, FRANZ-JOSEF SCHMITT¹, HANS JOACHIM EICHLER¹, ATHINA ZOUNI², and GERNOT RENGER² — ¹Institute of Optics and Atomic Physics, Berlin Institute of Technology, Germany — ²Max-Volmer-Laboratory for biophysical chemistry, Berlin Institute of Technology, Germany

In this work a generalised PS II model for the simulation of fluorescence induction curves is presented. Fluorescence induction curves were measured with continuous laser illumination on isolated core complexes from the thermophilic cyanobacterium *Thermosynechococcus elongatus* and hole cells of the green algae *Chlorella pyrenoidosa* chick. Perfect data fit was achieved within the framework of a model for the PS II reaction pattern comprising electron transfer reactions to the exogenous electron acceptor $K_3Fe(CN)_6$ in core complexes and to the endogenous plastoquinone in *Chlorella* cells. Based on data reported in the literature a consistent set of rate constants was obtained for electron transfer at the donor and acceptor side of PS II. The simulations based on the model of the PS II reaction pattern provide information on the time courses of population probabilities of different PSII states in photosynthetic samples under various conditions (e.g. presence of herbicides, other stress conditions, excitation with actinic pulses of different intensity and duration).

Acknowledgement: Financial support by DFG project Sfb 429 and Federal Ministry of Education and Research (BMBF)

BP 29.9 Thu 16:45 H45

Photocycle Dynamics of the E149A Mutant of Cryptochrome 3 from *Arabidopsis thaliana* — PEYMAN ZIRAK¹, ●ALFONS PENZKOFER¹, JUDIT MOLDT², RICHARD POKORNY², ALFRED BATSCHAUER², and LARS-OLIVER ESSEN³ — ¹Institut II - Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstr. 31, 93053 Regensburg — ²Fachbereich Biologie, Pflanzenphysiologie/Photobiologie, Philipps-Universität, Karl-von-Frisch-Str. 8, 35032 Marburg — ³Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Str., 35032 Marburg

The E149A mutant of the cryDASH member cryptochrome 3 (cry3) from *Arabidopsis thaliana* was characterized *in vitro* by absorption and emission spectroscopy. The mutant protein non-covalently binds the cofactor flavin adenine dinucleotide (FAD), but not the second cofactor 5,10-methenyl-tetrahydrofolate (MTHF). Thus, the photo-dynamics caused by FAD is accessible without the intervening coupling with MTHF. In dark adapted cry3-E149A, FAD is present in the oxidized form (FAD_{ox}), semiquinone form (FADH[•]), and anionic hydroquinone form (FAD_{red}H⁻). Blue-light photo-excitation of previously unexposed cry3-E149A transfers FAD_{ox} to the anionic semiquinone form (FADH[•]) with a quantum efficiency of 0.02 and a back recovery time of 10 s (photocycle I). Prolonged photo-excitation leads to an irreversible protein re-conformation leading to a change in the photocycle dynamics with photo-conversion of FAD_{ox} to FADH[•] (efficiency 0.00032), of FADH[•] to FAD_{red}H⁻ (efficiency 0.016), and thermal back equilibration in the dark on a minute timescale (photocycle II).

BP 30: Networks: From Topology to Dynamics V (joint DY, BP, SOE)

Time: Thursday 16:00–17:15

Location: H44

BP 30.1 Thu 16:00 H44

Eat the specialist: Some results on the stability of 100 billion food webs — ●THILO GROSS — Max-Planck Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden

Ecological food webs are complex networks of feeding interactions, describing who-eats-who in an ecosystem. Previous theoretical results suggest that the dynamical stability of these webs should decrease with increasing number of species and network connections. Yet, large and densely-linked webs found in nature are highly stable. Identification of the properties promoting stability is therefore an important goal of ecological research. The approach of generalized modeling enables us to investigate the local stability of steady states in these webs with a higher degree of generality and efficiency than previous simulative approaches. Because of the complexity of the problem, a general food web model contains several thousand unknown parameters. However, the numerical efficiency of the generalized models is such that tens of billions of different realizations of plausible webs can be analyzed in reasonable computational time. This provides a sound basis for the statistical exploration of the high-dimensional parameter space. In this talk I will demonstrate the application of generalized modeling, in simple examples and in large food webs. The latter reveals certain topological properties having a strong impact on network stability.

BP 30.2 Thu 16:15 H44

Regular graph properties of the plasmodial vein network of the slime mould *Physarum polycephalum* — WERNER BAUMGARTEN and ●MARCUS HAUSER — Otto-von-Guericke-Universität Magdeburg, Abteilung Biophysik, Institut für Experimentelle Physik, Universitätsplatz 2, 39106 Magdeburg, Germany

The plasmodium of the slime mould *Physarum polycephalum* is a single multi-nucleate giant amoeboid cell. It forms a characteristic two-dimensional vein network, where the apical end of the plasmodium extends to search for new food sources, while the dense network of tubular veins is in charge of transport of protoplasm throughout the giant cell.

A graph theoretical analysis of the vein network of the *Physarum polycephalum* strain HU195×HU200 reveals that the nodes have exclusively the degree 3, i.e., each node connects to exactly three veins. This means that the vein network of this slime mould forms a regular cubic graph, and hence does not show small-world properties. The intensities of the edges (the vein segments) connecting a pair of nodes differ, thus forming a weighted graph. The distributions of the lengths and areas of the veins follow exponential distributions, while their widths are distributed either log-normally or normally. Interestingly, these functional dependencies are robust during the entire evolution of the growing plasmodial vein network of *Physarum polycephalum*.

BP 30.3 Thu 16:30 H44

Feedback-mediated control of a spiral wave in a bidomain model of cardiac tissue — ●EKATERINA ZHUCHKOVA, VLADIMIR ZYKOV, and HARALD ENGEL — Institut für Theoretische Physik, Technische Universität zu Berlin, Berlin, Germany

At the moment anti-tachycardia pacing (ATP) is the only low-energy therapy for ventricular tachyarrhythmias and it would be desirable since it prevents adverse side effects. However, ATP is not robust since its success/failure depends on many factors [1]. Using realistic

bidomain model for simulation of electrical activity in cardiac tissue together with a simplified Fenton-Karma ionic model for a cell, we show that spiral waves in the heart could be eliminated by repetitive extracellular stimulation. A spiral wave core can be guided towards boundaries by feedback forcing along a one-dimensional registering electrode [2]. Every time the spiral wave front is tangent to the registering electrode, an extracellular current is applied through stimulating electrodes. The amplitude of the stimulation is much less than the single-shock defibrillation threshold, which gives a possibility to use the proposed method as an alternative low-voltage defibrillation strategy.

[1] E. Zhuchkova and H. Engel, Robustness of local forcing in inhibition of reentry, IPACS Open Access Library (2009), accepted.

[2] J. Schlesner, V. S. Zykov, H. Brandtstädter, I. Gerdes and H. Engel, Efficient control of spiral wave location in an excitable medium with localized heterogeneities, NJP 10, 015003 (2008).

BP 30.4 Thu 16:45 H44

Linking Molecular Simulations and Systemic Modelling — ●TIHAMER GEYER and VOLKHARD HELMS — Zentrum für Bioinformatik, Universität des Saarlandes, D-66123 Saarbrücken

When modeling biological systems there is a gap of scales between the systemic models that try to describe the metabolism of a complete cell and the molecular biological descriptions focussing on the detailed processes of a single enzyme. We therefore proposed an agent based approach that allows to bridge between the two regimes.

For this, we set up the individual enzymes from their microscopic elementary reactions like the binding of a metabolite molecule to a binding site or the transfer of an electron from one site inside the protein to another. The respective numbers of these protein "building blocks" are then connected to metabolite pools via standardized connectors to set up the metabolic system under consideration. This pools-and-proteins model can thus be used to "convert" detailed molecular biological knowledge into a systems biological model for analysis of the complete system.

To develop and test our approach we used the bacterial photosynthetic apparatus. But even for the "boringly" well-known system, many of the detailed kinetic constants were unknown. By comparing the behavior of the complete system to time-dependent experiments, we could determine the values and sensitivities of all parameters of our model. The thus parametrized protein modules allowed for new insights into their inner working and can be re-used to set up other, related systems.

BP 30.5 Thu 17:00 H44

About scaling in the growth of clubs and communities — LU XIN¹, DIEGO RYBSKI², and ●FREDRIK LILJEROS¹ — ¹Department of Sociology, Stockholm University, S-106 91 Stockholm, Sweden — ²Potsdam Institute for Climate Impact Research, P.O. Box 60 12 03, 14412 Potsdam, Germany

Many systems comprise emergent power-laws in the growth rates with respect to the size of the units such as companies or cities. Here we study online communities and investigate the growth properties of clubs and social communities. We find power-law relations for the average growth rate and for the standard deviation. The quality of the data permits to analyze the growth – complementary to (temporal) correlations – on the basis of individuals behaving in a social context.

BP 31: Posters: Membranes and Vesicles

Time: Thursday 17:15–20:00

Location: Poster B1

BP 31.1 Thu 17:15 Poster B1

Investigation of Erythrocytes Cell-Cell Adhesion using Holographic Optical Tweezers — ●PATRICK STEFFEN and CHRISTIAN WAGNER — Universität des Saarlandes, Saarbrücken

In the classical model, the role of red blood cells (erythrocytes) in blood clot formation is thought to be passive. It is supposed that they get caught into a fibrin-network, generated in the clotting process, just for reasons of geometrical restrictions. Additionally, it is commonly

believed that there exist no adhesion forces among the cells. The main part in clot formation take activated platelets. Lysophosphatidic acid (LPA) is a messenger released from these activated platelets. Treating red blood cells (RBC) with LPA leads to a Ca²⁺ influx into the cells. The consecutive rise of internal calcium level activates the Scramblase protein whereby the negatively charged Phosphatidylserine (PS) gets to the outer leaflet of the cell membrane. Thus the objective is to investigate the contribution of red blood cells in blood clot formation.

In order to test this hypothesis we built up an integrated microfluidic holographic optical tweezers setup to study this cell adhesion. Measurements with LPA and the calcium Ionophor A23187 showed that by this increased intracellular calcium level an adhesion of the cells among each other occurs. Thus, we postulate that the response of RBCs on LPA reveals a direct and active participation of these cells in blood clot formation.

BP 31.2 Thu 17:15 Poster B1

Near membrane particle fluctuations and single receptor bindings — ●TIM MEYER¹, HOLGER KRESS², and ALEXANDER ROHRBACH¹ — ¹Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany — ²Yale University, New Haven, USA

The usage of optical traps combined with arbitrary microscopy methods has a decisive advantage especially in biology: rare events can be turned into frequent events by bringing e.g. interaction partners into close proximity to each other. New insights especially in cell biology are enabled by recording the relevant processes in a small volume at ultra-high speed and with nanometer precision. Here we investigate phagocytosis, which is the process by which bacteria are internalized into macrophages. This process, which is a central mechanism in the immune system, was so far mainly investigated by conventional light and electron microscopies. However, its mechanical properties were barely known up to now. The motion of an optically trapped bead was tracked interferometrically in 3D with nanometer precision at a microsecond timescale. The measurement of the thermal bead fluctuations during the binding to the cell membrane enabled the observation of individual receptor-ligand bond formation. Comparison with Brownian Dynamic Simulations confirm the feasibility of several new types of experiments, which enable fast and precise images of local interactions - information which is not accessible with current light microscopy techniques!

BP 31.3 Thu 17:15 Poster B1

Oscillations in the lateral pressure of lipid monolayers induced by the second messengers MARCKS and Protein Kinase C — ●SERGIO ALONSO¹, MARKUS BÄR¹, UNDINE DIETRICH², and JOSEF A. KÄS² — ¹Physikalisch-Technische Bundesanstalt, Berlin, Germany — ²University of Leipzig, Leipzig, Germany

The binding dynamics of the peptide MARCKS to the lipid PIP2 modulated by protein kinase C leads to damped oscillations in lateral pressure of a lipid monolayer. These periodic dynamics can be attributed to changes in the crystalline lipid domain size. We elaborate a mathematical model to explain the observations based on the changes in the physical structure of the monolayer by the translocation of MARCKS peptides. The model equations are numerically integrated and reproduce the experimental observations.

BP 31.4 Thu 17:15 Poster B1

Multi-Bilayer Substrates for Cellular Mechanosensing Assays — ●PHILIPP RAUCH¹, DANIEL MINNER², LYDIA WOITERSKI¹, JOSEF KÄS¹, and CHRISTOPH NAUMANN² — ¹Universität Leipzig, Germany — ²Indiana University, Indianapolis, USA

Many processes in cell motility, morphogenesis and differentiation are influenced by mechanical signals and responses from the cellular environment. Similar mechanisms can be found in different types of cells, amongst others in neuroblasts moving to their final location in the brain, in fibroblasts responding to mechanical properties of the surrounding or in mesenchymal stem cells during differentiation. The development of in vitro systems to investigate the underlying mechanisms has been in focus of many research groups in different fields. Most present assays are based on functionalized hydrogels or polymeric substrates with variable elasticity which mimic the extracellular matrix. A viscous or viscoelastic environment, however, as it is found in organic tissue and especially in cell-cell contacts cannot be implemented with these methods. In order to overcome these limitations we developed and tested multi-stacked tethered lipid bilayer substrates with adjustable viscosity suitable for cell adhesion. The lateral mobility of lipid molecules in these layers can be varied from values close to the reduced diffusion in a typical fibroblast plasma membrane to that of a free floating bilayer. As we could show, different cell types respond to subtle changes within that range through altered morphology and growth behavior. Details of the composition and manufacturing process as well as the physical properties of the novel system will be presented.

BP 31.5 Thu 17:15 Poster B1

Microarray device for local electric recording of planar lipid bilayers — ●THERESA KAUFELD and CHRISTOPH F. SCHMIDT — Drittes Physikalisches Institut, Georg-August-Universität Göttingen

Mechanosensitive ion channels play an important role in cell function. They are involved in cell communication and act as emergency release valves to regulate osmotic pressure in cells. In order to understand their function and gating behaviour they can be reconstituted in artificial lipid bilayers and examined with electrophysiological and optical techniques such as single-channel recording and light microscopy.

We have here designed a device for simultaneous electrical recording, fluorescence microscopy and optical trapping experiments to stimulate and characterize the opening of mechanosensitive channels. We form phospholipid bilayers on microfabricated porous silicon substrates because they combine the stability of solid supported membranes and the accessibility to both sides of the bilayer, which is necessary for electrical recordings. We produced a microchip for electrical recording using standard cleanroom techniques.

Apertures of micrometer size were etched into a silicon substrate forming porous microarrays. To electrically isolate the substrate, an oxide layer was grown by thermal oxidation. Integrated Ag/AgCl electrodes surrounding each microarray were fabricated by vapour deposition to make them individually addressable for electrical recordings and to be able to switch between the microarrays during the measurement.

BP 31.6 Thu 17:15 Poster B1

An in-house x-ray scattering study of membrane fusion intermediates: Sample environment and the effect of cholesterol — ●TOBIAS REUSCH, SEBASTIAN AEFNER, BRITTA WEINHAUSEN, and TIM SALDITT — Institute for X-ray Physics, Göttingen, Germany

We have developed an x-ray scattering setup which allows to study membrane fusion intermediates or other nonlamellar lipid mesophases by laboratory-scale x-ray sources at quasi arbitrary degrees of hydration.

We report results of a study of pure lipid bilayers and phospholipid/cholesterol binary mixtures. Stalks, putative intermediate structures occurring during the membrane fusion process, can clearly be identified from reconstructed electron density maps. The choice of phases corresponding to the observed diffraction peaks can be narrowed down substantially by the application of the swelling method.

Phase diagrams of the lyotropic phase behavior of DOPC/cholesterol and DPhPC/cholesterol samples are presented. If cholesterol is present in moderate concentrations, it can substantially promote the formation of stalks at higher degrees of hydration or lower osmotic pressure respectively.

BP 31.7 Thu 17:15 Poster B1

Monte Carlo simulation of two-component membranes: Phase separation dynamics and anomalous diffusion — ●JENS EHRIG, EUGENE P. PETROV, and PETRA SCHWILLE — Biophysics, BIOTEC, TU Dresden, Tatzberg 47/49, 01307 Dresden

Anomalous subdiffusion is an intriguing phenomenon frequently observed in cell membranes, e.g. in SPT, FCS, and FRAP experiments. It is usually ascribed to the presence of membrane heterogeneities with dimensions below the optical resolution limit. In order to understand how the sub-micrometer-scale phase separation in the cell membrane can affect the lipid diffusion and manifest itself experimentally, we carry out dynamic Monte Carlo simulations of a two-component lipid membrane (DMPC/DSPC) with the size on the micrometer scale over time intervals of order of a second. Our model correctly reproduces the thermodynamic properties, as well as the phase diagram of the lipid mixture. Upon an abrupt temperature quench of the system into the two-phase coexistence region of the phase diagram, a power-law domain growth is observed, as predicted theoretically and observed experimentally. For certain ranges of the membrane compositions and temperatures it is found that the Brownian motion of lipid molecules shows strong deviations from the normal diffusion law. In cases where the membrane shows critical fluctuations, results of simulated single particle tracking and fluorescence correlation spectroscopy experiments show transient subdiffusion behavior spanning several orders of magnitude in time.

BP 31.8 Thu 17:15 Poster B1

Conformation of DNA molecules adsorbed on free-standing cationic lipid membranes — ●CHRISTOPH HEROLD, EUGENE P. PETROV, and PETRA SCHWILLE — Biophysics, BIOTEC, TU Dres-

den, Tatzberg 47/49, 01307 Dresden

We study ds-DNA fragments (5, 10, 20, and 48 kbp) electrostatically adsorbed on free-standing lipid membranes consisting of zwitterionic DOPC with added fractions of cationic DOTAP (1–10%). The free-standing bilayers are modeled using giant unilamellar vesicles of sizes $> 100 \mu\text{m}$. We found that DNA molecules are initially adsorbed on the cationic membrane in a coil conformation (gyration radius of ca. $2 \mu\text{m}$ for 48 kbp DNA) and then collapse into globules with a size below the optical resolution limit (gyration radius of ca. $0.3 \mu\text{m}$). The fraction of collapsed DNA globules depends on the cationic lipid concentration and the DNA fragment length. DNA collapse is favored for high DOTAP concentration and long DNA fragments. At low DOTAP concentration and for shorter DNA fragments a coexistence of DNA molecules in coil and globule conformation is observed. We present results of a systematic study of this phenomenon using fluorescence video microscopy with single particle tracking.

BP 31.9 Thu 17:15 Poster B1

Acyl chain correlation at the lamellar-to-rhombohedral phase transition in phospholipid membranes — ●BRITTA WEINHAUSEN, SEBASTIAN AEFNER, and TIM SALTIT — Institute for X-ray Physics, Göttingen, Germany

The poster has been withdrawn.

BP 31.10 Thu 17:15 Poster B1

Panta Rhei – Flow Behaviour in Phospholipid Membranes — ●SEBASTIAN BUSCH¹, CHRISTOPH SMUDA², LUIS CARLOS PARDO³, and TOBIAS UNRUH¹ — ¹Physik Department E13 and Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, Lichtenbergstraße 1, 85748 Garching bei München — ²Institut für Pharmazeutische Wissenschaften, ETH Zürich, CH-8093 Zürich — ³Grup de Caracterització de Materials, ETSEIB, Universitat Politècnica de Catalunya, E-08028 Barcelona

The long-range motion of phospholipid molecules in the membrane has been of major interest for many years not only because of its importance for processes in the cell membrane but also the puzzling fact that short- and long-time techniques observed vastly different mobilities: Neutron scattering experiments observed much faster motions on the picosecond time scale than macroscopic techniques.

We show that our new high-precision quasielastic neutron scattering experiments are compatible with recent molecular dynamics simulations which propose a flow-like motion of the phospholipid molecules on short times. The difference of observed mobilities can be explained by the transition from this ballistic regime to normal diffusive behaviour.

The influence of additives on the phospholipid mobility, measured on the same time scale, will also be briefly addressed.

BP 31.11 Thu 17:15 Poster B1

Lipid bilayers interacting with polymer chains: A Monte Carlo study — ●MARCO WERNER^{1,2} and JENS-UWE SOMMER^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden, Germany — ²Technische Universität Dresden - Institute for Theoretical Physics

We consider the interaction of amphiphile bilayers and polymer chains by a lattice based Monte Carlo method using the Bond Fluctuation Model [I. Carmesin and K. Kremer, 1988, *Macromol.* 21:2819]. To take advantage of the efficiency of this coarse graining method, we introduce explicit solvent to mediate the amphiphilic interactions. Therewith we observe stable bilayers spanned over the periodic boundary, which are formed spontaneously from a random initial state. We also obtain self-organized vesicles appearing in non-periodic boxes. By variation of bending stiffness for the hydrophobic tails we test the model to reproduce the crystalline phase as observed experimentally. We investigate the interactions between lipid bilayers and polymer chains for various chain lengths, chain densities and chain-solvent interactions. Our simulations show that hydrophobic chains are trapped within the hydrophobic layer of the membrane by changing conformations from dense globules into quasi 2D swollen coils. Manipulations of lipid bilayers using polymer chains can have interesting applications for drug delivery systems.

BP 31.12 Thu 17:15 Poster B1

Hydrodynamic interaction of particles in scanning line optical tweezers — ●BENJAMIN TRÄNKLE¹, MICHAEL SPEIDEL², and ALEXANDER ROHRBACH¹ — ¹Lab for Bio- and Nano-Photonics, University of Freiburg, Germany — ²Sick-Stegmann, Donaueschingen, Germany

In living cells, the distance of reaction partners determines whether biological processes take place or not. This is especially the case for the fusion of vesicles. Physical interactions within the cell, i.e. hydrodynamic and entropic forces play a crucial role in this context since the motion of vesicles is confined by the size of compartments inherent to the cell structure. Therefore, we are studying the dynamic interaction of at least 2 particles diffusing within a confined volume by using an optical trapping potential. This model system allows the particles to get in close contact to one another due to Brownian position fluctuations. The system is realized by an oscillating optical trap, with a scanning frequency up to 5 kHz and a lateral extension of about $10 \mu\text{m}$. The laser power is modulated while scanning. Thereby an elongated optical potential is generated. Artificially created volumes can simulate the cell compartments and the confined motion of particles within these bounding walls is expected to be influenced due to interaction potentials. By scanning the particles, their 3D position is obtained by back focal plane interferometry and recorded with up to 10 kHz. The particle trajectories can now be used to calculate the interaction potential and hydrodynamic coupling.

BP 31.13 Thu 17:15 Poster B1

formation of planar lipid bilayer in a microfluidic chip — ●JEAN-BAPTISTE FLEURY¹ and RALF SEEMANN^{1,2} — ¹Experimental Physics, Saarland University, D-66123 Saarbrücken, Germany — ²Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany

We propose a new microfluidic approach to produce extremely stable planar lipid bilayer (until days), which can be directly observed with high optical quality. We demonstrate the formation of planar lipid bilayer by producing membrane domains as report in the literature [1]. This method furthermore provides a convenient tool for the analysis of self organization properties of proteins (or other active compounds) which are embedded into planar lipid bilayer, as we will demonstrate explicitly using gold nanoparticles.

[1] S. Mukherjee and all. *Annu. Rev. Cell Dev. Biol.* 20, 839 866 (2004).

BP 31.14 Thu 17:15 Poster B1

Conformation of adhesion clusters — ●DANIEL SCHMIDT¹, UDO SEIFERT¹, and ANA-SUNCANA SMITH^{1,2} — ¹II. Institut für theoretische Physik, Universität Stuttgart — ²Institut für Theoretische Physik I, Universität Erlangen-Nürnberg

We model domains of ligand-receptor bonds that form when a membrane adheres to a functionalized substrate. The aim is to determine the optimum organization of bonds when the bonds maintain lateral mobility. The bonds are modeled as harmonic springs that are organized on a hexagonal or central hexagonal lattice. The membrane is described by the Helfrich free energy in the Monge representation whereas the nonspecific interaction with a wall is modeled by a harmonic well set at a well defined distance from the wall. The results of our modeling emerge from a variation of the total free energy, and provide both, the optimum membrane conformation and the appropriate spring deformation. We find that depending on both, the stiffness of the membrane and the springs there are three possible outcomes:

- (i) densely packed domains when the bonds try to minimize their distance,
- (ii) dilute clusters of bonds where optimum distance between the bonds is found,
- (iii) unstable domains.

Such results are in good agreement with recently performed experiments on avidin carrying vesicles that adhere to neutravidin carrying substrates.

BP 31.15 Thu 17:15 Poster B1

The role of diffusion on specific adhesion — ●TIMO BIHR, ELLEN REISTER, and UDO SEIFERT — Uni Stuttgart, II. Institute for Theoretical Physics

We analyse the adhesion of a flexible membrane to a flat substrate. Between the substrate and the membrane acts a confining potential in addition to reactions between receptors and ligands. The ligands in the membrane diffuse freely while the positions of the receptors in the substrate are kept fixed. The backbone of the receptor is modelled as a spring. The membrane fluctuations are described by a Langevin-Equation, which is numerically integrated in our simulation, the diffusion of the ligands is simulated by a simple random walk, and the reaction rate between ligands and receptors depends on the binding energy and the distance between receptor and ligand.

In equilibrium we find that higher binding energies are required to sustain adhesion than in models with fixed ligand positions because of a higher entropy contribution to the free energy. The simulations were run for different ligand concentrations, diffusion constants, reaction rates, binding energies and strain energies of the receptor. The adhesion process depends crucially on the diffusion constant of the ligands. For high diffusion constants bond clusters develop while for low diffusion constants bonds form independently from each other. This effect also has an influence on the average height of the membrane because evenly spread bonds pull the membrane closer to the substrate than bonds that are concentrated in one region.

BP 31.16 Thu 17:15 Poster B1

Observing the growth of lipid droplets in vivo and in vitro — ●MÁRIA HANULOVÁ and MATTHIAS WEISS — Cellular Biophysics Group, DKFZ, Im Neuenheimer Feld 280, 69120 Heidelberg

Lipid droplets (LD) are fat deposits of cells. In simple terms, they are balls of triglycerides (TG) and cholesteryl esters (CE) surrounded by a phospholipid monolayer into which proteins are embedded. Lipid droplets store excess fatty acids, release them in case of need, and are linked to many metabolic diseases. As of yet, the biogenesis and growth of LDs is poorly understood. According to the most popular model, TG and CE are synthesized at the endoplasmic reticulum (ER) and self-assemble as a globule between the leaflets of the ER membrane. Most likely, LDs then pinch off and carry away lipids from the ER membrane as a protecting monolayer. The growth of LDs has been hypothesized to rely on two (not mutually exclusive) mechanisms: (i) fusion with other LDs, or (ii) acquisition of newly synthesized lipids. To approach this problem, we observed the growth of lipid droplets in living HeLa cells by time-resolved confocal microscopy. Additionally, we used time-resolved fluorescence correlation spectroscopy in vitro to validate the physical possibility of fusion of lipid droplets. These experimental results are in favorable agreement with large-scale simulations

of ours.

BP 31.17 Thu 17:15 Poster B1

Computer simulations of membrane fusion — ●SANDRA FRANK — Universität Göttingen

Fusion of membranes is a universal phenomenon belonging to the basic physiology of higher cells. The process of fusion is essential for a multitude of biological processes like synaptic release, viral infection, and trafficking within cells. We use coarse-grained computer simulations to investigate membrane fusion depending on membrane tension and density of proteins or hydrophobic mismatch between protein and membrane.

BP 31.18 Thu 17:15 Poster B1

Mechanics of Small Unilamellar Vesicles — ●SAI LI, FREDERIC EGHIAIAN, and IWAN SCHAAP — III. Physikalisches Institut, Georg-August-Universität, 37077 Göttingen, Germany

Lysosomes, enveloped viruses, synaptic and secretory vesicles are all examples of natural nano-containers (diameter ~ 100 nm) which specifically rely on their lipid bi-layer to protect and exchange their contents with the cell. We have developed methods primarily based on atomic force microscopy that allow precise investigation of the mechanical properties of these vesicles. The mechanical properties of small, spherical vesicles were probed by applying very low forces (0.1-0.3 nN), which led to a maximum 30 % deformation. The effects of lipid composition, temperature, osmotic pressure and the radius of curvature were studied for liposomes with diameters between 30 and 150 nm. In order to extract the lipid bi-layer elastic constants we used finite element methods to model the measured deformations. The elastic constants we found for the lipid bi-layer were in very good agreement with previously reported experiments on micrometer-sized giant vesicles. We will discuss the effects of parameters that increase the stiffness in relation to the high curvature of the vesicles.

BP 32: Posters: Physics of Cells

Time: Thursday 17:15–20:00

Location: Poster B1

BP 32.1 Thu 17:15 Poster B1

Intra- and intercellular fluctuations in Min protein dynamics decrease with cell age — ●ELISABETH FISCHER-FRIEDRICH¹, GIOVANNI MEACCI², JOE LUTKENHAUS³, HUGUES CHATE⁴, and KARSTEN KRUSE⁵ — ¹Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — ²IBM T. J. Watson Research Center, P.O. Box 218, Yorktown Heights, NY 10598 — ³Department of Microbiology, Molecular Genetics, and Immunology, University of Kansas Medical Center, Kansas City, Kansas 66160 — ⁴CEA-Saclay, Service de Physique de l'Etat Condensé, 91191 Gif-sur-Yvette, France — ⁵Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

Self-organization of proteins in space and time is of crucial importance for the functioning of cellular processes. Often, this organization takes place in the presence of strong random fluctuations due to the small number of molecules involved. We report on stochastic switching of the Min-protein distributions between the two cell-halves in short *Escherichia coli* cells. A computational model provides strong evidence that the macroscopic switching is rooted in microscopic noise on the molecular scale. In longer bacteria, the switching turns into regular oscillations that are required for positioning of the division plane. As the pattern becomes more regular, cell-to-cell variability also lessens, indicating cell age-dependent regulation of Min-protein activity.

BP 32.2 Thu 17:15 Poster B1

High-speed dynamics of helical bacteria trapped in a light tube. — ●MATTHIAS KOCH and ALEXANDER ROHRBACH — University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

The helical bacterium *Spiroplasma melliferum* is a wall-less bacterium, where genome reduction has left these bacteria with a minimal set of genes - sufficient for independent life and self-reproduction. As a consequence they have an extreme structural simplicity and are among the smallest cells in size (~ 200 nm thin, 3-5 μ m long). However, they infect various plants and insects and thereby do tremendous harm to agriculture industry. Their motility, defined by helicity changes, kinking and propelling is very complex, and enables propagation in com-

plex environments. However, it is unclear how this ~ 500 gene machine works. Which molecular motors and which filament proteins cooperate at which forces on which time scales? What are the energetic of this apparatus and how do they change during external disturbances. We try to answer these questions by optically trapping the whole bacterium in a light tube, which consists of a high speed scanning line optical trap. Although propelling and kinking, the bacterium remains in the focal plane and can thereby be observed with video microscopy. In addition, trapping light scattered at the slopes of the helix gives precise 3D information about its dynamics, which is analyzed and modelled with Fourier-techniques. We show experimental results, including energies and forces involved in motility, and compare them to simulation data. Further, we present a first model of how this minimal machine could work and which amount of power it needs for self-propulsion.

BP 32.3 Thu 17:15 Poster B1

Elucidating the interaction of misfolded proteins with the quality control machinery in the endoplasmic reticulum — ●NINA MALCHUS and MATTHIAS WEISS — DKFZ, Heidelberg, Germany

A multitude of transmembrane proteins enter the endoplasmic reticulum (ER) as unfolded polypeptide chains. During their folding process they interact repetitively with the ER's quality control machinery. Here, we have used fluorescence correlation spectroscopy to probe these interactions for a prototypical transmembrane protein, tsO-45-G, in vivo [1]. While both, folded and unfolded tsO-45-G showed anomalous diffusion, the unfolded protein had a significantly stronger anomaly. This difference subsided when unfolded tsO-45-G was in a complex with its chaperone calnexin, or when a mutant form of tsO-45-G with only one glycan was used. Our experimental data and accompanying simulations suggest that the folding sensor of the quality control (UGT1) oligomerizes unfolded tsO-45-G, leading to a more anomalous/obstructed diffusion. In contrast, calnexin dissolves the oligomers, rendering unfolded tsO-45-G more mobile, and hence prevents poisoning of the ER. Additionally, we performed computer simulations to investigate the origin of the spread in the anomaly obtained from FCS

experiments on membranes [2].

[1] N. Malchus & M. Weiss, submitted.

[2] N. Malchus & M. Weiss, J. Fluoresc., in press.

BP 32.4 Thu 17:15 Poster B1

Cell Monolayer Rheology — ●MATHIAS SANDER and ALBRECHT OTT — Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken

The mechanics of living cells is a major determinant of cell behaviour (e.g. in wound healing, cell differentiation). Understanding its underlying principles would add to cell biology, medicine and biophysics. Here we use "Cell Monolayer Rheology (CMR)", which determines the properties of a monolayer of approximately 10^6 cells with the help of a commercial rheometer. This allows us an improved definition of cell-mechanical responses. As for dead matter, it is often assumed that cells respond linearly within certain ranges of mechanical stimuli. However, the highly complex and dynamic structure of the cytoskeleton, which mainly governs the cellular mechanical properties, suggests a more subtle mechanical behaviour. Therefore, in our experiments, we focus on the non-linear response of a cell monolayer. Another important topic is the rheological study of inorganic layers as adhesion-promoting surface coatings. These can serve as an alternative to usual protein coatings. We investigate the different coatings with respect to their adhesion properties using the CMR-technique.

BP 32.5 Thu 17:15 Poster B1

The contribution of microtubules to the mechanical properties of cells — ●KENECHUKWU DAVID NNETU, TOBIAS KIESSLING, ROLAND STANGE, ANATOL FRITSCH, and JOSEF KÄS — University of Leipzig, Institute of Experimental Physics I, Linnéstr. 5, 04103, Leipzig

A cell as a complex system is made up of various subcellular structures that allows it to sense and react to its environment. While a lot of studies on the mechanical properties of cells have been done with adherent cells, little is known about the behaviour of cells in suspension. Although the state of suspension is not the most physiological, cells do sometimes find themselves in suspension for example during cancer metastasis as they move to other parts of the body through the blood and lymph vessels. Using the microfluidic optical stretcher that probes the mechanical properties of cells in suspension we studied the effect of the drugs Taxol and Latrunculin A. This allows a deeper insight into the contribution of microtubules to cellular mechanics.

BP 32.6 Thu 17:15 Poster B1

The automated Microfluidic Optical Stretcher — ●ROLAND STANGE, TOBIAS KIESSLING, BERND KOHLSTRUNK, and JOSEF A. KÄS — University of Leipzig, Institute of Experimental Physics I, Linnéstr. 5, 04103 Leipzig

Measuring the deformability of biological cells can be done in different ways. The most accurate one is the optical deformability measurement with the microfluidic optical stretcher. Due to the optical differences of each single living cell the scattering of the result has to be compensated with large numbers of measurements. According to the fact that the optical stretcher is operating with suspended cells in microfluidic channels it is complicated to handle by hand and time consuming to get precise and reliable data.

To improve the way of measuring the optical deformability we fully automated the optical stretcher by using a Labview program to control the flow pumps, the lasers and the camera. The produced data is then automatically evaluated by a Matlab program which finds out the deformation values from the images by an edge detection process. Furthermore the computer controlled microfluidic and photo lithographic produced measure chambers allow us to get different parameters out of the cell and sort them after measurement in a precisely controllable way.

BP 32.7 Thu 17:15 Poster B1

Living cell interactions with nanostructures — ●FELIX KEBER, PHILIPP PAULITSCHKE, EVA WEIG, and DORIS HEINRICH — Fakultät für Physik und CeNS, LMU München, Germany

Cellular function is triggered by intracellular signaling cascades on small temporal and spatial scales. One prime example is cell migration, a process which is induced by actin polymerization, and which results in cellular force exertion in three dimensional environments. Cell migration reflects the cellular microarchitecture, as a complex interplay of cellular force exertion by actin polymerization pattern dynamics. We

investigate interactions of living cells with top-down-fabricated micro- and nanostructures. Our focus is set on the change in intracellular actin distribution as a reaction to our structured sample.

BP 32.8 Thu 17:15 Poster B1

Relating Cell Deformability to Cell Migration — ●FRANZISKA LAUTENSCHLAEGER¹, JOAKIM DA-SILVA¹, MICHAEL BEIL², and JOCHEN GUCK¹ — ¹Dep. of Physics, University of Cambridge, UK — ²Dep. of Internal Medicine I, University of Ulm, Germany

Mechanical properties of cells, mainly defined by the cytoskeleton, are closely related to cell function and can be measured with a dual-beam laser trap (Optical Stretcher). Functional changes which go hand in hand with changes of the cytoskeleton also occur during differentiation of stem cells. This suggests monitoring differentiation by the changing mechanical deformability of the cells. As a proof of principle, we compared the deformability of a haematopoietic precursor cell line (NB4) to ATRA differentiated NB4 cells. The differentiated cells were significantly softer. Surprisingly, the deformation behaviour of ATRA differentiated NB4 cells was not altered after treatment with the microtubule stabilizing drug Paclitaxel. In contrast, the relaxation after stress application changed significantly. In order to relate these rheology experiments to cell migration, all three cell types were observed migrating into 5µm large channels. It was observed that undifferentiated NB4 cells were not able to migrate into these channels, contrary to differentiated NB4 cells and cells treated with taxol. Differences between the two latter have been found in the time the cells needed to migrate fully into the channel. This result correlates cell deformability measurements and cell migration measurements and might constitute an explanation for a syndrome occurring in leukemia patients after treatment with ATRA.

BP 32.9 Thu 17:15 Poster B1

Mechanosensing by neurons and glial cells — ●KRISTIAN FRANZE^{1,2}, HANNO SVOBODA², POURIA MOSHAYEDI^{1,3}, ANDREAS F. CHRIST¹, JAMES FAWCETT³, CHRISTINE E. HOLT², and JOCHEN GUCK¹ — ¹Department of Physics, Cavendish Laboratory, University of Cambridge, UK — ²Department of Physiology, Development and Neuroscience, University of Cambridge, UK — ³Brain Repair Center, University of Cambridge, UK

Nervous tissue is densely packed with different types of cells. All these building blocks differ in their mechanical properties. Here we show how neurons and glial cells respond to the compliance of their environment. Primary retinal ganglion cells, astrocytes, and microglia were cultured on polyacrylamide gels with shear moduli between 0.1 and 30 kPa, and quantitative morphometric analysis was used to evaluate cell responses to the mechanically different substrates. While astrocytes and microglia cultured on stiffer substrates showed increased perimeter, area, diameter, elongation, number of extremities and overall complexity if compared to those cultured on more compliant substrates, the lengths and branching patterns of neuronal processes were not significantly changed. However, when cultured on substrates with a stiffness gradient, neurons preferentially grew towards soft. The observed cellular behavior may explain why glial scars formed after traumatic injury to the central nervous system impede neuronal regeneration. Ultimately, this impediment might be circumvented by using neural implants that incorporate mechanical properties based on our findings.

BP 32.10 Thu 17:15 Poster B1

Integrin alpha5beta1 increased cell invasion through enhanced contractile forces — ●CLAUDIA TANJA MIERKE¹, BENJAMIN FREY³, MARTINA FELLNER¹, MARTIN HERRMANN², and BEN FABRY¹ — ¹University of Erlangen, Biophysics Group — ²University Hospital Erlangen, Dpt. Internal Medicine III — ³University Hospital Erlangen, Dpt. Radiation Oncology

Cell motility is a fundamental biomechanical process in tumor growth and metastasis formation. Cell migration through dense connective tissue usually requires firm adhesion to the extracellular matrix through integrins. For some tumors, increased integrin expression is associated with increased malignancy and metastasis formation. Here, we studied the invasion of cancer cells with different α5β1 integrin expression levels into dense 3-D collagen fiber matrices. Using a cell sorter, we isolated α5β1-high and α5β1-low expressing sub cell lines from parental MDA-MB-231 breast cancer cells. Cells with higher α5β1 expression showed significantly (3-fold) increased cell invasiveness, whereas knock-down of the α5 integrin subunit lead to decreased tumor cell invasion. Interestingly, knock-down of the collagen receptor integrin subunit α1 did not alter invasiveness, indicating that the effect is integrin-type spe-

cific. Fourier transform traction microscopy revealed that the a5b1-high expressing cells generated 5-fold larger contractile forces. Cell invasiveness was reduced after addition of the myosin light chain kinase inhibitor ML-7 or the myosin II inhibitor blebbistatin in a5b1-high cells, but not in a5b1-low cells, suggesting that a5b1 integrins enhance cell invasion through enhanced generation of contractile forces.

BP 32.11 Thu 17:15 Poster B1

Increase of cell stiffness in single muscle cells from patients with primary desminopathies — ●NAVID BONAKDAR¹, PHILIP KOLLMANNBERGER¹, ROLF SCHRÖDER², and BEN FABRY¹ — ¹Center for Medical Physics and Technology, Biophysics Group, Dept. of Physics, University of Erlangen-Nuremberg, Erlangen, Germany — ²Institute of Neuropathology and Department of Neurology, University Hospital Erlangen, Germany

Desmin-related myopathies belong to the heterogeneous group of distal-onset skeletal myopathies characterized by large accumulation of desmin (IFs) (Goebel et al. 1997), which compromises the ability of desmin to assemble into intermediate filaments (Sjoberg et al. 1999). Myofibrillar myopathies (MFMs) are histopathologically characterized by desmin-positive protein aggregates and myofibrillar degeneration and are caused by mutations in genes encoding for extramyofibrillar proteins. The disease usually develops in the second to third decade of life with signs of muscle weakness in the lower extremities and sometimes the heart. (Schröder et al., 2007). The precise molecular pathways and sequential steps that lead from an individual gene defect to progressive muscle damage are still unclear. (Schröder et al. 2009) Here we present the results of rheological measurements of myoblasts with and without desmin aggregation. Cell rheology is measured using FN-coated beads forced in a high-force Magnetic Tweezers setup. Stiffness of cells with desmin aggregation is markedly increased, indicating that desmin is directly involved with mechanical cell alteration that may contribute to the progression of MFMs.

BP 32.12 Thu 17:15 Poster B1

Tumor cell invasion as a random walk with density dependent diffusivity — ●CLAUS METZNER, JULIAN STEINWACHS, FRANZ STADLER, MARTINA FELLNER, CLAUDIA MIERKE, ANDREAS KRONWALD, SEBASTIAN PROBST, and BEN FABRY — Biophysics Group, Department of Physics, University of Erlangen, Germany

An important problem in cancer research is to understand the migration of tumor cells through connective tissue. We investigate the invasion of a layer of carcinoma cells into a 3D collagen gel and measure the temporal development of the spatial cell distribution. The distributions do not resemble normal particle diffusion into a half space. In particular, a strong dependence on initial cell density is indicative of collective effects. We show that all characteristic features are captured by a simple model: cells detect the presence of close neighbors, form clusters, and have a reduced diffusion constant in this clustered state. By optimizing only three parameters, the diffusion constants and the detection range, quantitative agreement is obtained between measured and Monte-Carlo-simulated invasion profiles.

BP 32.13 Thu 17:15 Poster B1

Phase Transitions in Embryonic Development: How P-Granules Segregate — JÖBIN GHARAKHANI¹, ●CLIFFORD BRANGWYNNE^{1,2}, ANTHONY HYMAN², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany

In the nematode *C. elegans*, germ cells and their precursors carry P-granules which are aggregates of proteins and RNA. P-granules are important in the specification of germ line cells. During the first cell division of the fertilized egg, P-granules are segregated towards the posterior side and are subsequently found in the posterior daughter cell. A fundamental question is to understand the mechanisms of segregation during asymmetric cell division. It has recently been shown that P-granules segregate by preferentially nucleating and subsequently growing on the posterior side of the cell, thereby effectively localizing the granular material. This preferential condensation can be explained by a gradient which decreases the saturation point of this phase transition along the anterior-posterior axis of the cell. Using a simulation describing nucleation, droplet growth, and fusion, we study the P-granule segregation driven by a gradient of supersaturation in the cell.

BP 32.14 Thu 17:15 Poster B1

High-precision tracking of sperm swimming fine-structure provides strong test of resistive force theory — BENJAMIN M. FRIEDRICH^{1,3}, INGMAR H. RIEDEL-KRUSE^{2,4}, JONATHAN HOWARD², and ●FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany — ³Weizmann Institute of Science, Rehovot, Israel — ⁴Department of Bioengineering, Stanford University, Stanford, USA

Sperm cells are propelled in a liquid by regular bending waves of their whip-like flagellum. The shape of the flagellar wave determines the path along which a sperm cell swims. We have tested a simple hydrodynamic theory of flagellar propulsion known as resistive force theory: We conducted high-precision measurements of the head and flagellum motions during circular swimming of bull spermatozoa near a surface. We found that the fine-structure of sperm swimming represented by the rapid wiggling of the sperm head around an averaged path is, to high accuracy, accounted for by resistive force theory and results from balancing forces and torques generated by the beating flagellum. We determined the ratio between the normal and tangential hydrodynamic friction coefficients of the flagellum, to be 1.81 ± 0.07 (mean \pm s.d.). We also determined how the coarse grained curvature of the swimming path depends on the average curvature of the beat pattern. The observed ratio of these curvatures can be accounted for by resistive force theory. Hence, this theory accounts both for the fine-structure of sperm swimming as well as for the circular motion on larger scales.

BP 32.15 Thu 17:15 Poster B1

Theoretical and experimental studies of Protein Kinase C membrane translocation processes — ●MARTIN PEGLOW¹, MIKE BONNY¹, HEIKO RIEGER¹, KARSTEN KRUSE¹, and LARS KAESTNER² — ¹Theoretische Physik, Universität des Saarlandes, Campus, 66123 Saarbrücken — ²Institut für Molekulare Zellbiologie, Universitätsklinikum des Saarlandes, 66421 Homburg

Protein Kinase C α (PKC α) is a versatile key for decoding the cellular calcium toolkit. Once activated by cytosolic Ca²⁺ ions PKC α translocates to the plasma membrane and creates local patterns with limited spatial spread ($< 4\mu\text{m}$), the so-called local translocation events (LTEs). Two populations of LTEs exist, namely short lived events with lifetimes of 500-1500 ms and long lasting events with duration up to 10 seconds, which markedly exceeds the duration of the underlying calcium signals [1]. If we incorporate a possible interaction between membrane bound PKC α in our stochastic three-dimensional reaction-diffusion model, we can explain both LTE populations. In addition to our computer simulations, we perform fluorescence resonance energy transfer (FRET) measurements to give evidence for our assumption of a so far unknown interaction in between membrane bound PKCs molecules.

[1] Gregor Reither, Michael Schaefer, Peter Lipp, Journal of Cell Biology, 174, 521-533 (2006)

BP 32.16 Thu 17:15 Poster B1

Strain Dependent Cell Response to Optical Forces — ●TINA HÄNDLER, ROLAND STANGE, ANATOL FRITSCH, and JOSEF KÄS — University of Leipzig, Germany

The optical stretcher is a device to investigate global mechanical behavior of single cells in suspension. Cells are trapped between two counter-propagating laser beams. By increasing the laser power and hence the momentum transferred to the cell surface, the cells are measurably deformed. Since the cytoskeleton, a dynamic polymer network inside the cell, is responsible for cellular mechanical properties, changes in the cytoskeletal proteins are reflected in the cell's response to the stress applied.

For small deformations and low stresses, most of the cells deform viscoelastically. At higher stresses, some cells seem to respond actively to the applied forces and show contractive behavior. This temporary decrease in relative deformation can be observed by using a linearly increasing laser power. Modifying motor proteins and microtubules with chemical agents allows a differentiated investigation of the observed phenomena. The aim of the presented work is to explore the role of cytoskeletal components in possibly stress-induced active behavior.

BP 32.17 Thu 17:15 Poster B1

Cellular force generation and transmission in 3T3 fibroblasts — ●FLORIAN SCHLOSSER¹, DAISUKE MIZUNO², FLORIAN REHFELDT¹, and CHRISTOPH F. SCHMIDT¹ — ¹Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany — ²Organization for the Promotion of Advanced Research, Kyushu Univ., Fukuoka, Japan

Biological cells constantly communicate with their environment. Besides biochemical interactions, cells can also sense their mechanical micro-environment and external forces. Key players in the mechanosensing and -transduction processes are acto-myosin stress fibers that generate contractile forces.

To elucidate the mechanistic details of the physical interactions between cells and their surrounding, we use a dual optical trap to perform high-resolution measurements of cellular force fluctuations. Monitoring the displacement fluctuations of two fibronectin-coated beads attached to opposite sides of a cell and analyzing their correlated motions in conjunction with active probing of the cell with oscillating forces allows us to measure simultaneously the overall forces the cell generates and the fraction of that force transmitted to the environment. We present data of force fluctuations and cell stiffness of 3T3 fibroblasts obtained by such active and passive microrheology measurements. To distinguish non muscle myosin II - based activity from other effects, we used blebbistatin, a potent and specific inhibitor of non-muscle myosin II.

BP 32.18 Thu 17:15 Poster B1

Biomechanical Data Networks — ●TOBIAS R. KIESSLING, KENECHUKWU D. NNETU, ANATOL FRITSCH, ROLAND STANGE, and JOSEF A. KÄS — University of Leipzig, Institute of Experimental Physics I, Linnéstr. 5, 04103 Leipzig, Germany

The transition from benign tissue to malignant cancer is accompanied by various alterations of the cellular organization, amongst others of the cytoskeleton. This highly dynamic polymer network provides both, functional and mechanical stability to cells whereas small changes of the cytoskeletal composition are reflected in alterations of the mechanical properties of cells.

The Microfluidic Optical Cell Stretcher, built to monitor these cytoskeletal changes provides a fast and easy access to a range of physical parameters of thousands of cells. Methods derived from gene expression network analysis techniques will be discussed that help to reveal unbiased relations between measured physical properties and how these can be used to differentiate between benign and malignant cells without the need of any molecular marker.

BP 32.19 Thu 17:15 Poster B1

Quantification of hematopoietic stem cell and neutrophil chemotaxis using microstructured systems and ELISA — ●CHRISTINA LEINWEBER¹, RAINER SAFFRICH², ANTHONY D. HO², NICOLE NIEMEIER³, KATJA SCHMITZ³, MICHAEL GRUNZE^{1,3}, and AXEL ROSENHAHN^{1,3} — ¹Applied Physical Chemistry, University of Heidelberg — ²Department of Medicine V, University of Heidelberg — ³IFG/ITG, Karlsruhe Institute of Technology

The migration of hematopoietic stem cells (HSC) towards bone marrow, the so called homing process, plays an important role in modern leukemia therapy. HSC are supposed to be guided by a concentration gradient of chemokines which are expressed by marrow cells, the mesenchymal stromal cells (MSC). Therefore we investigate the chemotactic response and migration behavior of HSC using different in vitro chemotaxis assays with increasing intricacy, e.g. migration experiments in microwells, transwells and within microstructured systems. These chip systems allow studying single parameters, such as migration kinetics, thresholds, sensing sensitivity and swarm behaviour, by varying the geometry of the microchannel structures. In order to establish the methods, particularly the microstructures, we also used neutrophil granulocytes differentiated from HL-60 cell line as a model system. Additionally we performed ELISA experiments to analyze the expression of the chemokine SDF-1 by MSCs, as SDF-1 is already known to be involved in the signalling process and most likely controls HSC migration. We determined the SDF-1 concentration in dependence on expression time and on MSC culture media.

BP 32.20 Thu 17:15 Poster B1

A precise and rapid UV laser ablation system for developmental cell biology studies — ●FELIX OSWALD and STEPHAN GRILL — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

We are presenting a state-of-the-art laser ablation system for use in cell biology studies. Diffraction-limited dissection of biological samples is achieved by coupling a pulsed ultraviolet laser (355 nm) to a conventional inverted microscope equipped with a confocal imaging system. With this setup, we can thus perform photo and plasma-induced ablation in areas up to 100 μm^2 and at high rates (500 Hz) by directing the beam with a fast mirror scanning system. Ablation experiments of the

myosin-actin cytoskeleton of *Caenorhabditis elegans* embryos demonstrates the versatility and power of such a nanoscalpel in probing the mechanical properties of cellular structures during development.

BP 32.21 Thu 17:15 Poster B1

4D-Tracking of pathogens by Digital In-line Holographic Microscopy — ●SEBASTIAN WEISSE¹, MATTHIAS HEYDT¹, NIKO HEDDERGOTT², MARKUS ENGSTLER², MICHAEL GRUNZE^{1,3}, and AXEL ROSENHAHN^{1,4} — ¹APC, University of Heidelberg — ²Zoology I, University of Würzburg — ³ITG, Karlsruhe Institute of Technology — ⁴IFG, Karlsruhe Institute of Technology

Digital Holographic Microscopy (DHM) using the in-line geometry is based on the original idea of Gabor's 'new microscopic principle'. An interference pattern containing the three dimensional information of the object encoded in phase and amplitude is recorded. Using computers, real space information about the object can be restored from these holograms applying a reconstruction algorithm. We built a portable, temperature-controlled holographic microscope to study the motion patterns of pathogenic microorganisms such as the blood parasite *Trypanosoma brucei*, the causative agent of African sleeping sickness under physiological conditions. The directed self-propulsion of Trypanosomes in the bloodstream of a mammalian host is essential for the clearing of immunoglobulins from the parasite's cell surface by hydrodynamic drag force. This mechanism is one of the parasite's strategies to evade the host's immune system and thus directly linked to pathogenesis. So far the motility studies on this unflagellated microorganism have only been carried out using standard 2D microscopy techniques. In our system parasites were tracked at varying temperatures and viscosities with high spatial and temporal resolution and the obtained 3D motion patterns statistically analyzed.

BP 32.22 Thu 17:15 Poster B1

High Resolution Growth Cone Actin Dynamics — ●MELANIE KNORR¹, TIMO BETZ², DANIEL KOCH³, and JOSEF KÄS¹ — ¹University of Leipzig — ²Institut Curie, Paris — ³Georgetown University, Washington D.C.

Neuronal growth is one of the fundamental processes in brain development and nerve regeneration. During growth, neuronal cells form long extensions, called neurites, which are guided toward their target sites by a motile structure at their tip, the so called growth cone. These growth cones are able to rearrange their cytoskeleton for directed growth, following very small guidance cues. Former research suggests amplification of these chemical signals via stochastic fluctuations of the leading edge of growth cones. Betz and Koch et al. already showed that the stochastic lamellipodium dynamics are determined by the interplay of actin polymerization, pushing the edge forward and molecular motor driven retrograde actin flow retracting the actin network. They identify switching of "on/off" states in actin polymerization as the main determinant of lamellipodial advancement. Further quantification of the suggested stochastic signal amplification, however, is limited by the spatial and temporal resolution of their imaging technique. Novel techniques and their realization are presented and discussed, able to detect the edge dynamics in higher temporal and spatial resolution.

BP 32.23 Thu 17:15 Poster B1

Vinculin regulates cell mechanical properties through src phosphorylation on its lipid anchor — ●NADINE LANG, GEROLD DIEZ, WOLFGANG GOLDMANN, and BEN FABRY — Biophysics Group, FAU Erlangen-Nürnberg, Germany

The focal adhesion protein vinculin links the actin cytoskeleton to integrin adhesion receptors. It has been reported that vinculin also binds to the lipid bilayer of the cell membrane. Vinculin with mutated or missing lipid binding regions leads to reduced focal adhesion turnover and decreased cell motility. We investigated whether this effect is directly caused by impaired lipid binding, or indirectly by mutations of residues on the lipid binding regions that are important for signaling. Vinculin has two lipid binding regions on its tail: one located on helix 3 has no phosphorylation sites, and another at the C-terminal (lipid anchor) which harbors a src-kinase regulated phosphorylation site at residue Y1065. Cells with mutations on helix 3 showed no change in stiffness (demonstrated by magnetic tweezer), in tractions (measured by traction microscopy) and in adhesion strength (determined by FN-coated bead detachment from the integrin receptor). In contrast, cells with missing lipid anchor or impaired lipid binding by mutating residues R1060 and K1061 showed strongly reduced stiffness, tractions and adhesion strength. Nearly identical behavior was observed if only the src phosphorylation site on the lipid anchor was mutated. These data show that

lipid binding of vinculin's anchor is required for vinculin's mechano-coupling function, which in turn is regulated via src phosphorylation. Thus, vinculin is an important signaling protein in the FAC.

BP 32.24 Thu 17:15 Poster B1

Interaction between nanoparticles and living cells with force spectroscopy — ●SEBASTIAN ZÜNKELER, DANIEL WESNER, KATJA TÖNSING, and DARIO ANSELMETTI — Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University

Nanotechnology is regarded as a key technology of the 21st century and nanotechnological systems are already used in many applications. However, the interaction between nanoparticles (NP) and living cells is not yet fully understood in the context of toxicology and need therefore additional characterization. To analyze these interactions with AFM force spectroscopy we have used an epoxide resin as adhesive for different metal oxide NP and attach aggregates which consist of primary particles to AFM-cantilevers. The characterization of the tip is possible with electron microscopy and the use of AFM and an inverse grid. We have shown that the used NP bind most likely unspecific to RLE-6TN rat lung cells. The number of rupture events increase with the contact time between tip and cell membrane and the measured rupture forces in the range of 50 pN depend mainly on micromechanical membrane properties.

BP 32.25 Thu 17:15 Poster B1

Collective organization and separation of multicellular systems — ●ANATOL FRITSCH, TOBIAS KIESSLING, FRANZISKA WETZEL, MAREIKE ZINK, and JOSEF KÄS — University of Leipzig, Germany

For the spatial organization of tissue in multicellular organisms the mechanical properties of single cells and their environment are of great importance. In embryogenesis cells have to migrate to their future destinations and furthermore collectively separate from other cell groups. Biomedical studies indicate that these compartments of cells have sharp borders keeping even cancerous cells from migrating across. From a physical point of view this may be explained with differences in surface tension, migration or mechanical stiffness of the cells.

We study the mechanical properties of primary tumor cells of different tissues using optical surface forces on single cells as well as their adhesion forces. Primary cells from different compartments or cell types are labeled and mixed to form a multicellular tumor spheroid. Active demixing of the different cell types can lead to sharp borders separating them, which is then correlated to the single cell data acquired in precedent studies.

BP 32.26 Thu 17:15 Poster B1

Structure and dynamics of stress fibers in 3T3 fibroblasts — ●CONSTANTIN SPILLE, TIL DRIEHORST, FLORIAN REHFELDT, and CHRISTOPH F. SCHMIDT — Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany

Mechano-sensing and force transduction play an essential role in many cellular processes but the microscopic mechanisms are not yet understood. Acto-myosin stress fibers are key players in the physical response to the mechanical micro-environment as demonstrated in recent studies of cells spreading on elastic substrates. Stress fibers are composite structures of actin bundles, cross-linked by alpha-actinin, and mini-filaments of non muscle myosin II (NMM II) that generate contractile forces.

We here present data, obtained by confocal microscopy, on the structure of stress fibers in 3T3 fibroblasts adhering to elastic substrates of varying stiffness. Staining fixed cells at different time points for actin, NMM IIa, and alpha-actinin, has allowed us to quantitatively analyze the influence of the mechanical properties of the surrounding on the cell's cytoskeleton and on the architecture of stress fibers.

BP 32.27 Thu 17:15 Poster B1

Mechanical characterization of primary cilia of epithelial cells — ●CHRISTOPHER BATTLE and CHRISTOPH F. SCHMIDT — Drittes Physikalisches Institut, Georg-August Universität, Göttingen, Germany

Recent studies have shown that the primary cilium, long thought to be a vestigial cellular appendage with no function, has remarkable sensory abilities. Of particular interest, from both a biophysical and medical standpoint, are the primary cilia in kidney epithelial cells, which have been demonstrated to act as tiny flow sensors. The cilia are lined with mechanosensitive TRP channels (PC2), which allow the influx of cations into the cell in response to mechanical stimuli. We explore the

mechanical response of this system using fluorescence microscopy and optical trapping techniques.

BP 32.28 Thu 17:15 Poster B1

Confined Intermediate Filament Fluctuations in Live Cells — ●JANNICK LANGFAHL-KLABES¹, JENS NOLTING¹, ALEXANDER EGNER², and SARAH KÖSTER¹ — ¹Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany — ²Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

The cytoskeleton, which provides mechanical strength for the cell, contains three different types of fibrous proteins. Besides actin and microtubules intermediate filaments (IFs) play an important role. IFs are extremely flexible biopolymers that can be stretched to several times their initial length. The key to these large deformations is their hierarchical structure, which facilitates cascaded deformation mechanisms at different levels of strain. The filamentous structures in live cells are by no means static but undergo excessive fluctuations and show dynamics on many different time scales. We investigate keratin intermediate filament networks which are believed to play a key role in cell mechanics. To this end we carry out time-lapse fluorescent live cell imaging experiments on genetically enhanced carcinoma cells. These model cells express fluorescent keratin which forms thick cytoplasmic bundles. We perform fluctuation analyses based on the worm-like-chain model to investigate the influence of thermal versus active motion and retrieve mechanical properties like persistence length and bending rigidity. Our results show that keratin bundles are strongly confined within the surrounding network. This observation is further confirmed by a structural analysis using high-resolution STED microscopy.

BP 32.29 Thu 17:15 Poster B1

Influence of Microfluidic Shear on Keratin Networks in Live Cells — ●JENS NOLTING, JANNICK LANGFAHL-KLABES, and SARAH KÖSTER — Courant Research Centre Nano-Spectroscopy and X-Ray Imaging, University of Göttingen, Germany

Intermediate filaments (IFs) are a major component of the eukaryotic cytoskeleton along with microtubules and microfilaments. IFs show a hierarchical build-up which distinguishes them from other cytoskeletal filaments and leads to a pronounced flexibility. Here, we present a study of keratin intermediate filament networks in live cells which are believed to play a key role in cell mechanics, in particular with regard to external forces. We expose cells expressing fluorescent keratin proteins to shear forces applied by microfluidic methods and investigate the response of the keratin cytoskeleton. This approach enables us to apply well-defined flow fields due to controlled external parameters and variable microchannel layouts. Moreover, the shear flow can be established such that it acts on one individual cell or on groups of cells. In combination with finite element method simulations of flow conditions and fluid-cell-interactions and experimental flow-field analyses these experiments provide important steps towards an understanding of the rheological properties of whole cells.

BP 32.30 Thu 17:15 Poster B1

Modelling the Polymorphism of Bacterial Flagella — ●CHRISTOPH SPEIER, REINHARD VOGEL, and HOLGER STARK — Institut für Theoretische Physik, TU Berlin

Bacteria such as *E. coli* propel themselves using a bundle of long helical tails, known as flagella. The main part of the flagellum is a cylindrical structure made from 11 protofilaments that are assembled from thousands of copies of the protein flagellin. This subunit can assume two different states (R and L) with different RR and LL distances. Proteins of the same state are stacked onto each other to form one protofilament. The flagellum can adapt different helical forms (polymorphism). While flagella, in which all proteins are in the same state, form straight tails, they exhibit a helical structure when protofilaments of both R and L type occur. Transitions between different forms of the flagellum can be induced by changing the salt-concentration or the pH value of the solvent and by applying external torques.

The well established Calladine model explains the different possible helical states of the flagellum but provides no understanding why it conventionally assumes the so-called normal state. Refining an existing model, we consider the flagellin protein as a bistable rigid-body unit with state-dependent bonds to neighboring units. Whereas the outer bonds determine the helical form of the filament, the inner bonds are responsible for its structural stability. With our model we can verify that the normal state is only stable when the rigid-body unit assumes an elongated shape in accordance with the real form of flagellin.

BP 32.31 Thu 17:15 Poster B1

Hopf Bifurcation in Rotating Bacterial Flagella — ●REINHARD VOGEL and HOLGER STARK — TU Berlin

Many types of bacteria swim by rotating a bundle of helical filaments also called flagella. Each filament is driven by a rotatory motor. When its sense of rotation is reversed, the flagellum leaves the bundle and undergoes a sequence of configurations characterized by their pitch, radius and helicity (polymorphism). Finally the flagellum assumes its original form and returns into the bundle.

The flagellum of bacteria such as *E. coli* and *Salmonella* consists of three parts; the rotary motor embedded in the cell membrane, a short proximal hook that couples the motor to the third part, the long helical filament. The hook has a well regulated length of $0.055\mu\text{m}$ and a diameter of around $0.02\mu\text{m}$. The filament is up to $20\mu\text{m}$ long and like the hook about $0.02\mu\text{m}$ in diameter. It is relatively stiff but can switch between distinct polymorphic forms.

In this contribution, we demonstrate how the hook transmitting the torque of the motor to the filament can be modeled. We then investigate the shape of the flexible helical filament when the motor torque is applied. For small torques acting such that the cell body is pushed forward, the helix axis is approximately parallel to the torque and the filament is only slightly deformed. The thrust force assumes a stationary value. However, when the torque is increased, the filament starts to bend which is visible through a Hopf bifurcation in the thrust force. We discuss the importance of this bifurcation for the bundle formation and for the transitions between different polymorphic configurations.

BP 32.32 Thu 17:15 Poster B1

Calcium Signaling upon mechanical stimulus in the Optical Stretcher — ●MARKUS GYGER and JOSEF KÄS — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik I, Linnéstraße 5, 04103 Leipzig, Germany

Under physiological conditions many cells must react to mechanical stimuli. Calcium is one of the most important second messengers and is involved in most of the known mechano-activated cell responses. There are indications that during tumorigenesis the calcium signaling of a cell changes most likely leading to suppression of apoptosis and altered gene expression. The calcium influx can be made visible by appropriate fluorescent dyes, also chelating agents, quenching internal calcium signals as well as external calcium, are available. This provides a broad range of tools for the investigation of effects of calcium on the response of the cell to an external stimulus. The Optical Stretcher is a tool to probe global mechanical behavior of single cells in suspension. Cells are trapped by two anti-parallel laser beams. By increasing the laser power the momentum transferred to the cell surface causes visible deformations. Some cells, especially cancer cells, seem to respond actively to these deformations sometimes even resulting in a contraction of the cell relative to its initial, undeformed state counteracting the applied force. This raises interesting questions regarding the mechanisms by which cells register and respond to the applied forces. The aim of the presented work is to investigate the dependence of calcium influx on the forces applied to the cell surface in order to gain insight into the mechanisms of active responses to stretching.

BP 32.33 Thu 17:15 Poster B1

Continuous versus Boolean dynamics on simple networks — ●EVA GEHRMANN and BARBARA DROSSEL — Institut für Festkörperphysik, TU Darmstadt

We compare Boolean dynamics with continuous dynamics on simple network structures, which can be viewed as relevant modules of regulatory networks. The knowledge of regulatory and signaling processes in living cells is often only of qualitative nature, which gave rise to the description as Boolean networks, where the state of each gene is either "on" or "off". In recent years, experiments yielded more quantitative data for regulatory processes and their kinetic parameters. This leads back to the effort to describe processes in the cell with more realistic continuous models, which may give rise to dynamical phenomena that are not accessible with Boolean networks. Continuous models implement the switch-like dynamics of genes by using the sigmoidal Hill function and by using ordinary differential equations to evaluate the time course of the gene expression patterns. We use simple network components and a systematic rule for replacing Boolean functions with continuous functions in order to identify the main differences between the dynamical behavior and the attractor patterns of Boolean and continuous models.

BP 32.34 Thu 17:15 Poster B1

Chemotaxis model for bacteria with twitching motility — ●JOHANNES TAKTIKOS, VASILY ZABURDAEV, and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

We construct a model to study the characteristic motion of bacteria on a surface. Once bacteria, such as *Pseudomonas aeruginosa* or *Neisseria gonorrhoeae*, reach a surface they lose their helical flagella and instead use filaments, so-called type IV pili, to move forward. The resulting twitching motility represents an important and necessary mechanism that many types of bacteria use to form biofilms.

The main ingredient in our model is chemotaxis. This describes the bacterium's ability to orient its velocity direction along the gradient of the chemotactic field which is given by the concentration of a certain chemical. In our case, the chemical is produced by the bacteria themselves to attract each other and obeys a simple reaction diffusion equation. In a first approach, we neglect fluctuations in the absolute value of a bacterium's velocity and formulate a Langevin equation for the direction of the velocity. It consists of a deterministic part due to chemotaxis and a stochastic term representing both thermal and other sources of noise. The stochastic term alone would lead to rotational diffusion. Using computer simulations, we analyze possible time-dependent structures of bacterial paths and classify different patterns of collective motion.

BP 32.35 Thu 17:15 Poster B1

Contact-controlled amoeboid motility in microstructures induces topophoresis — ●CAROLIN LEONHARDT, DELPHINE ARCIZET, SOFIA CAPITO, SIMON YOUSSEF, SUSANNE RAPPL, JOACHIM O. RÄDLER, and DORIS HEINRICH — Center for Nanoscience, Ludwig-Maximilians-Universität, München

Amoeboid motility is crucial for functionality in many organisms. On a flat and homogeneous substrate, it is generally described as a random walk: Fast and directed migration alternates stochastically with phases of local random probing. To investigate the effect of surface topography on this search strategy, which is a key to understand the interplay between migration dynamics and cell-substrate interactions, we combined high resolution motion analysis and defined microstructured environments. We found that cells of the model organism *Dictyostelium discoideum* preferentially localise in contact with micropillars and that directed cell migration is biased towards the density gradient within arrays of varying pillar density: the cells undergo topophoresis. Our findings are consistent with a stabilisation of random protrusions that is induced by surface contact. This contact-reinforced motility may enable amoeboid cells to efficiently migrate in their natural habitat while searching for food. This effect could enable us to trap cells by topographical means only.

BP 32.36 Thu 17:15 Poster B1

Instabilities of Active Polar Gels in a Taylor-Couette Geometry — ●MARC NEEF and KARSTEN KRUSE — Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken

In many physiologically relevant situations, the dynamics of the cytoskeleton or of tissues in developing organisms occur in a confined geometry. From a physical point of view, both systems, the cytoskeleton of eukaryotic cells as well as ensembles of crawling cells, fall into the class of active polar gels. The generic behavior of such systems is captured by hydrodynamic equations that account for activity, stress generating processes and polar order. We employ the hydrodynamic theory to study instabilities of active polar gels confined to the space between two coaxial rotating cylinders, i.e., a Taylor-Couette geometry. In particular, we analyse the stability of states with orthoradial polarity and find that the system's activity together with its polarity can generate instabilities even in situations when neither of the cylinders rotates.

BP 32.37 Thu 17:15 Poster B1

Modelling protein accumulation at DNA damage sites — ●DANIEL LÖB and BARBARA DROSSEL — Technische Universität Darmstadt, Institut für Festkörperphysik

Cells react to DNA damage by rapidly accumulating and chemically modifying repair and signalling proteins. As a result of this, zones of massively increased repair protein concentrations, called foci, appear centered around the damage sites. The reaction processes that govern the formation of these foci are characterized by ongoing association and dissociation of proteins at specific rates.

We explore the protein accumulation dynamics using analytical cal-

culations as well as computer simulations based on ordinary differential equations and stochastic methods. It is a focus of our work to investigate the possibility of multistability and switching between different pathways.

We also discuss the implications this has on our understanding of the single-strand break repair mechanism Base Excision Repair (BER).

BP 32.38 Thu 17:15 Poster B1

Influence of subsurface composition on the adhesion of bacteria and the adsorption of proteins — ●PETER LOSKILL, YVONNE SCHMITT, HENDRIK HÄHL, and KARIN JACOBS — Saarland University, 66123 Saarbrücken, Germany

Biofilms are of special importance in various fields of the everyday life. Their initial formation is composed of two crucial steps: the adsorption of proteins and the adhesion of bacteria. These are complicated processes that depend on many factors.

So far, most studies focused on surface chemistry, hydrophobicity and surface roughness - factors which influence mainly the short range interactions.

Our studies concentrate on the impact of long range interactions, in particular van der Waals forces, which can be tuned by the use of tailored substrates. To characterize the processes, we follow two pathways: One way is to characterize protein adsorption on a fundamental level via ellipsometry. Another is to directly probe bacterial adhesion by AFM - force spectroscopy. As model systems we use *Staphylococcus aureus* bacteria and proteins like amylase, lysozyme and bovine serum albumin. The results of our experiments show that protein adsorption kinetics as well as bacterial adhesion are dependent on the subsurface composition of the substrate [1,2]. Hence it is of great importance for the design of anti-adhesive surfaces to consider not only the lateral but also the vertical composition of the substrate.

[1] A. Quinn et al., *Europhysics Lett.* 81 (2008) 56003

[2] M. Bellion et al., *J. Phys.: Condens. Matter* 20 (2008) 404226

BP 32.39 Thu 17:15 Poster B1

Bacterial probes with defined contact area for force spectroscopy — ●SEBASTIAN HÜMBERT, PETER LOSKILL, and KARIN JACOBS — Saarland University, 66123 Saarbrücken, Germany

Bacterial adhesion is a key factor in disease pathogenesis. Thus it is essential to understand the interaction of microorganisms with biological and artificial surfaces. A promising tool is to perform force-spectroscopy using an atomic force microscope (AFM) with the bacteria themselves as AFM probes. The aim of the studies presented is to create functionalized bacterial probes with a defined contact area to perform reliable force/distance measurements on various surfaces. Fundamental parameters are the tip geometry and the way the bacteria are 'glued' to the AFM tip. The adhesion protein must not alter the bacterial membrane, yet still has to be strong enough to hold the bacteria firmly onto the tip during the force/distance measurements. We show results for binding bacteria to the cantilever via charge effects, via covalent binding and via specific binding using different cantilever coatings. Our primary aim is to study the influence of the tip geometry and we present the outcome of experiments with single bacteria as probes and with bacteria-coated colloidal probes.

BP 32.40 Thu 17:15 Poster B1

A dynamic model for the morphogenesis of the Golgi apparatus — ●JENS KÜHNLE^{1,2}, JULIAN C. SHILLCOCK², OLE G. MOURITSEN², and MATTHIAS WEISS¹ — ¹German Cancer Research Center, Heidelberg — ²Center of Membrane Physics, University of Southern Denmark

The dynamic compartmentalization of eukaryotic cells is a fascinating phenomenon that is far from being understood. A prominent example for this challenge is the Golgi apparatus, the central hub for protein sorting and lipid metabolism in the secretory pathway. Despite major advances in elucidating its molecular biology, the fundamental question of how the morphogenesis of this organelle is organized on a system's level has remained elusive. Here, we have formulated a coarse-grained computational model that captures key features of the dynamic morphogenesis of a Golgi apparatus. In particular, our model relates the experimentally observed Golgi phenotypes, the typical turnover times, as well as the size and number of cisternae to three basic, experimentally accessible quantities: the rates for material influx from the endoplasmic reticulum, the anterograde and the retrograde transport rates. Based on these results, we elucidate which factors are crucial for the structure formation of the Golgi apparatus. Moreover, we propose which molecular factors should be mutated to alter the organelle's

phenotype and dynamics.

BP 32.41 Thu 17:15 Poster B1

Measuring Cytoskeletal Orientation Distributions of Large Cell Populations by Digital Image Processing — ●NORBERT KIRCHGESSNER, UTA ZEDLER, NICO HAMPE, WOLFGANG RUBNER, BERND HOFFMANN, and RUDOLF MERKEL — Institute of Bio- and Nanosystems 4: Biomechanics, Forschungszentrum Jülich GmbH, 52425 Jülich

Cell adhesion is vital for most cell types and supported by various proteins forming defined adhesion structures. These complex structures bind to both the cellular environment and to intracellular actin filaments. This direct interaction enables cells to actively sense and to respond to varying mechanical conditions. Cyclic stretch is such a mechanical signal with thereby induced cellular reorientations. Cell orientation given by the major axis of the cell shape is distinguished from cytoskeletal orientation defined by stress fibers. However, exact whole cell and cytoskeletal reorientation angles are difficult to determine.

Our approach applied the gradient based structure tensor method to bandpass filtered fluorescence microscopy data. In combination with a segmentation step this yielded accurate histograms of cytoskeletal orientations for individual cells. Subsequently, we obtained the predominant cytoskeletal orientation of each cell and intracellular orientation variations of stress fibers. Cellular orientations were determined as the major direction of the ellipse with equal normalized second central moment as the segmentation results for each cell. Application of these algorithms to large numbers of cells (n>200) yielded results with high statistical relevance.

BP 32.42 Thu 17:15 Poster B1

Construction and dynamics of a bistable genetic switch in E. coli — ●CHRISTOPH KLINGNER, SUSANN BERTHOLD, RALF JUNG-MANN, EIKE FRIEDRICH, and FRIEDRICH C. SIMMEL — Lehrstuhl für Bioelektronik, E14 TU München, James Franck Str., 85748 Garching, Germany

Standard genetic engineering tools can be utilized for the development of artificial gene regulatory circuits. Synthetic gene circuits can be used to "reprogram" bacterial cells in order to achieve artificial functions and behavior. In addition, they may prove useful for the elucidation of gene regulatory dynamics within a controlled setting. Among the simplest possible regulatory circuits, bistable or multistable genetic systems are of particular interest, as they may be utilized to switch between several distinct "states" of a cell. Furthermore, switching mechanisms are a key ingredient of more complex genetic programs. We here present the construction of a simple genetic switch based on the LacI and pTetR promoters, which can be switched chemically between two possible states. The regulatory dynamics of each of the two subsystems are investigated in the bacterium *Escherichia coli* in terms of stability, reproducibility and velocity while toggling with the inducers isopropyl thiogalactoside (IPTG) and anhydrotetracycline (aTc). The inhibition as well as positive auto-regulation of gene expression are studied and compared to model simulations.

BP 32.43 Thu 17:15 Poster B1

Magnetic Resonance Imaging (MRI) of tumor cell migration in animals — ●CHRISTIAN WEISS¹, BEN FABRY¹, and ANDREAS HESS² — ¹Biophysics Group, FAU Erlangen-Nürnberg — ²Lehrstuhl für Pharmakologie und Toxikologie, FAU Erlangen-Nürnberg

The process of metastasis formation involves the migration and 3-D invasion of tumor cells from a primary tumor to distant sites. Our aim was to monitor the dynamics of cell migration and invasion in animals over prolonged time periods using MRI. Human breast carcinoma cells were labeled with superparamagnetic $\gamma\text{Fe}_2\text{O}_3$ iron oxide nanoparticles. Particles were stabilized and biofunctionalized with poly-L-lysine. Approximately 10,000 cells were incubated with 1 μg of particles for 24 h. Particles are readily taken up by cancer cells and stored in intracellular clusters. During cell division, the nanoparticle clusters are divided and split between daughter cells. Nanoparticles remain stable for at least 3 weeks. In-vitro collagen gel assays show that there is no difference between the spreading or invasion behavior of tumor cells with and without nanoparticles. MRI imaging (conventional multi-spin sequences with a repetition time of 1000 ms and 8 echo times between 11 and 165 ms) of cells suspended in 2% agar gave a detection limit of the R2 relaxation rate of 20 μM Fe_2O_3 , equivalent to 70 cells/mm². The minimal detection volume of tumor cells in agar was 25 μl . Detection limit and minimal volume were verified by injecting labeled cancer

cells in dead mice. To achieve high sensitivity in mice, however, a slice thickness of less than 250 μm was necessary, which leads to whole-body scans with physiologically unacceptable duration ($> 4\text{h}$).

BP 32.44 Thu 17:15 Poster B1

Nonlinear Cell Mechanics Is Plastic Mechanics — LARS WOLFF, ●ANDREA KRAMER, and KLAUS KROY — Institut f. Theoretische Physik, Universität Leipzig

Recent investigations of the dynamical linear and nonlinear mechanical properties of single living cells have identified (at least) three major universal patterns of cell rheology: (i) power-law rheology, (ii) viscoelastic stiffening, and (iii) inelastic softening or "fluidization". We present a polymer-physics based minimal model that robustly reproduces all of these features and suggests their close mutual interdependence. In particular, the supposedly antagonistic effects of viscoelastic stiffening and fluidization are predicted to actually reinforce each other and the structural damping. The highly redundant nonlinear dynamical shear response of living cells is traced back to inanimate material properties shared by much simpler *in vitro* models of the cytoskeleton, notably by pure F-actin solutions, which has so far been experimentally validated only for (i) & (ii). According to the model, the core mechanism responsible for the mechanics of living cells and tissues is comprised by a small set of equations coupling semiflexible polymer dynamics as described by the glassy wormlike chain model with "bond"-kinetics in the highly degenerate free energy landscape of an "Arrhenius gel". The good quantitative agreement of model predictions for viscoelastic and inelastic protocols with experimental data from both *in vitro* model systems and living cells suggests intriguing new directions for future experiments aiming to relate microscopic structural parameters with the mechanical response.

BP 32.45 Thu 17:15 Poster B1

Mechanisms of Parasitic Cell Motility in Blood Flow and Possible Impact on Host Infection — ●SRAVANTI UPPALURI¹, ERIC STELLAMANNS¹, NIKO HEDDERGOTT², STEPHAN HERMINGHAUS¹, MARKUS ENGSTLER², and THOMAS PFOHL^{1,3} — ¹Max Planck Institute for Dynamics and Self Organization, Göttingen — ²Biocenter, University of Würzburg — ³Chemistry Department, University of Basel

African trypanosomes, parasites responsible for devastating disease in sub-Saharan Africa, are found in the mammalian bloodstream and penetrate the central nervous system during late stages of African Sleeping Sickness. Trypanosomes are able to make their way past the tightly protected blood brain barrier despite significantly high blood flow velocities in vessels around the brain. We find that the parasite is able to swim closer to vessel walls with increasing blood flow velocities. Typical vessels have a cell free layer near the channel walls, we mimic this phenomenon using microfluidic techniques and investigate the trypanosome's ability to make turns at relatively high flow velocities and invade through confining gaps. Gradient based microfluidics is exploited to test if the turning frequency is enhanced by chemical attractants. Lastly, we find that cell orientation is velocity dependent. Together our results point to strong hydrodynamical effects on swimming behavior of trypanosomes which may play an important role in different stages of infection.

BP 32.46 Thu 17:15 Poster B1

Quantitative temperature analysis by micro-thermo capillaries for biological systems — ●MICHAEL STÜHRENBURG¹, RENE HEIMBUCH¹, MIRIAM GIESGUTH², KARL-JOSEF DIETZ², SIMONE HERTH¹, and GÜNTER REISS¹ — ¹Fakultät für Physik, Universität Bielefeld — ²Fakultät für Biologie, Universität Bielefeld

Thermocouples based on the Seebeck effect between two metals are widely used for various applications. However, these thermocouples usually consist of wires of hundreds of nanometer thickness measuring the temperature in large objects and voluminous bulk phases. In a new setup, the two metals for the thermocouple are sputtered onto a

glass micro capillary with an outer diameter of about 450 nm leading to very small contact and measurement areas. These thermo capillaries can be used in a micro manipulation system to measure the temperature in small tissues, single cells, or other biological objects, e.g. leaf epidermis and trichomes. This poster reports the fabrication of micro-thermo capillaries and demonstrates its calibration and use for quantitative measurements.

BP 32.47 Thu 17:15 Poster B1

Local quantitative temperature measurements on silicon nitride membranes for biological applications — ●MAKSYM KOCH¹, NADINE EWERS¹, CARSTEN BUDKE², BRITTA RIECHERS², THOMAS KOOP², SIMONE HERTH¹, and GÜNTER REISS¹ — ¹Fakultät für Physik, Universität Bielefeld — ²Fakultät für Chemie, Universität Bielefeld

Thermocouples based on the Seebeck effect between two metals are widely used for various applications. However, these thermocouples usually consist of wires hundreds of nanometer thick measuring the temperature in large objects and voluminous bulk phases. In order to determine local temperatures, e.g., in single cells, thermocouples can be sputtered through special masks on top of a silicon nitride membrane. These membranes are only 50 or 100 nm thick and avoid extensive heat dissipation necessary for a quantitative analysis. Local quantitative temperature measurements were performed with Pd/Cr and Pd/NiCr with Seebeck coefficients of 27 $\mu\text{V}/\text{K}$ and 35 $\mu\text{V}/\text{K}$, respectively, using various types of heating processes.

BP 32.48 Thu 17:15 Poster B1

Dynamics of cell shape on micropatterned substrates — ●JEROME SOINE¹, ACHIM BESSER^{1,2}, and ULRICH SCHWARZ^{1,3} — ¹Karlsruhe Institute of Technology, Theoretical Biophysics Group — ²Harvard Medical School, MA, USA — ³University of Heidelberg, Institute for Theoretical Physics

Free edges of adherent cells often adopt the shape of inward directed circular arcs. Combining experiments with cells on micropatterned substrates, quantitative image processing and modeling, recently it has been shown that the values for the arc radii can be explained by the interplay between tension in the cell envelope and elastic strain along the cell periphery (Bischofs et al., Biophysical Journal 95: 3488, 2008). Here we extend this model to predict the dynamics of shape changes on micropatterned substrates. The free edge of a cell between two adhesion sites is modeled as a actively contracting visco-elastic beam. Intrinsic isotropic surface tension pulls in the edge and leads to the circular arc shape. Inhibition of actin polymerization or myosin II motor activity leads to changes in arc radius which can be predicted by our model. Special focus is given to the effect of positive feedback loops involving signaling through the small Rho-GTPases.

BP 32.49 Thu 17:15 Poster B1

Cells on different substrates. An investigation with AFM and optical microscopy. — ●DANIELE MARTINI¹, MICHAEL BEIL², OTHMAR MARTI¹, and THOMAS SCHIMMEL^{3,4} — ¹Institute of exp. physics, Ulm University — ²Institute of internal medicine I, Ulm University Hospital — ³Forschungszentrum Karlsruhe — ⁴Karlsruhe University

The main task of epithelial cells is to form a physical barrier, which is characterized by the properties of the cytoskeleton and cell-cell contacts. The principal aim of the first part of this project is to modulate the structure of these macromolecular complexes, optimizing the mechanical properties of the cells by a spatially hierarchically ordered and t-variable nanostructured culture substrate. Thus, at first, we have to investigate and control the growing and arrangement of these cells on different surfaces and, later, to define and influence the subcellular structure with chemically nanostructured culture substrates. In this poster we show AFM and optical microscopy experiments on adherent cells on different substrates. We discuss the influence of the substrate on cell morphology and on AFM images.

BP 33: Posters: Neurobiophysics

Time: Thursday 17:15–20:00

Location: Poster B1

BP 33.1 Thu 17:15 Poster B1

Influence of bilayer substrate fluidity on neuronal growth — ●LYDIA WOITERSKI¹, PHILIPP RAUCH¹, DAN MINNER², CHRISTOPH NAUMANN², and JOSEF KAES¹ — ¹Universität Leipzig, Germany — ²Indiana University, Indianapolis, USA

For cell motility it is crucial that cells sense the viscoelasticity of their environment. An important role in this process play focal adhesion complexes where transmembrane proteins of the integrin family bind to proteins of the extracellular matrix or within the cell to the cytoskeleton. Although it is known that the stability of these complexes depends on the stiffness of substrate, the complete mechanism of cell adhesion has not yet been fully understood. A suitable system mimicking the cell surface are tethered bilayers, where the membrane viscosity can be easily modulated by the polymer linker density or the number of bilayer stacks, was established by D. Minner and C. Naumann at the University of Indiana. They showed that the bilayer substrates are stable, have reproducible diffusion properties and that fibroblasts sense the surrounding viscosity of the substrate and change their morphology according to the membrane fluidity. In the present study neuronal cell lines were plated on single tethered bilayers with varied linker density. Preliminary results show that the neurons adhere at all densities but exhibit different dendritic growth - for low bilayer viscosity the growth seems to be faster which is in good agreement with the inverse durotaxis of neurons. This biomimetic system represents a versatile tool that allows for the quantification of cellular outgrowths, their velocities and can help to understand how these processes form.

BP 33.2 Thu 17:15 Poster B1

Light propagation through the vertebrate retina — ●SILKE AGTE^{1,2}, SABRINA MATTHIAS^{1,2}, STEPHAN JUNEK³, ELKE ULBRICHT¹, INES ERDMANN¹, DETLEV SCHILD³, JOSEF KÄS², and ANDREAS REICHENBACH¹ — ¹Paul-Flechsig-Institute for Brain Research, Department of Neurophysiology, Jahnallee 59, 04109 Leipzig, Germany — ²Institute of Physics, Department of Soft Matter Physics, Linnèstrasse 5, 04103 Leipzig, Germany — ³Center of Physiology and Pathophysiology, Department of Neurophysiology and Cellular Biophysics, Humboldtallee 23 37073 Göttingen, Germany

The retina of the vertebrates has an inverted design. Therefore the light has to pass several tissue layers before hitting the signal transducing photoreceptor cells. These layers include structures with sizes on the order of the wavelength of visible light which would result in a scattering and reflection of the photons. We suppose that the Müller cell of the retina is responsible for the light transport where this glial cell channels the light from the vitreous body to the nuclei of the photoreceptor cells. The Müller cell occupies several features which point to the lightguidance ability: e.g. its strategic position in the path of light through the tissue, its funnel shape, its rareness of highly scattering objects and its refractive index. This project investigates the optical properties of the retinal glial cell in its normal tissue by illuminating a single Müller cell endfoot. While the retina is moving with respect to the light source there are changes of the beam structure and thus the Müller cell channels the light to the photoreceptor cells similar to an optic fiber.

BP 33.3 Thu 17:15 Poster B1

Hidden Markov Models reveal distinct mobilities of synaptic vesicles — ●JAN-PHILIPP SPIES¹, CHRISTOPH ERLINKÄMPER¹, MATHIAS PASCHE², DETLEF HOF², KARSTEN KRUSE¹, JENS RETTIG², and UTE BECHERER² — ¹Theoretische Biologische Physik, Universität des Saarlandes, 66041 Saarbrücken — ²Physiologisches Institut, Universität des Saarlandes, 66421 Homburg

In neurons, release of neurotransmitter occurs through fusion of synaptic vesicles with the plasma membrane. Electrophysiological methods, e.g. membrane capacitance measurements, provide indirect information about distinct vesicle states ("docking" and "priming"). At present, the molecular origin of these states is unknown. To characterize them on the level of individual vesicles, we investigate their mobility using total internal reflection fluorescence (TIRF) microscopy. Employing Hidden Markov Models, we identify several states of different mobilities and propose possible underlying molecular mechanisms.

BP 33.4 Thu 17:15 Poster B1

Up- down state switching in a conductance- based cortical model — HONG-VIET NGO, ●ARNE WEIGENAND, and JENS CHRISTIAN CLAUSSEN — Institut für Neuro- und Bioinformatik, Universität zu Lübeck

In recent experiment [1] investigated the on- and off switching of bursting activity in ferret brain slices. This experiment is seen as a paradigmatic system towards the understanding of the emergence of cortical slow waves. The basic dynamics can be modeled by a simplified discretized integrate-and-fire model including inhibitory currents [2]. Here we use a conductance-based model to reproduce the spike-burst dynamics and the triggering of on-states as observed in [1].

[1] Y. Shu, A. Hasenstaub & D.A. McCormick. Nature 423, 288 (2003)
[2] Hong-Viet Ngo et al., submitted.

BP 33.5 Thu 17:15 Poster B1

Triggering bursts in all-to-all coupled neurons with global inhibition — ●HONG-VIET NGO¹, JAN KÖHLER², JÖRG MAYER², JENS CHRISTIAN CLAUSSEN¹, and HEINZ GEORG SCHUSTER² — ¹Institut für Neuro- und Bioinformatik, Univ. zu Lübeck — ²Univ. Kiel

Slow-wave sleep in mammals is characterized by a change of large-scale cortical activity currently paraphrased as cortical up-down states. Recently [Y. Shu, A. Hasenstaub & D.A. McCormick. Nature 423, 288 (2003)] demonstrated experimentally a bistable collective behaviour in ferret brain slices, with the remarkable property that the up states can be switched on and off with excitations, whereby the effect of the second pulse significantly depends on the time interval between the pulses. Here we present a time-discrete model of a neural network that reproduces this type of behavior, as well as reproduces the time-dependence found in the experiments. This class of models could be of general interest to various types of coupled systems if control pulses of negative signs cannot be realized, and offers new possibilities to control cortical slow waves.

BP 33.6 Thu 17:15 Poster B1

Critical micellar concentration (CMC) dependence of pluronic effects on neuronal cells in culture — ●VICENTE D. SAMITH^{1,2,3}, MARÍA J. RETAMAL², IGNACIO VERGARA², ESTEBAN RAMOS-MOORE², ULRICH G. VOLKMANN², and RICARDO B. MACCIONI^{1,4} — ¹Laboratory of Cellular and Molecular Neurosciences, Faculty of Sciences, Universidad de Chile, Santiago de Chile — ²Dept. of Physics, P. Universidad Católica de Chile, Santiago de Chile — ³Dept. of Chemistry, Universidad Andrés Bello, Santiago de Chile — ⁴International Center for Biomedicine (ICC), Santiago de Chile

We are evaluating triblock copolymers, referred to as pluronics, for delivery of anti-inflammatory drugs that normally do not cross the blood-brain barrier. We studied the cytotoxicity of pluronic F68 in human neuroblastoma cells in culture, and analyzed physicochemical parameters of this type of polymeric matrixes such as the critical micellar concentration (CMC). Atomic force microscopy (AFM) was used to investigate the morphological changes in the lipid monolayer as a function F68 concentrations from 0.5×10^{-4} M to 10×10^{-4} M, adsorbed on a solid substrate (hydrophilic silicon). We observe a gradual change in the morphology of the polymer, from a 'dendritic' to a supramolecular structure (clusters). The analysis of morphological changes of F68 is complemented by measurements of the percentage of film coverage on the silicon substrate as a function of the molar concentration of F68.

This work is supported by MECESUP, FSM 0605 and FONDECYT 1060628 (UGV) and 1080254 (RBM).

BP 33.7 Thu 17:15 Poster B1

Mechanosensitive Behavior of Neuronal Growth Cones — ●STEVE PAWLIZAK¹, KRISTIAN FRANZE², and JOSEF A. KÄS¹ — ¹Institute for Experimental Physics I, Soft Matter Physics Division, University of Leipzig, Germany — ²Cavendish Laboratory, Biological and Soft Systems, University of Cambridge, UK

Neuronal pathfinding is essential for the development of the central nervous system. Although it is generally accepted that chemotaxis is the major guidance factor, it seems unlikely that this is the only mechanism directing developmental neurons to their target sites, especially when considering the length of some pathways.

In [1], we support the idea that durotaxis also plays a non-negligible

role in this complex process. Our *in vitro* studies show that neurons actively palpate their mechanical environment with the help of their growth cones and retract their neurites from contacts they cannot mechanically deform. After mechanical stimulation of the neuronal growth cones using a modified scanning force microscope (SFM) probe, the neurons retract their processes and re-extend them into a

new direction when the exerted mechanical stress exceeds ~ 300 Pa. This threshold corresponds to the maximum substrate stiffness that neurons can visibly deform. Furthermore, an immediate calcium influx through stretch-activated ion channels seems to be correlated with neurite retraction.

[1] K. Franze et al., *Biophys. J.* **97** (7): 1883–1890 (2009)

BP 34: Posters: New Technologies

Time: Thursday 17:15–20:00

Location: Poster B2

BP 34.1 Thu 17:15 Poster B2

A novel efficient and fast method to reconstruct free energy landscapes — ●JENS SMIATEK and ANDREAS HEUER — Westfälische Wilhelms-Universität Münster, Institut für Physikalische Chemie, 48149 Münster, Germany

We present a novel method to efficiently explore and calculate free energy landscapes inspired by the Well-tempered Metadynamics algorithm [1]. The technique which is called "Weighted Histogram Metadynamics on a grid" is grid-based and allows a very fast computation in contrast to Well-tempered Metadynamics and further methods. The underlying free energy landscape is reconstructed on a grid as an estimate for a biasing potential. An exact histogram reweighting scheme is finally applied to compute the free energy landscape and for the demand of thermodynamic consistency. Furthermore by filling the free energy minima our method allows a rapid decrease in simulation time in the calculation of rare events. In addition, the calculated free energy landscape is not restricted to the actual choice of collective variables and can in principle be extended on the fly to all variables of interest. As an example for our method, we present the free energy landscape of the alanine dipeptide in solution for several collective variables.

[1] Barducci A., Bussi M. and Parrinello M., *Phys. Rev. Lett.* **100**, 020603 (2008)

BP 34.2 Thu 17:15 Poster B2

BioRef - a time-of-flight reflectometer for soft matter applications at HZB — ●MARKUS STROBL^{1,2}, ROLAND STEITZ², MARTIN KREUZER^{1,2}, REINER DAHINT¹, and MICHAEL GRUNZE¹ — ¹Universität Heidelberg — ²Helmholtz Zentrum Berlin

BioRef, a time-of-flight reflectometer at Helmholtz Zentrum Berlin (HZB) is currently under construction. Combined with an in-situ infrared spectrometer it will be optimised for soft matter applications at solid-liquid interfaces. A flexible double-chopper set-up together with a wavelength band chopper will enable the selection of well defined wavelength bands at different defined wavelength resolutions in order to optimize measurements with regard to the given application [1]. A state-of-the-art 2D position sensitive 3He detector will be used for the reflectivity measurements in horizontal scattering geometry. The time-of-flight mode is also chosen to realise the investigation of dynamic interface processes under shear and flow conditions. A choice of different wavelength bandwidths with at the same time constant wavelength resolution enables to focus on defined features in the reflection curve depending on the requirements of the specific measurements utilizing the highest possible efficiency. A q-range spanning 3 orders of magnitude and reflectivity measurements over more than 6 orders of magnitude are envisaged and their feasibility is supported by Monte Carlo simulations [2].

BP 34.3 Thu 17:15 Poster B2

Phase estimation from interferograms with few photons — ●DENNIS MÜLLER¹, THOMAS HOTZ², and RAINER G. ULBRICH¹ — ¹IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — ²Institut für Mathematische Stochastik, Georg-August Universität Göttingen, Germany

We report interferometric tracking of nanoparticles with subwavelength accuracy in the limit of low light intensities. With only few photons contributing to the far-field interferogram the ultimate accuracy of a position measurement which can be achieved from phase reconstruction is limited by shot noise of the detected photons. We have studied the precision of such a phase estimation, based on the maximum likelihood method, for different experimental configurations. Its dependence on the form of the interference pattern, the number and relative position of detection channels, and the total number of detected photons has been analyzed.

BP 34.4 Thu 17:15 Poster B2

The Optical Cell Rotator: Image propagation through fibers for contact-free rotation of cells — ●MICHAEL SCHMIDBERGER, MORITZ KREYSING, and JOCHEN GUCK — Cavendish Laboratory, Department of Physics, University of Cambridge

The Optical Cell Rotator (OCR) is a dual-beam laser trap that allows to hold and orient living cells stable in 3D. Unlike earlier versions of fiber-based traps, OCR uses fibers supporting more than one optical mode. Combined with adaptive optics, this allows for the generation of non-trivial trapping geometries while still having all the advantages of fibers.

We provide detailed analysis of the problems one faces when trying to propagate images through optical fibers. We then present solutions specifically interesting for optical trapping applications and show how these results can be used to rotate living cells stepwise through the focal plane of practically any optical microscope. Finally, we discuss how this feedback independent rotation mechanism can serve as basis for already established, but so far impractical tomographic imaging techniques.

BP 34.5 Thu 17:15 Poster B2

STED microscopy: High-resolution imaging of dynamic processes — ●CHRISTIAN OSSEFORTH¹, JEFFREY MOFFITT², and JENS MICHAELIS¹ — ¹Ludwig-Maximilians Universität München, Department Chemie und Biochemie, Butenandtstr.11, 81377 München — ²FAS Center for Systems Biology, Harvard University, Cambridge, MA 02138

Stimulated emission depletion microscopy has been shown to overcome the diffraction limit of normal confocal fluorescence microscopes by resolving structures down to 19 nm in x and y [1]. While for a long time the application of STED microscopy has been hindered due to the necessity of using complicated laser systems, the recent development of commercially available supercontinuum lasers have significantly lowered the cost and complexity of operating such a setup in a lab environment [2]. Here we present our current STED microscope setup using the aforementioned compact laser source in conjunction with a highspeed scanning stage. This allows for observing dynamic processes *in vitro* and *in vivo* with nanoscale resolution. Restrictions in scanning speed are set by the repetition rate of the laser source (1 MHz at the moment) but are thought to improve as the demand for fast, high power super-continuum lasers rises. We will discuss general design considerations as well as practical considerations for building a STED system.

[1] Wildanger D et al.; *J. Microsc.* 2009; 236(1):35-43

[2] Wildanger D et al.; *Opt Express* 2008; 16(13): 9614-9621

BP 34.6 Thu 17:15 Poster B2

Combined SERS/AFM microscopy on single gold nanoparticle clusters — ●DENNIS STEINIGEWEG, MOHAMMAD SALEHI, MAGDALENA GELLNER, MAX SCHÜTZ, and SEBASTIAN SCHLÜCKER — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück

Surface-enhanced Raman scattering (SERS) is an ultrasensitive technique of Raman spectroscopy for molecules on or near metallic nanostructures that support localized surface plasmon resonances. Single noble metal nanoparticle clusters exhibit extremely high and very localized near-field enhancements in the junctions between adjacent particles ("hot spots").

We employ SERS from self-assembled organic monolayers (SAM) on the surface of single gold nanoparticle clusters for probing their optical/plasmonic properties. Atomic force microscopy (AFM) on the same objects provides the corresponding topographic information.

BP 34.7 Thu 17:15 Poster B2

New Carbohydrate-based Protein Sensor Realized with Cantilever Arrays — ●KATHRIN GRUBER¹, TIM HORLACHER², PETER H. SEEBERGER², and BIANCA A. HERMANN¹ — ¹CeNS and Walther-Meißner-Institute, Walther-Meißner-Str. 8, 85748 Garching, Germany — ²Max Planck Institute of Colloids and Interfaces, Department of Biomolecular Systems, Arnimallee 22, 14195 Berlin, Germany

Cantilever based detection opens new means for the label-free analysis of biomolecular interactions in real-time and up to eight channels. In the static operation mode, the biomolecular interaction is transduced into a deflection of a micrometer thin silicon beam that can be read-out with nanometer precision via optical beam deflection. Owing to recent advances in carbohydrate sequencing and synthesis, glycomics is catching up fast to the more established fields of genomics and proteomics. Measuring carbohydrate interactions is key to understand carbohydrate function requiring the development of reliable, sensitive and selective sensor surface chemistries. Cantilever array have been successfully used in gene fishing, single base pair recognition, and antigen-antibody assays. We design a purely carbohydrate based sensing layer to single out the central glycoconjugate recognition. Using a reference sensor to account for non-specific binding, we detect carbohydrate-protein interactions down to nanomolar concentrations. We verify the selective binding of proteins to carbohydrate functionalized cantilevers by a competitive inhibition assay. Our results pave the way for carbohydrate based cantilever sensors as a robust, scalable and label-free method to study medically relevant carbohydrate-protein interactions.

BP 34.8 Thu 17:15 Poster B2

Magnetic Tweezers Setup for Single Molecule Experiments — ●CAROLIN RADEMACHER, SEBASTIAN HORSTMEIER, CHRISTOPH PELARGUS, ANDY SISCHKA, and DARIO ANSELMETTI — University of Bielefeld, Department of Physics, Experimental Biophysics and Applied Nanosciences

Besides atomic force microscopy and optical tweezers magnetic tweezers are a powerful tool for micromanipulations and single molecule force spectroscopy. We introduce a magnetic tweezers setup, that is based on a multipole-alignment operating with electromagnets to accomplish drag- and rotation-experiments with individual magnetic beads and allow operation at low mechanical vibrations. Since a wide range of applications is wanted, the pole pieces of the setup are manufactured through contact-lithography and electro-deposition [1], so that alterations are easy to accomplish in form and size. In the future we want to apply the magnetic tweezers to study rotating motor proteins under in vitro conditions. Here we present and discuss our setup and show the first data of our calibration experiments.

[1] A. H. B. de Vries, B. E. Krenn, R. van Driel, and J. S. Kanger. Patterned Electroplating of Micrometer scale Magnetic Structures on glass substrate. *Journal of Microelectromechanical Systems (JMEMS)*, 13:391 - 395, 2004.

BP 34.9 Thu 17:15 Poster B2

Single nanoparticle detection and the use of holographic optical tweezers for object manipulation in micro-fluidic devices — JULIA S. GEBAUER and ●LENNART TREUEL — Universität Duisburg-Essen, Essen, Germany

A Single NanoParticle Sensor (SNPS) has been developed on the basis of a modified optical tweezers approach and is used to count single NPs in micro-channels with high time resolution. The direction of a particle passing through the focus point can be determined by a suitable signal evaluation.

Laser pumps generated by optical tweezers can be used to establish controlled flow conditions in micro-fluidic devices. The flows generated by this approach are used to purposefully pump nano- and micro-objects in selected directions. The utilisation and characterisation of these micro pumps will be presented in this work. The combination of the ability to selectively pump nano- and micro objects with the single nanoparticle counter described above is expected to strongly enhance the use optical tweezers and their derivatives in new Lab-on-a-chip developments.

BP 34.10 Thu 17:15 Poster B2

Atomic scale magnetometry using single defects in diamond — ●THOMAS WOLF¹, HELMUT RATHGEN¹, ROLF REUTER¹, GOPALAKRISHNAN BALASUBRAMANIAN¹, FEDOR JELEZKO¹, DIRK BALD², and JÖRG WRACHTRUP¹ — ¹3. Physikalisches Institut, Universität Stuttgart, Germany — ²Structural Biology Group, Vrije Universiteit Amsterdam, Netherlands

Diamonds contain natural defect centers in their lattice structure known as color centers. Electron spin states in these centers (e.g. the Nitrogen-Vacancy or NV-center) can be changed and measured with optical techniques at room temperature. Using magnetic fields and magnetic field gradients the centers can be located spatially on the nanometer scale and allow for directional analysis. The potential for sub-nm precision by using magnetic resonance techniques has been shown by our group and collaborators.

Diamonds with diameters of a few nanometers containing a NV-center are comparatively cheap and can be produced in large scale. By chemical treatment functionalization of these can be achieved.

Using small nanosized diamond crystals containing a NV-center we intend to use diamond as non-toxic biological marker for a new magnetic resonance imaging technique having potential to overcome the classical resolution limit of light microscopy under physiological conditions.

BP 34.11 Thu 17:15 Poster B2

A hazardfree fabrication process for arbitrarily shaped microparticles — ●LUKAS BOGUNOVIC, JAN REGTMEIER, and DARIO ANSELMETTI — Experimental Biophysics and Applied Nanoscience, Physics Faculty, Bielefeld University, Bielefeld

The use of micro- and nanoparticles impacts applications in biotechnological, chemical and physical sciences like the manipulation and transport of objects in microenvironments or as model migrants in microfluidic systems [1,2]. However, most of the commercially available particles are spherical. Therefore their field of application with respect to shape dependent phenomena is strongly limited.

Here, we propose a novel simple and inexpensive method for the production of arbitrarily shaped microparticles with a manufacturing spreading better than 2.5%. Comparable methods essentially need hazardous acids like hydrofluoric acid (HF) or complicated processing setups which are therefore delicate to handle. Our process involves structuring of the particles in SU-8, which can be doped with tracers like magnetite or fluorescent dyes. Afterwards they are released from their substrate into a surfactant solution with a treatment in an ultrasonic bath.

[1] I. Safarik, M. Safarikova, *Chemical Papers*, **63**, 497-505, 2009

[2] J. Hanes et al., *Advanced drug delivery reviews*, **28**, 97-119, 1997

BP 34.12 Thu 17:15 Poster B2

Measuring rotational diffusion of proteins by fluorescence correlation spectroscopy — ●ANASTASIA LOMAN, INGO GREGOR, and JOERG ENDERLEIN — Third Institute of Physics "Biophysics", Georg-August-Universität, Göttingen

Translational and rotational diffusion are thermally driven processes which depend on molecular parameters as size and shape but also on interaction between molecule and solvent environment. Fluorescence correlation spectroscopy (FCS) is a well known technique to measure translational diffusion coefficients of fluorescent molecules thus monitoring intramolecular changes and intermolecular interactions.

Here we apply fluorescence correlation to measure rotational diffusion. In contrast to conventional fluorescence anisotropy measurements, a correlation based method will work also when the rotational diffusion time is much longer than the fluorescence decay time. Thus, the method is ideally suited to study the rotational diffusion of macromolecules in aqueous solutions having rotational diffusion times of dozen to hundred nanoseconds. By using a pulsed interleaved excitation scheme with crossed excitation polarization, we are able to maximize the temporal dynamics of the measured correlation curve as caused by rotational diffusion. The method is exemplified on sizing the large globular proteins such as amylase, ovalbumin and human serum albumin.

BP 34.13 Thu 17:15 Poster B2

Fluorescence spectroscopic studies of protein conformational dynamics — ●PHILLIP KROEHN — Drittes Physikalisches Institut, Georg August Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Proteinfolding is the physical process by which a polypeptidechain folds into its functional three dimensional structure from a random coil.

The WW-domain is the smallest betasheet known. It consists of a lightly hydrophobic core and takes part in protein-protein interactions by binding of proline rich regions. By singlemolecule FRET studies we want to analyse the folding/unfolding dynamics of the WW-domain

and its intermediate states. The unfolding of the protein will be accomplished by chemical or thermal denaturation.

To use smFRET we are going to label the WW-domain specifically with fluorophoric dyes by employing the orthogonal system. This new technique allows us to use a stopcodon as a codon for an unnatural aminoacid, like para-acetylphenylalanine, whereby it is placed in the polypeptide chain. We are able to specifically label these unnatural aminoacid in the protein.

BP 34.14 Thu 17:15 Poster B2

Fabrication of hybrid nano-micro-fluidic channels with extreme aspect ratios — ●EUGENIE FREDRICH, MARTINA EVERWARD, JÖRG KÄSEWIETER, DARIO ANSELMETTI, and JAN REGTMEIER — Experimental Biophysics & Applied Nanoscience, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

In the micro- and nanofluidic analysis of single molecules, often complex 3D geometries with high aspect ratios are required. Among the basic preconditions for the production of the structures, stability is the most fundamental one, but hard to realize with soft lithography. Furthermore, a spatial accuracy within the range of a few nanometers is especially required for nanofluidics.

In the novel method presented here, contact lithography with the photoresist SU8 is employed to create negative relief structures as small as 670 nm. The microfluidic device is molded with a polydimethylsiloxane (PDMS) bilayer. The first thin layer consists of h-PDMS, which accounts for the stability of the fabricated structures, whereas the second thicker layer is made of the more elastic Sylgard-184 PDMS allowing for flexibility and experimental handling. The resulting channels have a width of 200 μm and free hanging barrier structures forming a flow-through gap of 670 nm, i.e. an aspect ratio of about 300:1.

BP 34.15 Thu 17:15 Poster B2

Applications for fluorescence lifetime imaging: Fast genomic characterization and lifetime measurements on zero-mode waveguide — ●MIRA PRIOR, INGO GREGOR, and JÖRG ENDERLEIN — Third Institute of Physics "Biophysics", Georg-August-University Göttingen

Previous studies showed that the lifetime of the DNA-intercalating dimeric cyanine dye TOTO depends on the insertion of the dye into AT or GC base pairs of the nucleic acid sequence. Utilizing this characteristic we want to develop a fast and simple method of characterizing

unknown double-stranded DNA. With time-correlated single-photon counting (TCSPC) and fluorescence lifetime imaging (FLIM) we want to directly determine the lifetime of the dye YOYO in the DNA-strand depending on the insertion into an AT or GC base pair. A second application for FLIM is the detection of lifetimes of a dye on a zero-mode waveguide. The zero-mode waveguide consists of a circular aperture in an aluminum layer on a microscope slide. The detection volume is confined by the small aperture, which allows single-molecule measurements of high dye concentration in the micromolar range. TCSPC and FLIM allow us to determine the lifetime of the dye ATTO647 in dependence of the aperture diameter. The principle of the analysis of the detected photons and the identification of the single-molecules is based on a multi-exponential curve fitting and a maximum likelihood principle for the DNA-analysis. We want to analyze whether the distribution of lifetimes on the length of the ds-DNA strand correlates with the sequence of this DNA.

BP 34.16 Thu 17:15 Poster B2

Towards solid state nanopores with single walled carbon nanotube contacts — CAMILLE RAILLON¹, SUDHIR HUSALE¹, ●MATTHIAS HEISE², JURI ALLERDINGS², CHRISTOPH STRUNK², and ALEKSANDRA RADENOVIC¹ — ¹LBEN, IBI EPFL Lausanne 1015 Switzerland — ²Institut für experimentelle und angewandte Physik, 93040 Regensburg

We integrate nanoelectrodes with solid state nanopores for detection of passing molecules, e.g., DNA. To control the translocation speed we use optical tweezers [1], to increase spatial resolution of the sensor electrodes made from single walled carbon nanotubes (SWNT) comparable in thickness and distance to a single nucleotide are desirable. We used dielectrophoresis (DEP) method to attach nanotubes in the lithographically defined nanogaps. DEP is well known method and can potentially be used as an efficient trapping tool in the fabrication of such molecular devices. When an electric field is applied, we have observed that density of SWNTs in the nanogap can be tuned with the applied voltage (~ 0.1 V to 0.5 V). Nanogaps < 10nm have been achieved in this way. In a complementary way we grow SWNT from e-beam predefined catalyst particles deposited on our Si₃N₄ membranes. We then drill a hole through the membrane using the focused beam of a transmission electron microscope (TEM) at a position where a nanotube was grown. By this we cut the tube in half, resulting in a nanopore with a pair of SWNT nanoelectrodes. [1] E. H. Trepagnier et al., Nano Letters 7, 2824 (2007).

BP 35: Posters: Statistical Physics, Evolution, and Networks

Time: Thursday 17:15–20:00

Location: Poster B2

BP 35.1 Thu 17:15 Poster B2

Semiflexible polymers under the influence of a pressure driven Poiseuille flow — ●SEBASTIAN REDDIG and HOLGER STARK — Institut für Theoretische Physik, TU-Berlin

We introduce two different models for a semiflexible polymer under the influence of a pressure driven Poiseuille flow between two planar walls. In the first model we describe the polymer as a bead-spring model and use a discretized representation of the wormlike chain model for its bending elasticity. We neglect hydrodynamic interactions with the bounding walls but investigate the influence of the non-zero bead size which disturbs the external flow field. We explicitly calculate this disturbance from a series expansion following J.K.G. Dhont¹. It leads to additional terms in the equations of motion that cause cross-streamline migration in the Stokesian dynamics of the polymer. The direction of this migration can be controlled by varying the bead sizes. In the second model we approximate the beads by point particles and describe their hydrodynamic interactions with the two-wall Green tensor, derived by R.B. Jones², taking into account the no-slip condition at the bounding walls. Because the evaluation of the two-wall Green tensor consumes much computer time, we describe the polymer in this model by a simple dumbbell. Using Brownian dynamics simulations, we measure the center-of-mass probability density of the dumbbell and compare the results with theoretical predictions.

¹An Introduction to Dynamics of Colloids, Elsevier, (1996).

²Spherical particle in Poiseuille flow between planar walls, J. Chem. Phys, 121, 483 (2004).

BP 35.2 Thu 17:15 Poster B2

Systematic Microcanonical Analyses of Polymer Adsorption Transitions — ●MONIKA MÖDDEL¹, WOLFHARD JANKE¹ and MICHAEL BACHMANN² — ¹Institut für Theoretische Physik, Universität Leipzig — ²Institut für Festkörperforschung, Theorie II, Forschungszentrum Jülich

Regarding the advances in processing and manipulating molecules at solid substrates, an understanding of the cooperative effects of finite chains is particularly desirable. We investigate this problem focusing on the adsorption transition [1,2] of a single chain near an attractive substrate. This is conveniently and to our knowledge for the first time done by a detailed microcanonical analysis [2] of densities of states obtained by extensive multicanonical Monte Carlo computer simulations. A remarkable consequence of the convexity of the microcanonical entropy is that for short chains and strong surface attraction the transition is accompanied by a decrease of the microcanonical temperature with increasing energy. Since this is a characteristic physical effect it might not be ignored in analyses of cooperative macrostate transitions in finite systems.

[1] M. Möddel, M. Bachmann, and W. Janke, J. Phys. Chem. B 113, 3314 (2009).

[2] M. Möddel, M. Bachmann, and W. Janke, preprint.

BP 35.3 Thu 17:15 Poster B2

Spontaneous spiking in presence of delayed feedback — ●YUNYUN LI¹, GERHARD SCHMID¹, PETER HÄNGGI¹, and LUTZ SCHIMANSKY-GEIER² — ¹University of Augsburg, Augsburg, Germany — ²Humboldt-University Berlin, Berlin, Germany

Autapse is an interesting phenomena on neurons where axons synapsing on the same neuron's dendrites. This serves as delayed feedback mechanism in the dynamics of neuronal firing. Due the stochastic ion channel gating, there is intrinsic noise presented in the system which leads to spontaneous spiking[1]. Our modeling is done within a stochastic Hodgkin-Huxley model with self-delayed feedback of Pyragas-type. The delayed feedback introduced another time scale leading a competition between the delay time and characteristic intrinsic time of the Hodgkin-Huxley dynamics. Upon the intrinsic noise level and the coupling strength of the delayed coupling the firing exhibits bursting leading a multimodal structure in the interspike interval histogram. For the spontaneous spiking, both the mean interspike interval, and the coherence exhibits modulations upon varying the delay time.

[1] G. Schmid, I. Goychuk, P. Hänggi, *Europhys. Lett.* **56**, 22 (2001).

BP 35.4 Thu 17:15 Poster B2

Advection and Reaction in Open Flows — ●MITJA KLEIDER, IZABELLA BENCIK, and JÜRGEN VOLLMER — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Particles transported by blood flow can exhibit chaotic motion when wall irregularities are present [1]. This chaotic motion can influence physiological processes in the blood, for instance the activation and deposition of platelets that are involved in the thrombus formation.

To clarify the role played by chaotic advection in this process, we study a spatial model of a chaotic flow in which we define an activation and deposition region. Platelets can be deposited only if they are active when they enter the deposition region, i.e. if they have visited the activation region at a previous time. In this communication we discuss how chaoticity influences the deposition rate of platelets and enhances the growth of plaques and thrombi.

[1] Chaotic advection in blood flow, A. B. Schelin, Gy. Karolyi, A. P. S. de Moura, N. A. Booth, and C. Grebogi, *Phys. Rev. E* **80**, 016213 (2009)

BP 35.5 Thu 17:15 Poster B2

Finite-time thermodynamics and cyclic engines — ●DAVID ABREU and UDO SEIFERT — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

We study the finite-time thermodynamics of two simple systems and optimize the efficiency of a cyclic engine based on those two models. In the first case, the particle has two energy levels, one of which controlled by an external parameter ; in the second case, the particle is trapped in a harmonic potential whose position and stiffness are two externally controlled parameter. In both cases, we perform a measurement at the beginning and consider identical initial and final boundary conditions in energy. We show that optimization leads to discontinuous protocols. The second step consists in conceiving an optimal cyclic engine based on those two finite-time models. As opposed to the two-level model where the initial position is binary, the continuous model presents a different initial distribution at the beginning of each cycle, which leads to different solutions of the Fokker-Planck equation i.e. different optimal protocols. We emphasize the role of the measurement in the process and analyze the consequences of a feedback control during one cycle.

BP 35.6 Thu 17:15 Poster B2

Extended Fluctuation-Dissipation Theorem for Sheared Colloidal Suspensions — ●BORIS LANDER¹, THOMAS SPECK², and UDO SEIFERT¹ — ¹II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — ²Department of Chemistry, University of California, Berkeley, CA 94720, USA

We consider suspensions of interacting colloidal particles driven by simple shear flow. For arbitrary strain rates, the recent extension of the fluctuation-dissipation theorem (FDT) to nonequilibrium steady states [1,2] enables us to study the response of single particles (tracer particles) perturbed by a small force. For particles interacting with a screened Coloumb potential, we obtain response and correlation functions through extensive numerical simulations for different densities and strain rates. For higher densities these curves show oscillations, which are explained qualitatively. The time-integrated version of the extended FDT connects the single particle mobility with the diffusion coefficient through an integrated excess function. In addition, we analyze features of this system analytically in the simple model of a single particle in a harmonic potential driven by shear flow.

[1] T. Speck and U. Seifert, *Europhys. Lett.* **74**, 391, (2006)

[2] T. Speck and U. Seifert, *Phys. Rev. E* **79**, 040102(R), (2009)

BP 35.7 Thu 17:15 Poster B2

Effect of thermostating and electrostatics on the solution structure and dynamics of signal transduction of the wildtype-LOV1 domain of phototropin — EMANUEL PETER, BERNHARD DICK, and ●STEPHAN BAEURLE — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, Universitätsstr. 31, 93053 Regensburg, Deutschland

Phototropins are photoactive proteins in plants and algae, which consist of 2 LOV-(light oxygen voltage sensitive)-domains and 1 kinase domain. Each LOV-domain contains a noncovalently bound flavin-mononucleotid-(FMN)-chromophor, which after absorption of blue light at around 450 nm undergoes a photoreaction with a cysteine-residue attached to an apoprotein, inducing a signal in the organism via the kinase-domain. Both the signal transduction as well as the mechanism of the photoreaction of these domains are still only poorly understood. In this presentation we show results of molecular dynamics simulations, where we investigated the effect of thermostating and long-range electrostatics on the solution structure and dynamics of signal transduction of the wildtype LOV1-domain of the green algae *Chlamydomonas reinhardtii*. By comparing our calculation results with recent simulation and experimental data, we demonstrate that these issues have an important influence on the equilibrium structure and the time-evolution of the system.

BP 35.8 Thu 17:15 Poster B2

Thermodynamics of polymers anchored to fluctuating tethered membranes — ●STEFFEN KARALUS^{1,2}, WOLFHARD JANKE¹, and MICHAEL BACHMANN² — ¹Institut für Theoretische Physik, Universität Leipzig, Germany — ²Soft Matter Systems Research Group, Institut für Festkörperforschung (IFF-2), Forschungszentrum Jülich, Germany

By means of extensive Monte Carlo simulations we study a coarse-grained model for a bead-and-spring polymer anchored to a two-dimensional tethered (polymerized) membrane embedded into three-dimensional space [1]. Our model includes interactions within the polymer and the membrane as well as an attractive polymer-membrane potential. In order to identify structural transitions, we investigate fluctuations of thermodynamic quantities in dependence of the polymer-membrane interaction strength. Applied methods include generalized ensemble methods such as multicanonical simulations and parallel tempering.

[1] H. Popova and A. Milchev, *J. Chem. Phys.* **127**, 194903 (2007); *J. Chem. Phys.* **129**, 215103 (2008)

BP 35.9 Thu 17:15 Poster B2

Role of hydrodynamic anisotropy for protein-protein encounter — ●JAKOB SCHLUTTIG, CHRISTIAN KORN, and ULRICH SCHWARZ — Institut für Theoretische Physik, Universität Heidelberg, 69120 Deutschland

Protein-protein interactions in cells comprise both transport and reaction steps. Although both single proteins and intermediate complexes are usually not spherical, the role of anisotropy for protein-protein encounter has not been systematically studied before. Using a Langevin equation approach, we quantify the influence of anisotropy on the encounter rate of model particles. We consider a purely geometric definition of the encounter complex by introducing spherical encounter patches located on the surface of ellipsoidal particles. We investigate the encounter rate k at various aspect ratios ξ for different locations of the encounter patches and different concentrations. We show that the dependence of k on ξ can be mainly attributed to steric effects while the altered diffusion behaviour has a rather small effect. In general one expects that rotational diffusion crosses over to isotropic behaviour for sufficiently long times. We analytically calculate the three-dimensional crossover time and show that it is much smaller than typical protein encounter times, in good agreement with our simulation results.

BP 35.10 Thu 17:15 Poster B2

Die zelluläre Proteinsynthese, ein kosmisches Fraktal der E8-Grp. — ●NORBERT SADLER — 85540 Haar ; Wasserburger Str. 25a

Die Struktur des expandierenden Universums kann mit der E8-Gruppe algebr. definiert werden: $E8=1/(5/9 \cdot H)=8,56 \cdot 10^{17}$ mit $H=64,7 \text{ km/mpcs}$. Die E8-Symmetriegruppe kann als ein synth. kosm. Ribosom verstanden werden, dass unter Wechselwirkung mit der beschl. kosmischen Expansion H , in einer fraktalen Selbstorganisation, $E8/c=2,86 \cdot 10^9$ Basen-Paare translatiert. Das kosm. E8-Analogon zur zellulären Umsetzung der

Erbinformation ist ein synth. Ribosom, (4Basen**1Tripl)=64 Wörter, durch die die 20 Aminosäuren, unter Einwirkung der kosm. Expansion, gefädelt, transkribiert und synthetisiert werden. Die algebraisch-kosm. Darstellung der E8-Translation: $E8/c = (H=64,7\text{km/mpcs}) * (4\text{Bas}^{**1}\text{Tripl}) * (4/3\text{Prot}) * (2^{**19}\text{Aminos.})$

Algebra E8: $64,7 * 64 * 4/3 * 2^{**19} = 2,86 * 10^{**9}$ Basen-Paare

Die algebra. Darstellung über die 32 Kristall-Klassen:

$E8/c = (\text{alfa}(\text{QCD})/\text{alfa}(\text{QED})) * (32\text{Kr.Kl.}) * (4^{**3}) * (2^{**19}\text{Aminos.})$

Algebra E8: $8/3 * 32 * 64 * 2^{**19} = 2,86 * 10^{**19}$ Basen-Paare. Die Menge der über E8 tranlatierten Basen-Paare entspricht in etwa der des Human-Genoms. Erkenntnis: Das expandierende Universum ist in der E8-Darstellung ein kosmisches Organell

BP 35.11 Thu 17:15 Poster B2

The influence of spatial correlations and fractal properties of bacterial patterns on colony extinction — ●FLORENTINE MAYER and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München, Germany

Bacterial communities represent complex and dynamic ecological systems. They appear in the form of free-floating bacteria as well as biofilms in nearly all parts of our environment. They are highly relevant for human health and disease. Spatial patterns arise from heterogeneities of the underlying landscape or are self-organized by the bacterial interactions, and play an important role in maintaining species diversity. We investigate mechanisms for extinction of the population with our automaton model for a bacterial biofilm in fluctuating environments, where each bacterium can take two different phenotypes, whose growth and death rates depend on the environmental conditions. Employing stochastic simulations we find that the typical time until extinction occurs depends on the system size. We study the maximum of cluster mass over time during an extinction process. Furthermore the fractal properties of the patterns that existed before the extinction are characterized in regard to their influence on the extinction behaviour.

BP 35.12 Thu 17:15 Poster B2

Fixation time in zero-sum and non zero-sum cyclic coevolution — ●MARKUS SCHÜTT and JENS CHRISTIAN CLAUSSEN — Inst. für Neuro- und Bioinformatik, Universität zu Lübeck

In the territorial and mating behavior of *Uta stansburiana*, as well as in the colicin secretion and resistance, cyclic coevolutionary dynamics is observed. The coevolutionary payoff matrix has the structure of the rock-paper-scissors (RPS) game, which typically is zero-sum: what one player loses, equals the gain of the winning opponent. In biology, payoffs are difficult to measure, but in general the game can deviate from the zero-sum condition, and the examples mentioned above represent the positive and negative sum cases. In previous work, we have shown that a positive-sum game can stabilize the coexistence (and therefore preserve biodiversity) for a population size below a critical value [1], similar as for the Moran process in cyclic bimatrix games [2]. Here [3], we investigate the scaling of the fixation time and show that the crossover from polynomial to exponential scaling is consistent with the drift reversal as demonstrated in [1].

[1] JC Clausen and A Traulsen, Phys. Rev. Lett (2008)

[2] JC Clausen, Eur. Phys. J. (2007)

[3] M Schütt and JC Clausen (in preparation)

BP 35.13 Thu 17:15 Poster B2

Investigating the chemo-mechanical properties of two-dimensional actin networks — KAI UHRIG^{1,2}, RAINER KURRE^{1,2}, ●MARTIN STREICHFUSS^{1,2}, FRIEDRICH ERBS^{1,2}, SIMON SCHULZ^{1,2}, ANABEL CLEMEN^{1,2}, TAMAS HARASZTI^{1,2}, CHRISTIAN BÖHM^{1,2} und JOACHIM SPATZ^{1,2} — ¹MPI for Metals Research, Dept. Spatz, Heisen-

bergstr. 3, 70569 Stuttgart — ²Univ. of Heidelberg, Biophys. Chem. Dept., INF 253, 69120 Heidelberg

The actin cortex, a quasi two-dimensional network of actin, plays an important role in cell stability, motility and viscoelasticity. In vivo, its characteristic properties are controlled by various crosslinkers, such as actin binding proteins or ions. To investigate the influence of a specific crosslinker on the network's behaviour exclusively we create and probe biomimetic models of the actin cortex. This is realized using microbeads trapped by holographic optical tweezers (HOTs) as scaffold for the actin filaments. With this technique we are able to create actin networks in arbitrary geometry and determine the forces exerted by different crosslinkers. Using a special microfluidic flowcell we have full control over the chemical environment in our experiments. The acting forces are measured by highspeed imaging, whereas simultaneous fluorescence microscopy yields information about the structure and density of the actin network. In another approach we use micropillars as framework and measure unzipping forces of crosslinked actin filaments.

BP 35.14 Thu 17:15 Poster B2

Coexistence and phenology of mass-selective predators — ●LAURIN LENGERT, BARBARA DROSSEL, and CHRISTIAN GUILL — TU Darmstadt, Hessen, Deutschland

We study the phenology of predator species, i.e. the chronological succession of species that consume the same prey species within a year. Phenology is modeled by using body-mass dependent attack rates. While prey individuals that are very small compared to predators can easily hide from predators, larger prey individuals have a higher chance to directly escape attacks. This leads to an unimodal capture rate as function of predator and prey size with a maximum at intermediate predator-prey body-mass ratios.

We model the prey to grow during the observed period while the larger predators have a constant body mass (assuming that new born predator individuals are hatching and growing during a different period of the year). Differently sized predator species thus differ in the time when their attack rates on the prey species are maximal.

We analyze the effect of predator phenology on the system's capability to support several predator species with different mean individual body masses and present results concerning minimal size differences between coexisting predators as well as potential invasion scenarios.

BP 35.15 Thu 17:15 Poster B2

The effect of body mass and adaptive foraging on food web robustness — ●LOTTA HECKMANN, CHRISTIAN GUILL, and BARBARA DROSSEL — Institut für Festkörperphysik, TU Darmstadt

Revealing the mechanisms promoting the stability of complex food webs remains a challenge for theoretical ecologists. One apparently stabilizing factor identified recently is the incorporation of allometric scaling, i.e., the influence of the body mass of a species on its metabolic rate, into the differential equations of population dynamics. By this, predator-prey interaction rates become body-mass dependent. Another mechanism contributing to the stability of food webs is adaptive foraging, that is, the capability of predators to focus on more profitable prey.

We numerically investigated the impact of the combined effects of allometric scaling and adaptive foraging on the robustness of food webs, considering different time scales of adaptation (evolutionary vs. behavioural changes) and different predator-prey body mass ratios. Our simulations include nonlinear population dynamics equations with Holling type II functional responses and intraspecific competition. The simulations were performed for different stochastic network structures, such as random graphs or the niche model. Additionally, we analyze in more detail the mechanisms by which adaptive foraging stabilizes food webs by using modules of a small number of interacting species.

BP 36: Posters: Tissue Dynamics, Charge Effects, and Anomalous Transport

Time: Thursday 17:15–20:00

Location: Poster B2

BP 36.1 Thu 17:15 Poster B2

Self-organized growth regulation in developing epithelia — ●PEER MUMCU¹, THOMAS BITTIG¹, ORTRUD WARTLICK², MARCOS GONZÁLEZ-GAITÁN², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany —

²Department of Biochemistry and Department of Molecular Biology, Geneva University, Switzerland

Developing tissues possess intrinsic growth control mechanisms which determine the final size and shape. The basic principles of growth regulation are still poorly understood but it is widely accepted that

certain morphogens act as growth factors that play a key role in this process. Morphogens are a special class of signaling molecules which are secreted from localized sources, spread throughout the tissue and provide cells with positional information. Focusing on the *Drosophila* fly wing as model system, we present a theoretical study of dynamical morphogen distributions in growing epithelia using a continuum theory and a description which is based on discrete cells. The discrete description combines a two-dimensional vertex model for the organization of cells with dynamic equations for the morphogen concentrations. Within this framework we discuss the scaling of morphogen profiles with tissue size. We introduce a growth rule which couples the decision to divide a cell with temporal changes of the cellular morphogen levels. We show that this growth rule can regulate growth in a self-organized way and compare the results to experimental data from the developing fly wing.

BP 36.2 Thu 17:15 Poster B2

An Asymmetric *her* Gene Regulatory Network in the Segmentation Clock — ●SAÚL ARES¹, CHRISTIAN SCHRÖTER², LUIS G. MORELLI^{1,2}, ANDREW C. OATES², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

The segmentation clock is a transcriptional oscillator that controls the sequential segmentation of the vertebrate body axis during embryonic development. Previous models of the zebrafish segmentation clock consisting of symmetric interactions of the cyclic genes *her1* and *her7* were based only on wild type gene expression data. We have combined genetic experiments studying mutations in both these genes and in the non-cyclic *hes6*, together with measurements of the period of oscillation of the several mutant conditions. Our results can not be explained by previous models. To understand them, we propose a new model where the *her* genes have distinct functions in the segmentation clock with asymmetric interactions between them. Our mathematical model is based on a genetic regulatory network where *her1/hes6* and *her7/hes6* heterodimers have opposing functions. This genetic network model is consistent with experiments and makes testable predictions of biochemical interactions in the clockwork. An important insight coming from our model is that heterodimer formation is a rate limiting step and hence plays a key role in control of the segmentation period.

BP 36.3 Thu 17:15 Poster B2

Intercellular coupling tunes the period and stability of a multicellular biological clock — ●LUIS G. MORELLI^{1,2}, SAÚL ARES², LEAH HERRGEN¹, CHRISTIAN SCHRÖTER¹, ANDREW C. OATES¹, and FRANK JÜLICHER² — ¹Max Planck Institute of Molecular Cell Biology and Genetics — ²Max Planck Institute for the Physics of Complex Systems

During vertebrate embryonic development, the body segments are formed in a sequential and periodic process controlled by a multicellular genetic clock. Single cells contain autonomous genetic oscillators, and communicate with their neighbors to produce a reliable rhythm that results in a precise segmented pattern. Intercellular communication involves a complex cascade of events that introduces time delays in the coupling, and coupling delays can have complex effects on the collective dynamics. We have developed a generic description of the segmentation clock using phase oscillators, coupled with a time delay. This theory predicted that coupling strength and delays can tune the period of the segmentation clock and produce changes in segment length and cyclic gene expression patterns. We have verified these predictions under experimental conditions affecting components of intercellular coupling in zebrafish embryos. The theory also predicts the existence of instabilities for certain ranges of the coupling delay. By altering the traffic of ligands involved in inter-cellular communication, we find evidence consistent with such an instability.

BP 36.4 Thu 17:15 Poster B2

Vertex Model for Mechanics and Dynamics of Epithelia — ●DOUGLAS B. STAPLE¹, REZA FARHADIFAR¹, SUZANNE EATON², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Epithelia are sheets of cells that organize into specific geometrical arrangements or morphologies essential for proper tissue functioning. Here we represent epithelia as networks of polygons: stable and stationary network configurations obey force balance and are represented as local minima of a work function. We describe the ground-state

phase diagram to our model, identifying transitions relevant to tissue growth, mechanics, and cell extrusion. The dynamics of cell extrusion and cell-boundary rearrangements depend critically on energetic barriers arising naturally in our model, and are well understood in terms of simple geometric arguments.

BP 36.5 Thu 17:15 Poster B2

Simulation and analysis of neuronal pattern formation in the visual cortex — ●GHAZALEH AFSHAR^{1,2}, DOMINIK HEIDE⁵, LARS REICHL^{1,2}, and FRED WOLF^{1,2,3,4} — ¹MPIDS, Göttingen — ²BCCN, Göttingen — ³Georg-August-Universität, Göttingen — ⁴IMPRS, Göttingen — ⁵FIAS, Frankfurt am Main

Orientation preference maps in the visual cortex, characterized by topological point defects called pinwheels, presumably develop by self-organization of neuronal circuits [1,2]. It was shown recently that the spacing of adjacent orientation columns exhibits a high degree of variability within the visual cortex [3]. We generalized a model based on Turing type instability proposed previously [1] to exhibit a map of local column spacing instead of a single fixed wavelength and studied this model numerically. In the homogeneous model defect densities of solutions split at a late stage of development filling a broad band of values. In the model with spacing heterogeneity this splitting is suppressed. In contrast to the homogeneous model in which the power spectrum of the stable solutions is composed of a finite number of Fourier components, in the heterogeneous model the power spectrum asymptotically shows a continuous band of modes around the critical circle with a finite width depending on the strength of spacing inhomogeneity. This closely resembles the experimental observation. We conclude that wavelength heterogeneity substantially increases the agreement between experimental observation and Turing type models of neural pattern formation. [1] Wolf. PRL (2005). [2] Kaschube et al. NJP (2008). [3] Kaschube et al. PNAS (2009).

BP 36.6 Thu 17:15 Poster B2

Solid tumor growth and fluid transport taking into account a hierarchical network of the host: a three-dimensional theoretical model — ●MICHAEL WELTER and HEIKO RIEGER — Universität des Saarlandes, 66041 Saarbrücken, Germany

Solid tumors like melanoma acquire sufficient nutrients by coopting the host vasculature and inducing angiogenesis in the surrounding tissue. Furthermore their growth is accompanied with a drastic reduction of vessels density and vessel dilation in the center of the tumor. Thus the original well organized hierarchical network becomes chaotic and a heterogeneously distributed tumor vasculature is formed. We develop a hybrid stochastic/continuum model for three-dimensional tumor growth which includes an explicit representation of the hosts vasculature and its remodeling via sprouting, vessel removal and dilation. The evolution of the tumor mass is captured by a diffusion-reaction model. The heterogeneity and leakiness of tumor vessels is highly relevant for the exavasation and interstitial transport of drugs since large non-vascularized regions exist and high interstitial fluid pressures may impede flow through the vessel walls. Therefore we analyze the flow of a tracer through the interstitial space coupled to our tumor networks by means of a convection-diffusion-reaction model.

BP 36.7 Thu 17:15 Poster B2

Ion Transport through OmpF and OmpC Channels Simulated using Molecular Dynamics — SOROOSH PEZESHKI, ISTVAN BIRO, MATHIAS WINTERHALTER, and ●ULRICH KLEINEKATHÖFER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

The outer membrane porins F and C (OmpF and OmpC) are major pores in the cell membrane of the Gram-negative bacterium *Escherichia coli*. They are considered the main pathways for ions and molecules through the membrane. Using the crystal structures, it is possible to study OmpF and OmpC in computer simulations. The ion conductance through these nano pores is simulated in all-atom molecular dynamics and the temperature dependence of the conductance is calculated for different salt concentrations. Good agreement can be observed in the comparison between simulations and experiments [1]. The advantage of molecular dynamics simulations is that they allow a deeper view on the molecular interactions leading to the macroscopic observation. Ion pathways can be followed and the interaction of ions with certain residues can be observed [2].

[1] S. Pezeshki, C. Chimere, A. Bessenov, M. Winterhalter, U. Kleinekathöfer, Biophys. J. **97**, 1898 (2009).

[2] C. Chimere, L. Movileanu, S. Pezeshki, M. Winterhalter, U. Kleinekathöfer, Eur. Biophys. J. **38**, 121 (2008).

BP 36.8 Thu 17:15 Poster B2

Charge induced liquid-liquid phase separation in protein solutions — ●MARCELL WOLF, ZHANG FAJUN, and SCHREIBER FRANK — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The liquid-liquid phase separation (LLPS) in concentrated protein solutions plays an important role for protein crystallisation as well as protein-association related diseases, such as the sickle cell anemia and eye cataracts, etc. Here, we show that the LLPS in protein solutions can be induced by using a multivalent salt, using Human Serum Albumin (HSA) and Yttrium Chloride (YCl₃). The phase diagram of HSA with YCl₃ was determined; it shows a re-entrant phase behaviour [1], i.e. the protein solution undergoes a phase-separation upon adding salt up to a critical value c^* , c^{**} , causes the precipitate to dissolve and the system turns back to a homogeneous solution. In the condensed phase between c^* and c^{**} the solution exhibits a (L-L) phase separation. After centrifugation, a protein-poor and a protein-rich phase were obtained and the protein concentration for each phase was determined using UV-visible spectroscopy. We also discuss the effect of the LLPS conditions for protein crystallisation.

[1] F. Zhang et al., Phys. Rev. Lett. 101 (2008) 148101

BP 36.9 Thu 17:15 Poster B2

Reentrant Condensation of protein solutions induced by Fe³⁺ and Al³⁺ — ●BENJAMIN HECK, FAJUN ZHANG, and FRANK SCHREIBER — Auf der Morgenstelle 10, Universität Tübingen, 72076 Tübingen, Germany

The trivalent ions such as Fe³⁺ can be physiologically important and also relevant in the context of protein-aggregation diseases such as Alzheimer. Therefore it is important to understand their impact on protein interactions and phase behavior in solution. Using model globular proteins, we found that addition of Fe³⁺/Al³⁺ into protein solution leads to a reentrant phase behavior [1]. When salt concentration, c , is below a critical value, $c < c^*$, proteins are negatively charged. The repulsive Coulomb interaction is dominating which stabilizes proteins in solution. Above c^* , aggregation occurs because the effective surface charge of proteins is significantly reduced due to the binding of cations on the protein surface. Further increase salt concentration above a second critical value, c^{**} , one finds redissolution which in a simple picture is interpreted as effective inversion of charges [1]. Charge inversion takes place only for multivalent ions. Electrophoresis experiments confirm the effective charge inversion of proteins as a function of salt concentration. Small-angle X-ray scattering data further reveal a clear transition of interactions from repulsive to attractive and to repulsive again at $c < c^*$, $c^* < c < c^{**}$ and $c^{**} < c$, respectively. [1] F. Zhang et al., Phys. Rev. Lett. 101 (2008) 148101

BP 36.10 Thu 17:15 Poster B2

Anomalous transport in living cells — ●DORIS HEINRICH — Biophysics of Cell Dynamics Group, Fakultät für Physik und CeNS, LMU München, Germany

Living cells exhibit exceptional dynamic properties, caused by the presence of ATP-driven motion. In particular, intracellular transport of cargos proceeds by successive phases of diffusion and active movement along microtubules via dynein and kinesin motors. While passive Brownian motion allows for intracellular transport of molecules on the nanoscale, it becomes inefficient for transport of large proteins, vesicles and organelles on the scale of a whole cell. We developed an automated and reliable time-resolved identification method for motility state signatures of cytoplasmic tracers. Such an approach is both experimentally challenging and of fundamental importance for our understanding of intracellular transport processes. We investigated the motion of micron- and nanosized particles in the amoeba *Dictyostelium discoideum* (Dd). The distribution of active transport durations is found to decay exponentially with a characteristic time $t = 0.65$ s. The velocity distribution of active events exhibits several peaks, revealing the signature of a finite number of molecular motors working collectively. By further applying spatially and temporally defined external boundary conditions to these cells, like drugs, precisely monitored magnetic field gradients or by cell motility essays on pre-ordered 3D topologies, we induce changes in cellular function.

BP 36.11 Thu 17:15 Poster B2

Non-ballistic and subdiffusive nanoparticle transport in living cells — ●MARCUS OTTEN¹, AMITABHA NANDI², DELPHINE ARCIZET¹, BENJAMIN LINDNER², and DORIS HEINRICH¹ — ¹Ludwig-Maximilians-Universität and Center for NanoScience (CeNS), München, Germany — ²Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

Intracellular transport of vesicles, macromolecules and organelles relies on ballistic and diffusive (including subdiffusive, Brownian and superdiffusive) motion. Local mean square displacement (MSD) analysis allows for the time-resolved separation of these two motion types and their respective motion parameters. It has been established that the ballistic regime is determined by molecular motors. The diffusive regime is of particular interest for inferring information about the cytoskeleton's role in transport.

The non-ballistic phases of intracellular transport are characterized experimentally using nanoparticles in *Dictyostelium discoideum* cells. Local MSD analysis yields the distributions for the effective diffusion coefficient and the local MSD exponent. These statistics can be reproduced by simulating a Brownian motion the increments of which are negatively correlated over short times. Very good agreement of the experimental and simulated statistics yields valuable information about the short-timescale subdiffusive behaviour and an underlying biophysical picture.

BP 37: Biomaterials

Time: Friday 10:00–13:00

Location: H43

Invited Talk BP 37.1 Fri 10:00 H43
Pearls and Feathers: New Concepts and Inspiration for Plant's Design — ●INGRID WEISS, EDUARD ARZT, and HELMUT KIRCHNER — INM - Leibniz Institute for New Materials gGmbH, Campus D2 2, D-66123 Saarbrücken, Germany

Pearls and nacre are at the forefront of understanding the earliest genetic routes towards high-performance composite materials. Also the display function of birdfeathers for sexual attraction implies very specific needs of evolutionary relevance. Our work demonstrates that various functions are achieved by the composite structure of biological materials, which is better than the sum of its parts. While pearls consist of micro- and nano-patterned aragonite with low organic content, the cortex material of feathers, beta-keratin, is homogeneous over about 80% of the length of the rachis. Our ongoing research on chitin in pearls [1,2], and on keratin in feathers [3] aims at understanding what exactly happens in feather follicles under load, and in pearl forming tissue during the process of biomineralization thus creating a basic link between gravity, materials properties, and life. This would as well be relevant for understanding complex structured materials such as plants.

References [1] I.M. Weiss, Jewels in the pearl, ChemBioChem, in

press (2010) [2] I.M. Weiss et al., The chitin synthase involved in marine bivalve mollusk shell formation contains a myosin domain, FEBS Lett. 580, 1846-1852 (2006) [3] I.M. Weiss & H.O.K. Kirchner, The peacock's train (*Pavo cristatus* and *Pavo cristatus mut. alba*) I. Structure, mechanics, and chemistry of the tail feather coverts, J. Exp. Zool. A, submitted, (2009)

BP 37.2 Fri 10:30 H43

New functional ceramic composites through biomineralisation? — ●KATHARINA GRIES^{1,2}, MALTE LAUNSPACH¹, MEIKE GUMMICH¹, TANJA DODENHOF¹, ANDREAS ROSENAUER², and MONIKA FRITZ¹ — ¹Pure and Applied Biomineralisation, Biophysics Institute, Universität Bremen, Germany — ²Electron Microscopy Group, Solid State Physics, University Bremen, Germany

The biogenic polymer/mineral composite nacre is grown by a self-organisation process, where a few weight percent of organic material governs the specific crystallization of the calcium carbonate polymorph aragonite. The thus developed material shows a dense packing of thin layers (500nm) of mineral platelets interdispersed by a few nanometer of organics, acting like a glue to improve the mechanical properties of this biogenic ceramic by making it non-brittle. In order to be able to

make use of this self-organised structure formation for future purposes and applications we have to understand this process, which results in the microstructure with mineralized platelets embedded in bioorganic nanolayers. In direct atomic force microscopy experiments and in crystallization experiments, on the interaction of model polymers and purified proteins with the mineral calcium carbonate, crystal nucleation and inhibition properties of the different polymers and proteins were discovered. We employ SEM (scanning electron microscopy), AFM (atomic force microscopy), precipitation assays, contact angle measurements and theoretical simulations to investigate the interaction processes between organic and inorganic material in the natural and synthetic composites.

BP 37.3 Fri 10:45 H43

The nanostructure of biogenic calcite: a 3D SAXS/WAXS study. — ●CHRISTOPH GILOW¹, BARBARA AICHMAYER¹, CHENGHAO LI¹, STEFAN SIEGEL¹, OSKAR PARIS², EMIL ZOLOTYABKO³, and PETER FRATZL¹ — ¹Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Research Campus Golm, 14424 Potsdam, Germany — ²Institute of Physics, University of Leoben, A-8700 Leoben, Austria — ³Department of Materials Engineering, Technion - Israel Institute of Technology, Haifa 32000, Israel

Biogenic crystals grow in the presence of organic macromolecules which influence their shape and internal structure, often resulting in superior material characteristics. Calcitic prisms from the shell of the *Pinna nobilis* scatter like single crystals, despite containing significant amounts of intra-crystalline organic macromolecules which cause anisotropic distortions of the calcite unit cells. Individual prisms were investigated by means of 3D wide- and small-angle scattering (SAXS/WAXS) using synchrotron radiation at the μ -Spot beamline, BESSY II, Helmholtz Zentrum Berlin. The SAXS signal was also found to be strongly anisotropic and had a fixed orientation correlation to the WAXS pattern. Additional insights into the nanostructure of calcitic prisms and the organic-mineral interfaces were gained by laboratory SAXS measurements on powdered samples as well as by SEM studies on etched samples. Annealing the prisms at 300°C, a temperature which was chosen to mainly affect the organic macromolecules, led to substantial structure rearrangements on a nano-scale.

BP 37.4 Fri 11:00 H43

The ordered arrangement of secondary osteons in long bones — ●CAROLIN LUKAS¹, RON SHAHAR², JOHN DUNLOP¹, SHARON PAPO², and RICHARD WEINKAMER¹ — ¹Max Planck Institut of Colloids and Interfaces, Potsdam — ²The Hebrew University of Jerusalem, Rehovot, Israel

Bone remodeling, the renewal process of bone, leads in compact bone to the formation of cylindrical structures called osteons. In the central cavity (haversian canal) of the osteon a blood vessel is responsible for the supply of nutrients to the bone cells. This work aims (i) to quantify the order in the arrangement of haversian canals and (ii) to use a simple model to explain the measured order. Using microscopy we studied different long bones (radius, metacarpal) from horses and dogs at different anatomical locations. The spatial arrangement of osteons was quantified by the use of the autocorrelation function (ACF) and by the shortest distance distribution (SDD) which describes how far away bone is from its nearest haversian canal. In our model the arrangement of osteons is created by a random sequential addition process. Each osteon is characterized by an haversian canal surrounded by a circular exclusion zone within which the creation of another osteon is prohibited (cherry-pit model). The radii of the exclusion zone are assumed to be normally distributed. The analysis of the microscopic images showed that the ACFs and SDDs are independent of the anatomical location in the horse radius, but not in the metacarpal bone. These differences could be explained by the model, by either increasing the mean value of the exclusion radius or the standard deviation.

BP 37.5 Fri 11:15 H43

Bioactive surfaces from polymeric films aiming at near IR-light triggered cellular response — ●DMITRY VOLODKIN^{1,3}, ANDRE SKIRTACH¹, NARAYANAN MADABOOSI¹, JENIFER BLACKLOCK¹, REGINE VON KLITZING³, ANDREAS LANKENAU², CLAUS DUSCHL², and HELMUTH MÖHWALD¹ — ¹MPIKG, Am Mühlenberg 1, 14476 Potsdam-Golm, Germany — ²IBMT, Am Mühlenberg 13, 14476 Potsdam-Golm, Germany — ³TU Berlin, Strasse des 17. Juni 124, 10623 Berlin, Germany

The layer-by-layer (LbL) polymer self-assembly based on consecutive polymer adsorption has emerged as a powerful and versatile strategy to

engineer surface films for bio-applications. Here we present composite LbL-assembled dynamic films possessing high loading capacity, remote release functionalities, and controlled cellular response. The film has been formed using two biopolymers, namely hyaluronic acid (HA) and poly-L-lysine (PLL). The film able to embed material of different nature (from flexible macromolecules such as DNA and proteins to nano- and microparticles) in extremely high amounts (tens of mg per cm²) that is related to spontaneous "polymer doping". Here we present remote release of film-entrapped material by "biofriendly" near-infrared light. Composite HA/PLL film with embedded gold nanoparticles and biomacromolecules or microcapsules hosting biomolecules can be activated by infrared light resulting in biomolecules* release. The films can be constructed to be cell (fibroblasts) adhesive or cell resistant depending on its intrinsic properties. Light-triggered DNA transfection to individual cell is demonstrated.

15 min. break

BP 37.6 Fri 11:45 H43

The Effect of Large Strain Deformations on the Non-linear Material Properties of Collagen — ●STEFAN MÜNSTER^{1,2}, LOUISE JAWERTH², DAVID WEITZ², and BEN FABRY¹ — ¹Department of Physics, University Erlangen-Nuremberg, Germany — ²Department of Physics, Harvard University, Cambridge, USA

Collagen is the most abundant protein in vertebrates, and its mechanical properties govern the structure and function of many tissues. When subjected to large strain, collagen shows strain-stiffening behavior typical for biopolymers. Here, we investigate how the strain-stiffening response of collagen changes as the material undergoes repeated large strain oscillations. We shear *in vitro* reconstituted collagen gels in a plate-plate rheometer by applying sinusoidal strain oscillations, and analyze the non-linear stress-strain relationship. With each cycle, the maximum stress and the linear modulus of the material decrease, and the strain-stiffening response occurs at higher strains. Surprisingly, the shape of each stress-strain response is similar to that observed during the previous cycle, only shifted towards larger strain values. Upon addition of covalent crosslinks by incubating the polymerized collagen gels with 2% glutaraldehyde solution, the stress-strain relationship becomes independent of the loading history. We hypothesize that the microscopic mechanism responsible for the history dependence is intra-fibrillar slip of adjacent collagen monomers, which increases the rest lengths of previously strained fibers. A simple visco-elastic model which takes the fibrillar structure of the gels into account shows remarkable similarity with our experimental data.

BP 37.7 Fri 12:00 H43

Using microtubules to measure actin viscoelasticity — FELIX ZÖRGIEBEL¹, ●MARCEL BREMERICH¹, FREDERICK C. MACKINTOSH², and CHRISTOPH F. SCHMIDT¹ — ¹III. Physikalisches Institut, Georg-August-Universität, 37077 Göttingen — ²Department of Physics & Astronomy, Vrije Universiteit, 1081 HV Amsterdam

In conventional active and passive microrheology techniques, micron-sized particles are embedded in biological samples for probing their viscoelastic properties. These methods are not always well suited for investigating the interior of living cells because the probe particles can perturb their neighborhood and because surface interactions can occur. Such problems can be elegantly circumvented by using natural constituents of the cellular system as local probes. The thermal bending fluctuations of microtubules, for instance, intrinsically carry information about the mechanical properties of the surrounding medium. It turns out that one can investigate local shear moduli and stress fluctuations in biopolymer networks by a detailed analysis of the spatial and temporal bending fluctuations of just one point of a microtubule, largely without introducing probe artifacts. To test this new method, we sparsely seeded an *in vitro* network of filamentous actin with microtubules which were again sparsely labeled with nanometer-sized gold particles. The displacements of these particles were then tracked by laser interferometry using an optical trap. Knowing the microtubule elastic properties, the observed bending dynamics allowed us to estimate the complex shear modulus of the surrounding actin network.

BP 37.8 Fri 12:15 H43

Micromechanical Properties and Structure of the Pericellular Coat of Living Cells — ●HEIKE BÖHM¹, TABEA MUNDINGER¹, VALENTIN HAGEL¹, UWE RAUCH², JENNIFER CURTIS³, and JOACHIM SPATZ¹ — ¹Max-Planck-Institute for Metals Research, Department New Materials & Biosystems & University of Heidelberg, Department

of Biophysical Chemistry, Heisenbergstr. 3, 70569 Stuttgart, Germany — ²Vessel Wall Biology, Department of Experimental Medical Science, Biomedical Center, Lund University, 221 84 Lund, Sweden — ³School of Physics, Georgia Institute of Technology, 837 State Street, Atlanta, GA

Most mammalian cells are enveloped by a coat of polysaccharides and proteins, the pericellular coat (PCC). It plays a vital role in biological processes such as adhesion and proliferation. The PCC's backbone is composed of hyaluronan (HA), a highly hydrated polysaccharide that anchors the coat to the cell membrane. The molecular interaction of hyaluronan with different HA binding proteins determines the architecture of the PCC. Their mesoscopic arrangement influences not only the cell's perception of its environment but also its ability to withstand compression. This is especially important for our cells of interest: chondrocytes living and maintaining the load-bearing cartilage. In order to study the mesoscopic structure of the PCC, we employ a toolbox of different biophysical techniques, including confocal microscopy, particle tracking microrheology [1] and adhesive nanostructured surfaces. T [1] H. Boehm, T. A. Munding, C. H. J. Boehm, V. Hagel, U. Rauch, J. P. Spatz, J. E. Curtis, *Soft-Matter* 2009, DOI: 10.1039/B905574F.

BP 37.9 Fri 12:30 H43

Linker Induced Actin Network Formation under Cell-Sized Confinement — ●FLORIAN HUBER, SEBASTIAN EHRIG, CARSTEN VOGT, DAN STREHLE, and JOSEF KÄS — Division of Soft Matter Physics, Department of Physics, University of Leipzig, Linnéstr. 5, D-04103 Leipzig, Germany

Cross-linked actin networks are decisively involved in the overall mechanical properties of cells. The networks' architecture ranges from densely packed bundles to networks with high crossing angles and is typically assigned to specific linker proteins. Recently, however, it was found that weak cross-linkers give rise to both extended networks and bundles. We used multivalent ions as model-linkers to study actin fil-

ament aggregation in cell-sized geometries. Small droplets filled with actin filaments are sealed by a thin oil film to control droplet evaporation. At a critical concentration of multivalent ions their potential turns attractive. This implies a phase transition from isotropic or nematic f-actin solutions to cross-linked actin networks.

In addition to the well-known bundle formation, we obtained regularly spaced networks of star-like astern patterns. These networks display many features of cellular networks in the actin cortex and may serve as a model system for the cortical actin layer. Moreover, by altering the linker properties it was possible to switch between different network architectures. Observed phase transitions are fast (seconds to few minutes) which is of high interest concerning the known ability of living cells to quickly modify their morphology.

BP 37.10 Fri 12:45 H43

Active polar gels in a Taylor Couette Geometry — ●MATTHIAS MUSSLER and ALBRECHT OTT — Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken

The Taylor Couette Geometry is a well researched system for polymer-suspensions and many other inactive fluids. Our experimental approach starts with the assumption that, if a fluid or suspension has active components, the critical Taylor Number is influenced by these active processes, i.e. filament de-/polymerisation, and the phase diagram will change. This is observable by the formation of Taylor Vortices or other flow figures and calculable by the stimulus in relation to the flow variation. For these experiments we use an extract of *Xenopus* Oocytes as an example for acellular but nonetheless active fluid and Macrophages as an example for highly active living cells in a coaxial cylinder geometry in a commercial rheometer. The calculus of these experiments is based on the theory of active polar gels described by Kruse et al. This theory describes an active fluid with several components. It takes into account polar order and considers the case when one component is viscoelastic.

BP 38: Focus: Charge Effects in Soft and Biological Matter III (joint CPP, BP, ST)

Time: Friday 10:15–12:00

Location: H45

Invited Talk

BP 38.1 Fri 10:15 H45

Charge inversion in macromolecular systems — ●CHRISTIAN HOLM — Institut für Computerphysik, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany

We discuss our current understanding of the phenomenon of charge inversion in macromolecular systems, based on simulational results in recent years. In this approach the solvent has been incorporated only as an implicit dielectric background, whereas all charges and salt ions are treated explicitly. We will also discuss our recent work on modelling electrophoresis of charged polymers within a coarse grained approach, where the solvent degrees of freedom have been modelled using a Lattice-Boltzmann algorithm.

[1] R. Messina, C. Holm, K. Kremer, *Ground state of two unlike charged colloids: an analogy with ionic bonding*, *Euro. Phys. Lett.*, **51**, 461 (2000).

[2] O. Lenz, C. Holm, *Simulation of charge reversal in salty environments: Giant overcharging?*, *Euro. Phys. J. E* **26**, 191-195 (2008).

[3] K. Grass, C. Holm *Mesoscale modelling of polyelectrolyte electrophoresis*, *Faraday Discuss.* **144**, 57-70 (2010).

BP 38.2 Fri 10:45 H45

Counterion condensation and effective charge of linear and globular macromolecules — UTE BÖHME and ●ULRICH SCHELER — Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden

The charge density on charged macromolecules is usually so high, that the thermal energy of the respective counterions is insufficient to escape the electric field generated from the charges on the macromolecule. Therefore a fraction of counterions condenses on the macromolecule, lowering the effective charge of the macromolecule. The combination of diffusion and electrophoresis NMR provides an unambiguous possibility for the experimental determination of the effective charge, which is in good agreement with molecular simulations [1, 2]. This approach has been applied to flexible and stiff polyelectrolytes as well as proteins and other globular molecules [5]. Because PAMAM dendrimers exhibit only two types of chargeable groups, counterion condensation

can easily be quantified, where the degree of protonation of the amino groups is inferred from proton NMR spectra. The fraction of condensed counterions increases with increasing molecular weight to level at about 70%. The effect of the variation of the solvent properties is studied with variation of the ionic strength and the dielectric constant of the solution.

[1] K. Grass, U. Böhme, U. Scheler, H. Cottet, C. Holm, *Physical Review Letters* **100**, (2008) 096104 [2] U. Scheler, *Current opinion in Colloid & Interface Science*, **14** (2009), 212 [3] U. Böhme, U. Scheler, *Coll. & Surf. A.*, **222**, (2003), 35

BP 38.3 Fri 11:00 H45

Detection of multilayer formation of charged macromolecules by field-effect devices: from experiment to theory — ●ANDREY CHERSTVY¹, MARIAM ABOUZAR², and ARSHAK POGHOSSIAN² — ¹IFF-2, FZ Jülich, Germany — ²IBN-2, FZ Jülich, Germany

Field-effect based semiconductor devices for label-free detection of adsorption of charged macromolecules are widely used for biosensor applications. The quantitative understanding of signals measured is however still missing in many cases. We use a capacitive electrolyte-insulator field-effect device for electrical detection of layer-by-layer adsorption of oppositely charged polyelectrolyte PE PSS/PAH chains onto the sensor surface [1]. We measure the thickness of PE layers formed as well as the changes in morphology and wettability of the modified sensor surface. We also study the effects of ionic strength on the sensor signal detected upon PE multilayer formation. We observe progressively decaying oscillations of the sensor potential upon repetitive PE adsorption. To analyze these zig-zag variations, we develop a theoretical model that accounts for the Debye screening by mobile ions within the PE layer. The model predicts that potential oscillations monitored by the sensor originate from the sign and the charge density of last PE layer. These variations depend strongly on bulk electrolyte concentration and physical parameters of PE multilayers. At lower salt, the oscillations predicted are much larger and more persistent with number of PE layers deposited. The magnitude and decay length of oscillations are in good agreement with experimental

observations.

[1] A. G. Cherstvy et al., submitted to J. Phys. Chem. B.

BP 38.4 Fri 11:15 H45

Electrostatic interactions control the permeability of biological hydrogel filters — •OLIVER LIELEG^{1,3}, LUCY COLWELL^{1,2}, REGINA BAUMGÄRTEL^{1,3}, IOANA VLADSCU¹, MICHAEL BRENNER², ANDREAS BAUSCH³, and KATHARINA RIBBECK¹ — ¹FAS Center for Systems Biology, Harvard University, Cambridge, USA — ²School of Engineering and Applied Sciences, Harvard University, Cambridge, USA — ³Lehrstuhl für Zellbiophysik E27, Technische Universität München, Germany

The controlled exchange of molecules between biological entities (organelles, cells, or organisms) and their environment is critical for life. Biological hydrogels appear well suited to achieve such selective exchange: A hydrogel within the nuclear pore controls the passage of material between the nucleus and the cytoplasm. Mucus hydrogels lining the uterus, the stomach or the lung allow us to expel ingested particles and defend the cells beneath from a variety of pathogens. Extracellular matrix hydrogels in the connective tissue regulate the distribution of growth factors, proteins or drugs. Although hydrogel based filters are integral parts of biology, clear concepts of how their barrier function is controlled on a microscopic level are missing. Here, we discuss three biological hydrogels which differ in terms of their composition and biological function, but nevertheless seem to share a common physical design principle that regulates their microscopic barrier function: We demonstrate that particle translocation in these hydrogels is based on electrostatic interactions between diffusing particles and the hydrogel polymers rather than size exclusion effects.

BP 38.5 Fri 11:30 H45

Diffusion and charge transport in ionic liquids: the role of ion-ion interactions — •JOSHUA SANGORO, CIPRIAN IACOB, JÖRG KÄRGER, and FRIEDRICH KREMER — Institute of Experimental

Physics I, University of Leipzig, Linnéstr. 5, 04103, Leipzig

Self-diffusion in a variety of glass-forming ionic liquids (ILs) are investigated in a wide frequency and temperature range by means of Broadband Dielectric Spectroscopy (BDS) and Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR). It is experimentally shown that in the time-scale characterising the cross-over from sub-diffusive to diffusive ion dynamics, the hopping lengths are of the order of molecular diameters determined from quantum-chemical calculations. This provides a direct means - via Einstein-Smoluchowski relation - to determine diffusion coefficients by BDS over more than 8 decades unambiguously and in quantitative agreement with independent PFG NMR measurements. Unprecedented possibilities in the study of charge transport and dynamic glass transition are thus opened.

BP 38.6 Fri 11:45 H45

Collapse of highly charged polyelectrolytes triggered by attractive dipole-dipole interactions — •ANDREY CHERSTVY — IFF-2, FZ Juelich

We study the collapse of flexible highly charged polyelectrolyte PE chains induced by attractive dipole-dipole interactions [1]. The latter emerge due to formation of dipoles between the chain monomers and counterions condensed on PE from solution. Using the statistics of slightly perturbed Gaussian polymers, we obtain the scaling relations for PE dimensions as a function of PE charge density in the limit of compacting chains. The results are in good agreement with the outcomes of MD simulations of collapse of flexible PEs with explicit counterions. Then, we analyze the results of MD simulations for complex formation by two highly charged PEs carrying opposite charges. We use the scaling arguments based on the picture of complexation of electrostatic blobs to rationalize the size of complexes of the two chains in the collapsed state. We also analyze PE linear charge densities required for the onset onto collapse. [1] A. Cherstvy, submitted to JPCB.