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Overview of Invited Talks and Sessions

(lecture rooms C 243 and PC 203; Poster A)

Invited Talks

BP 1.1	Mon	9:30–10:00	C 243	**Chemotaxis and Cell Migration: Sensing and Intracellular Dynamics** — •Eberhard Bodenschatz, Carsten Beta, Albert Bae, Gabriel Amselem
BP 1.2	Mon	10:00–10:30	C 243	**Regulation of Growth during Development: Role of Mechanics** — •Lars Hufnagel
BP 3.1	Mon	14:00–14:30	C 243	**How to Take a Quick Look—Rapid Neural Coding of Visual Information in the Retina** — •Tim Gollisch
BP 8.1	Tue	9:30–10:00	C 243	**Active stress fluctuations in biopolymer networks driven by molecular motors** — •Gijsje H. Koenderink, Marina Soares e Silva, Frederick C. MacKintosh
BP 8.2	Tue	10:00–10:30	C 243	**Regulation of microtubule sliding by antagonizing microtubule motors and crosslinkers** — •Marcel Janson
BP 20.1	Thu	9:30–10:00	C 243	**Modeling noisy concentration gradients inside single cells** — Filipe Tostevin, Pieter ten Wolde, •Martin Howard
BP 20.2	Thu	10:00–10:30	C 243	**Non-equilibrium dynamics of gene expression** — •Johannes Berg
BP 24.1	Thu	14:00–14:30	C 243	**A biochemical reconstitution approach of the coordinated actin assembly dynamics in motile and morphogenetic processes.** — •Marie-France Carlier, Louis Renault, Guillaume Romet-Lemonne, Emmanuele Helfer, Beata Bugyi, Kim Ho Diep Le, Dominique Didry, Stéphane Romero
BP 27.1	Fri	10:15–10:45	C 243	**Secretion of protein-coated vesicles** — •Pierre Sens

Invited talks of the joint symposium SYSM

See SYSM for the full program of the Symposium.

SYSM 1.1	Tue	14:00–14:30	H 0105	**Two-Focus Fluorescence Correlation Spectroscopy: A versatile tool for precise measurements of molecular diffusion** — •Jörg Enderlein, Anastasia Loman, Thomas Dertinger, Iris von der Hocht, Bernd Müller, Victor Pacheco, Konstantin Komolov, Karl-Wilhelm Koch, Ingo Gregor
SYSM 1.2	Tue	14:30–15:00	H 0105	**Tracking and Manipulating Single Molecule Diffusion in Liquids** — •Frank Cichos
SYSM 1.3	Tue	15:00–15:30	H 0105	**Single Molecule Studies on Myosin Motors** — •Claudia Veigel
SYSM 1.4	Tue	16:00–16:30	H 0105	**Real-time observation of bacteriophage T4 gp41 helicase reveals unwinding mechanism** — M. Manosa, T. Lionnet, M. M. Spiering, S. J. Benkovic, D. Bensimon, •V. Croquette
SYSM 1.5	Tue	16:30–17:00	H 0105	**From valleys to ridges: Exploring the dynamic energy landscape of single membrane proteins** — •Daniel Müller

Invited talks of the joint symposium SYMP

See SYMP for the full program of the Symposium.

SYMP 1.1	Thu	9:30–10:00	H 0105	**Hydrodynamic cooperativity in active fluids** — •Ignacio Pagonabarraga
SYMP 1.2	Thu	10:00–10:30	H 0105	**Hydrodynamic Effects on Molecular Motion** — •Raymond Kapral
SYMP 1.5	Thu	11:15–11:45	H 0105	**Proton transport through water-filled narrow pores** — •Christoph Dellago
SYMP 1.6	Thu	11:45–12:15	H 0105	**Role of fluctuations in the selectivity mechanism for the KcsA potassium channel** — •Michael E. Paulaitis, Dilip Asthagiri, Lawrence R. Pratt
SYMP 2.1	Thu	14:00–14:30	H 0105	**DNA mechanics and dynamics** — •Richard Lavery
SYMP 2.2	Thu	14:30–15:00	H 0105	**Charge mobility of discotic mesophases of polyaromatic hydrocarbons: a multiscale quantum/classical study** — •Denis Andrienko
SYMP 2.4	Thu	15:30–16:00	H 0105	**Simulation of coarse-grained membrane models** — •Marcus Müller
SYMP 2.5	Thu	16:00–16:30	H 0105	**Fragments of a computational cell: mesoscopic simulations of soft matter** — •Julian C. Shillcock

Invited talks of the joint symposium SYDN

See SYDN for the full program of the Symposium.

SYDN 1.1	Fri	10:10–10:50	H 0105	**Volunteering and Punishment in Public Goods games** — •Christoph Hauert
SYDN 1.8	Fri	12:20–13:00	H 0105	**Inequity Concerns in Social Networks** — •Pablo Branas-Garza

Sessions

BP 1.1–1.11	Mon	9:30–13:00	C 243	**Cell Migration and Tissue Dynamics**
BP 2.1–2.10	Mon	10:30–13:15	PC 203	**DNA and Chromatin**
BP 3.1–3.11	Mon	14:00–17:15	C 243	**Neuronal Systems**
BP 4.1–4.6	Mon	14:30–16:00	PC 203	**Novel Methods**
BP 5.1–5.4	Mon	16:15–17:15	PC 203	**Photobiophysics**
BP 6	Mon	14:30–16:45	MA 001	**Statistical Physics in Biological Systems (joint session DY/BP)**
BP 7.1–7.54	Mon	17:00–19:30	Poster A	**Posters I**
BP 8.1–8.11	Tue	9:30–13:00	C 243	**Active Filament Networks**
BP 9.1–9.9	Tue	10:30–13:00	PC 203	**Membranes and Interfaces**
BP 10.1–10.4	Tue	14:00–15:00	C 243	**Self Propulsion**
BP 11.1–11.8	Tue	15:15–17:15	C 243	**Transport Processes**
BP 12.1–12.5	Tue	17:30–18:45	C 243	**Cellular Force Generation**
BP 13.1–13.6	Tue	17:15–18:45	PC 203	**Biopolymers**
BP 14	Tue	17:00–19:00	C 230	**Single Molecules (joint session CPP/BP)**
BP 15.1–15.12	Wed	14:00–17:15	C 243	**Single Molecules**
BP 16.1–16.6	Wed	17:30–19:00	C 243	**Pattern Formation and Developmental Processes**
BP 17.1–17.7	Wed	14:00–15:45	PC 203	**Physics of Cells**
BP 18.1–18.5	Wed	16:00–17:15	PC 203	**Biomaterials**
BP 19.1–19.8	Wed	17:30–19:30	PC 203	**Semiflexible Polymers and Networks**
BP 20.1–20.8	Thu	9:30–12:00	C 243	**Regulation and Signaling**
BP 21.1–21.4	Thu	12:15–13:15	C 243	**Population Dynamics and Evolution**
BP 22.1–22.5	Thu	10:30–11:45	PC 203	**Cell Mechanics**
BP 23.1–23.5	Thu	12:00–13:15	PC 203	**Electrical Stimulation and Recording**
BP 24.1–24.9	Thu	14:00–16:45	C 243	**Actin Dynamics**
BP 25.1–25.10	Thu	14:30–17:00	PC 203	**Protein Structure and Folding**
BP 26.1–26.55	Thu	17:00–19:30	Poster A	**Posters II**
BP 27.1–27.8	Fri	10:15–12:45	C 243	**Membrane Morphology and Adhesion**
BP 28.1–28.8	Fri	10:45–12:45	PC 203	**Molecular Recognition**

Annual General Meeting of the Biological Physics Division

Tuesday 19:00–20:00 C 243

- Bericht

BP 1: Cell Migration and Tissue Dynamics

Time: Monday 9:30–13:00 Location: C 243

Invited Talk BP 1.1 Mon 9:30 C 243

Chemotaxis and Cell Migration: Sensing and Intracellular Dynamics — •Eberhard Bodenschatz, Carsten Beta, Albert Bae, and Gabriel Amselem — MPI for Dynamcis and Self-Organization, Goettingen, Germany

We report on chemotaxis and cell migration of the eukaryote Dictyostelium d.(Dicty) under well-controlled spatial and temporal stimuli in microfluidic devices. First the chemotactic response to stationary, linear gradients of cAMP will be reported. In shallow gradients of less than 10ˆ-3 nM/μm, the cells showed no directional response and exhibited a constant basal motility. In steeper gradients, cells moved up the gradient on average. In very steep gradients, above 10 nM/μm, the cells lost directionality and the motility returned to the sub-threshold level. We found cells to be able to chemotact well even when the average difference in receptor occupancy at the front and back of the cell is estimated to be only about 10 receptor molecules. Then we report experiments on the intracellular response of of PH-domain proteins to well controlled chematractant gradients. We use the photo-chemical release of caged cAMP in microfluidic devices to expose single chemotactic cells to spatio-temporally well controlled chemoattractant stimuli (switching time approx. 0.5 sec and arbitrarily shaped gradients). We found that the translocation signal sets in with a finite response only for steep gradients. At shallow gradients no translocation signal could be measured. A theory describing polarization of the intracellular signaling system will be presented. This work is in collaboration with W. Loomis, H. Levine and W. Rappel at UCSD.

Invited Talk BP 1.2 Mon 10:00 C 243

Regulation of Growth during Development: Role of Mechanics — •Lars Hufnagel — EMBL Heidelberg, Heidelberg, Germany

A fundamental and unresolved problem in animal development is the question of how a growing tissue knows when it has achieved its correct final size. A widely held view suggests that this process is controlled by morphogen gradients, which adapt to tissue size and become flatter as tissue grows, leading eventually to growth arrest. I will discuss the spatio-temporal dynamics of that the decapentaplegic (Dpp) morphogen distribution in the developing Drosophila wing imaginal disk and present an alternative model for wing size determination and proliferation control in tissues.

15 min. break

BP 1.3 Mon 10:45 C 243

A generalized Laplace law describes cell and tissue shape — •Ilka Bischofs[1], Franziska Klein[2], Dirk Lehnert[2], Martin Bastmeyer[2], and Ulrich Schwarz[3] — [1]Department of Bioengineering, UC Berkeley, USA — [2]Institute of Zoology I, University of Karlsruhe, Germany — [3]BIOQUANT, University of Heidelberg, Germany

Cues from adhesion geometry, tension and elasticity are important decision factors controlling cell and tissue differentiation. Here we study biological shape determinants across cell and tissue scales. Quantitative microscopy reveals that in both cases edges spanning adhesion sites form circular arcs with a distance dependent curvature. Computer simulations suggest that this is a universal result from isometric tension generated in a filamentous network whose mechanics is controlled by a cable-like, asymmetric response to tension and compression. The model yields a generalized Laplace law that maps onto an elastic contour model of competing line and surface tension. Actomyosin inhibition experiments in conjunction with model fitting are then used to address how cells control shape by actively modulating motor tension and contour elasticity.

BP 1.4 Mon 11:00 C 243

Pattern formation by biological cells: the influence of mechanical boundary conditions — •Pablo Fernández and Andreas R. Bausch — E22 Biophysik, Technische Universität München, D-85748 Garching, Germany

Mechanotransduction, the ability of living cells to sense mechanical tension and accordingly modify their phenotype, is drawing increased attention both from biologists and physicists as a general phenomenon in eukaryotic cells, comparable to chemotaxis in its physiological importance. As most cells spontaneously exert contractile forces under adhesive conditions, the possibility arises of their mechanical cross-talk through the extracellular matrix, with fascinating implications for the formation of tissues. Here, we study pattern formation in cell collections as a function of the mechanical boundary conditions. We place osteoblasts inside collagen gels of sizes 0.3–3 mm with various shapes. Within 1–2 days cells elongate into patterns following the asymmetries dictated by the gel shape. The edges of the gel are free and thus provide "zero tension" boundary conditions. Inclusion of pillars to anchor the gel renders them "zero displacement" and changes the cell pattern. As expected for a cooperative effect based on mechanical interactions, a strong effect of cell density is observed. The experiment thus offers a possible approach for a quantitative characterisation of mechanical interaction between cells.

BP 1.5 Mon 11:15 C 243

Strain Energy during Cell Invasion in Three-Dimensional Collagen Gels — •Thorsten M. Koch[1], Stefan Münster[1], Claudia T. Mierke[1], Philip Kollmannsberger[1], James P. Butler[2], and Ben Fabry[1] — [1]Department of Physics, University of Erlangen-Nuremberg, Germany — [2]Physiology Program, Harvard School of Public Health, Boston, USA

Cell invasion through a dense 3-dimensional matrix is believed to sensitively depend on the ability of cells to generate traction forces. To quantify cell tractions, we measured the strain energy of MDA-MB-231 breast carcinoma cells that invaded into a reconstituted collagen gel ($G' = 80$Pa, 500μm thickness, average mesh size 1μm). Alternatively, we also suspended cells in the collagen solution prior to polymerization. In both cases, cells assumed an elongated spindle-like morphology and locally contracted the gel. The undeformed state of the gel was measured after addition of the actin-disrupting drug cytochalasin-D. Gel deformations were quantified by tracking the spatial positions of fluorescent beads (⌀1μm) embedded in the gels. The bead positions served as nodes for a finite element tessellation. From the local strain of each element and the elasticity of the collagen, we computed the local strain energy stored in the collagen gel surrounding the cell. This technique was verified by indenting the surface of the gel with a steel sphere (⌀100μm, gravitational force 35.4nN). The strain energy of invaded cells was 14pJ, compared to only 1.01pJ of cells on a 2-D planar surface. These results demonstrate that tumor cells exert substantial traction forces during invasion.

BP 1.6 Mon 11:30 C 243

Cell migration through connective tissue in 3-D — •Claudia Tanja Mierke, Philip Kollmannsberger, Thorsten Koch, Daniel Paranhos-Zitterbart, and Ben Fabry — Universität Erlangen, Biophysik, Erlangen, Deutschland

A prerequisite for metastasis formation is the ability of tumor cells to invade and migrate through connective tissue. We analyzed the role of matrix-degrading enzymes, adhesion receptor expression, contractile force generation, and remodeling of cytoskeletal structures for cell invasiveness. We studied 51 well-established tumor cell lines regarding their ability to migrate through a collagen matrix. 27 cell lines were found to be non-invasive, and 24 cell lines were invasive to different degrees that we quantified by the number density of cells that invaded into the gels, multiplied with the average invasion depth. 2-D and 3-D traction microscopy was used to measure contractile forces. Adhesion strengths, cytoskeletal stiffness and molecular turn-over rates were measured using magnetic tweezer microrheology. The speed of cytoskeletal remodelling processes was characterized using nanoscale particle tracking. MMP-14 matrix metalloproteinase and 14 integrin adhesion receptor expression was measured using FACS analysis. We found that cell invasiveness correlated with increased expression of MMP-14 matrix metalloproteinase and integrin receptors (alpha3 and 5), increased contractile force generation, and increased speed of cytoskeletal reorganization. In summary, our results may help identify molecules and signal transduction pathways that control tumor invasion and metastasis formation.

BP 1.7 Mon 11:45 C 243

Stochastic Lamellipodium Dynamics and Forces in Cell Motility — •Daniel Koch[1], Melanie Knorr[1], Thomas Fuhs[1],

Timo Betz[2], Ulrich Behn[1], and Josef Käs[1] — [1]University of Leipzig, Leipzig, Germany — [2]Institute Curie, Paris, France

Cell motility is fundamental for cell migration and cell growth and therefore it is a basis for the understanding of many processes in natural phenomena such as development, neuronal plasticity, and cancer metastasis. The dynamics and forces in the lamellipodium of cells, a thin veil-like structure at the leading edge, are governed by the polymerization of actin filaments and the forces generated by the molecular motor myosin.

Investigation of the leading edge dynamics in combination with flow and force measurements in neuronal growth cones, fish keratocytes, and fibroblasts, gives new insight into the interplay of actin polymerization and retrograde flow and allows comparing the differences and similarities in motility in these different cell systems. We have developed a stochastic model that consistently describes actin polymerization, retrograde flow and edge dynamics in these cell systems. Furthermore, the measurement of the internal flow as well as the viscoelastic material properties of the cell allows calculating the internal force field acting within the lamellipodium. Finally, the measurement of the external traction forces completes the picture of the forces acting on a cell. All this information is combined into a complete picture of cell motility to address the question of universal mechanisms in the motility machinery of cells.

BP 1.8 Mon 12:00 C 243

Phase transitions in tissue growth — •Reza Farhadifar[1], Jens-Christian Röper[2], Benoit Aigouy[2], Suzanne Eaton[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauer Straße 108, 01307 Dresden

We present a theoretical study of growing epithelia using a vertex model. The network of adherence junctions is represented by a network of polygons. The mechanics of cells and their adhesive interactions are described by area elasticity, perimeter contractility and line tension. The ground state diagram of the model reveals a solid-liquid transition. Simulating tissue growth by repeated division of randomly selected cells we generate epithelial tissue morphologies. These tissue morphologies exhibit phase transitions between solid and soft network as a function of parameter values. We study the behavior of the order parameter of the transition which is the shear modulus of the network. The solid network first becomes semi-soft and subsequently it becomes fluid. In the fluid phase, T1 transitions can occur without work which permits the network to shear at vanishing shear modulus.

BP 1.9 Mon 12:15 C 243

Kinetics and scaling laws of growing cell populations — •Markus Radszuweit[1], Michael Block[1], Eckehard Schöll[1], and Dirk Drasdo[2] — [1]Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]INRIA, Rocquencourt, France

We study the growth kinetics and the critical surface dynamics of cell monolayers by a class of computationally efficient cellular automaton models avoiding lattice artifacts [1]. Our numerically derived front velocity relationship indicates the limitations of the Fisher-Kolmogorov-Petrovskii-Piskounov (FKPP) equation for tumor growth simulations. The critical surface dynamics corresponds to the Kardar-Parisi-Zhang (KPZ) universality class, which disagrees with the interpretation by Bru et al. [2] of their experimental observations as generic molecular-beam-epitaxy (MBE)-like growth. By comparison with a new cellular automaton for three-dimensional growth we demonstrate the agreement of the cell population kinetics in two and three dimensions.

References:
[1] M. Block, E. Schöll, and D. Drasdo, Phys. Rev. Lett. (accepted) 2007.
[2] A. Brú, S. Albertos, J. L. Subiza, J. L. García-Asenjo, and I. Brú, Biophys. J. 85, 2948 (2003).

BP 1.10 Mon 12:30 C 243

Dynamics of Anisotropic Tissue Growth — •Thomas Bittig[1], Ortrud Wartlick[2], Anna Kicheva[2], Marcos González-Gaitán[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Department of Biochemistry and Department of Molecular Biology, Geneva University, Sciences II, Quai Ernest-Ansermet 30, 1211 Geneva 4, Switzerland

During the development of multicellular organisms, organs grow to well-defined shapes and sizes. The proper size and patterning of tissues are ensured by signaling molecules as e.g. morphogens. Secreted from localized sources, they form graded concentration profiles in the target tissue which provide positional information to the cells.

We describe the growing tissue as a viscous fluid medium in which cell division induces active stresses that drive cell rearrangements. We focus on the case where cell division is anisotropic and a preferred orientation of cell division exists. We determine cellular flow fields using both analytical and numerical methods. If cell division and cell death balance, there is no net growth, but for anisotropic cell division the tissue undergoes spontaneous shear deformations. This is an example of convergence-extension movements which are often observed in developing tissues. Our theory of tissue growth provides a basis for the study of the transport of signaling molecules in growing tissues. Using our theory, we discuss the diffusion and degradation of morphogens in the growing Drosophila wing disk, a precusor of the fly wing.

BP 1.11 Mon 12:45 C 243

Simulations and model validation by measurements in an isolated rabbit heart — •Steffen Bauer[1], Inaki Romero[1], Rodrigo Weber dos Santos[2], Hans Koch[1], and Markus Bär[1] — [1]PTB Berlin — [2]Univ. Juiz de Fora, Brazil

Time-resolved surface activation time maps recorded from isolated rabbit hearts were analyzed in order to compare them with analogue maps generated by a computer model. Recordings were obtained under normal conditions as well as after the administration of ajmaline and palmitoleic acid (PA). In parallel, the measured quantities were simulated in a realistic computer model of the rabbit heart. The effect of ajmaline was reproduced by reducing the conductivity of sodium channels G_Na in the model. It was observed that addition of a given amount of ajmaline leads to an increase of the QRS time of up to 33 % and a decrease of typical velocities by 20-40 % with respect to normal conditions. A velocity decrease of about 20 % was reproduced in the computer model by a reduction of the G_Na by 60 %. Such a change in the model induces a corresponding increase of the QRS time by 20%. In contrast, administration of PA leaves the QRS time unchanged, while it reduces the speed by a similar margin as the ajmaline.

BP 2: DNA and Chromatin

Time: Monday 10:30–13:15 Location: PC 203

BP 2.1 Mon 10:30 PC 203

Structure and dynamics of interphase chromosomes — Angelo Rosa[1] and •Ralf Everaers[2] — [1]Institute for Biocomputation and Physics of Complex Systems, Corona de Aragón 42, 50009 Zaragoza (Spain) — [2]Université de Lyon, Laboratoire de Physique, École Normale Supérieure de Lyon, CNRS UMR 5672, 46 allée d'Italie, 69364 Lyon Cedex 07, France

During interphase chromosomes decondense, but FISH experiments reveal the existence of distinct territories occupied by individual chromosomes inside the nuclei of most eukaryotic cells. We use computer simulations to show that the existence and stability of territories is a kinetic effect which can be explained without invoking an underlying nuclear scaffold or protein-mediated interactions between DNA sequences. In particular, we show that the experimentally observed territory shapes and spatial distances between marked chromosome sites for human, *Drosophila* and budding yeast chromosomes can be reproduced by a parameter-*free* minimal model of decondensing chromosomes. Our results suggest that the observed interphase structure and dynamics are due to generic polymer effects: confined Brownian motion conserving the local topological state of long chain molecules and segregation of mutually unentangled chains due to topological constraints.

BP 2.2 Mon 10:45 PC 203

Higher-order folding of chromatin and the Random Loop Model — •Manfred Bohn[1], Dieter W. Heermann[1], and Roel van Driel[2] — [1]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 19, 69120 Heidelberg — [2]Swammerdam Institute for Life Sciences, University of Amsterdam, Kruislaan 318, 1098 SM Amsterdam

Remarkably little is known about the higher-order folding motifs of the chromatin fiber inside the cell nucleus. Folding depends among others on local gene density and transcriptional activity and plays an important role in gene regulation. Strikingly, at fiber lengths above 5 to 10 Mb (mega base pairs) the measured mean square distance $< R^2 >$ between any two points on the chromatin fiber is independent of genomic distance. The formation of loops on different length scales seems to play an important role in transcriptional regulation. We analyze the data with respect to different polymer models on short fiber lengths. For long fiber lengths above 10 Mb, where simple models fail in explaining experimental results, we propose a polymer model that explains the leveling off by means of random looping. An analytical expression is calculated for the mean square displacement over the thermal ensemble. The quenched average over the disorder of loops is performed numerically. A detailed investigation of this model shows that only a small number of loops on all scales are necessary to fit experimental data.

BP 2.3 Mon 11:00 PC 203

Genome size variation in eukaryotes: its causes and consequences — •A. G. Cherstvy — FZ Juelich, IFF, 52425 Juelich

The genome size - C value - of animals reveals about 10000 fold variation. The DNA length in fishes varies about 350, while in mammals/birds only 2-4 times. Complexity of organisms and number of genes are not related to DNA content (C value paradox). The genomes of salamanders and lungfishes are 20-40 times longer than of humans, while the gene numbers are quite close. Even some invertebrates have much longer DNA (grasshoppers and amphipods). In higher eukaryotes, only a couple of percent of DNA are actually coding for proteins. The rest, "useless", DNA is probably needed to organize DNA in chromatin/chromosome. It also determines the cell/nucleus size and speed of cellular processes. A naive expectation that evolution should remove this parasitic DNA does not work. On the contrary, the genome of lungfishes, remained unchanged over last 200-300 million years, is known to grow in some eras. But, the genome of Latimeria chalumnae - another living fossil - remained constant at about the human size. C-value can vary strongly between closely related species (some fishes, crustaceans amphipods, etc). E.g., amphipods of cold waters live longer, mature/grow slower, and produce less broods than their hot water colleagues. We will compare and contrast some extreme examples of the genome sizes known, discuss physical/biological mechanisms affecting C-value, outline the role of genome duplication and repetitive DNA sequences, study longevity vs genome size correlations for some species, and speculate about developmental consequences.

BP 2.4 Mon 11:15 PC 203

Phase diagram of chromatin within the two angle model for spherical and cylindrical shape of the nucleosomes — •Dieter Heermann and Philipp Diesinger — University of Heidelberg, Institute of Theoretical Physics, Philosophenweg 19, D-69120 Heidelberg

We have studied the phase diagram for chromatin within the framework of the two-angle model. We reveal the fine-structure of the excluded-volume borderline for spherical type nucleosomes and for cylindrical shape nucleosomes. Thus we where able to give a Ramachandran like diagram for the chromatin fiber. Furthermore, we examined how fluctuations in the distribution of the H1 histones or changes of the vertical distance between the in and outgoing DNA strand affect the chromatin fiber and its biophysical properties.

BP 2.5 Mon 11:30 PC 203

Time resolved access to linker histone/DNA structure formation — •Rolf Dootz, Heather Evans, and Thomas Pfohl — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany

Linker histones H1 are of central importance in genome organization and regulation. Combining small angle X-ray microdiffraction and microfluidics allowed for time resolved access to H1/DNA interaction dynamics and structure formation on relevant molecular length scales. The observed X-ray patterns indicate that the interaction of H1 with DNA is a two step process: an initial unspecific binding of H1 proteins to DNA is followed by a rearrangement of molecules in the formed assemblies. Our results suggest that the conformational transition of H1 tails from their rather extended conformation in aqueous solution to their fully folded state upon interaction with DNA may be responsible for the conformational phase transition of H1/DNA assemblies. We believe those findings have a direct bearing on the understanding of chromatin fiber folding into higher order structures.

15 min. break

BP 2.6 Mon 12:00 PC 203

Gold Nano-Stoves for Microsecond DNA Melting Analysis — •Calin Hrelescu[1], Joachim Stehr[1], Ralph A. Sperling[2], Gunnar Raschke[1], Michael Wunderlich[3], Alfons Nichtl[3], Dieter Heindl[3], Konrad Kürzinger[3], Wolfgang J. Parak[2], Thomas A. Klar[1], and Jochen Feldmann[1] — [1]Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Amalienstr. 54, 80799 Munich, Germany — [2]CeNS, Ludwig-Maximilians-Universität München, Amalienstr. 54, 80799 Munich, Germany and Fachbereich Physik, Philipps Universität Marburg, Renthof 7, 35037 Marburg, Germany — [3]Roche Diagnostics GmbH, Nonnenwald 2, 82372 Penzberg, Germany.

In diagnostics, medicine and biophysics, the melting analysis of DNA is a very important tool. In current temperature ramp techniques the typical time scales for a DNA melting analysis range from several minutes up to one hour. Especially for high throughput DNA analysis a faster detection of the DNA melting point is highly desirable, as well as the successful identification of mutants of the target DNA. We exploit the characteristic plasmonic properties of DNA bound gold nanoparticle aggregates to optically induce and detect the melting of double stranded DNA. The aggregates are used as very efficient light absorbers to locally convert optical energy from laser pulses into thermal energy. Pulsed optical experiments show that heating on a microsecond timescale is sufficient to melt DNA molecules. Only one single laser pulse is needed to distinguish between a perfectly matching target and a target with a point mutation.

BP 2.7 Mon 12:15 PC 203

Conformational DNA separation by dielectrophoresis — •Jan Regtmeier[1], Ralf Eichhorn[2], Alexandra Ros[1], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience, Bielefeld University, Universitaetsstr. 25, 33615 Bielefeld, Germany — [2]Condensed Matter Theory, Bielefeld University, Universitaetsstr. 25, 33615 Bielefeld, Germany

In modern biotechnology and pharmaceutics applications, topologically closed circular DNA plays an important role. For instance, plasmids are used as genetic vectors in DNA recombinants, and for in vivo gene therapy. The latter makes high purification and exact characterization of plasmid DNA indispensable.

We extend our previous studies [1] and present the separation of DNA fragments with equal number of base pairs according to their conformation (supercoiled from linear DNA fragments). The separation is performed in a microfluidic poly(dimethylsiloxane) (PDMS) chip within 210 s. The device consists of a cross injector and a microstructured separation channel with a periodic array of nonconducting posts. The application of an AC voltage induces dipoles in the DNA molecules, which couple to the inhomogeneous electric field in the post array (dielectrophoretic trapping). Superimposed application of a DC voltage induces DNA migration and separation, based on differences in DNA polarizabilities. A detailed analysis of the trapping times allows quantification of the DNA polarizabilities.

[1] Dielectrophoretic Manipulation of DNA: Separation and Polarizability, J. Regtmeier et al., Anal. Chem. 79, 3925-3932 (2007)

BP 2.8 Mon 12:30 PC 203

Thermodynamic Analysis of Interacting Nucleic Acids with Application to Biosensing Devices — •Justin Bois[1] and Niles Pierce[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]California Institute of Technology, Pasadena, CA, USA

DNA and RNA are versatile construction materials. By appropriately designing base sequences, synthetic nucleic acid systems can be programmed to self-assemble into complex structures. An understanding of the underlying free energy landscapes of these systems is crucial for their design, characterization, and control. This talk will focus

on theoretical and computational tools to characterize the equilibrium properties of an entire test tube of interacting nucleic acid strands. The utility of the approach will be demonstrated by elucidating the empirical behavior of a new class of DNA-based instrument-free biosensors currently under development.

BP 2.9 Mon 12:45 PC 203

DNA Melting: a combination of Poland-Sheraga and lattice models — •Ralf Everaers — Université de Lyon, Laboratoire de Physique, École Normale Supérieure de Lyon, CNRS UMR 5672, 46 allée d'Italie, 69364 Lyon Cedex 07, France

Key biological and nano-technological processes require the (partial) association and dissociation of complementary DNA strands. We present a variant of the Poland-Scheraga model which reproduces experimental data for melting temperatures for arbitrary strand length over the full experimental range of strand concentration and ionic strength of the solution. Furthermore, we show results for a corresponding lattice model of associating heteropolymers with identical melting behavior. The lattice model treats long-ranged excluded volume interactions between all parts of the molecule explicitly, provides access to an ensemble of three dimensional structures (and hence the response to external mechanical forces) and can be used for studying the kinetics of the melting transition.

R. Everaers, S. Kumar and Ch. Simm, **Phys. Rev. E** *75*, 041918 (2007).

D. Jost and R. Everaers, *submitted*.

BP 2.10 Mon 13:00 PC 203

Protein-DNA interactions: reaching and recognizing the targets — •A. G. Cherstvy[1], A. B. Kolomeisky[2], and A. A. Kornyshev[3] — [1]Theorie-II, IFF, FZ Juelich, D-52425 Juelich, Germany — [2]Department of Chemistry, Rice University, Houston, Texas 77005, USA — [3]Department of Chemistry, Imperial College London, SW7 2AY, London, UK

Searching and recognizing the targets by DNA binding proteins is one of the fundamental biological processes. Some proteins (e.g. the lac repressor) can find their targets 10-100 times faster than predicted by the 3D diffusion rate. However, recent single-molecule experiments showed that the 1D diffusion constants of protein motion along DNA are very small. This controversy pushed us to revisit the problem of target search. We present a theoretical approach which describes some physical-chemical aspects of the target search and DNA-protein recognition. We consider the search process as a sequence of cycles, with each cycle consisting of 3D and 1D track. It is argued that the search time contains three terms: for the motion on 3D, and 1D segments, as well as the correlation term. We show that the acceleration in search time can be reached by a parallel scanning for target by many proteins. Also, we show how the complementarity of charge patterns on a target DNA sequence and on the protein may result in electrostatic recognition of a specific track on DNA by the protein and lead to its subsequent pinning. We estimate the depth and width of the potential well near the recognition region and typical times proteins can spend in the well.

BP 3: Neuronal Systems

Time: Monday 14:00–17:15 Location: C 243

Invited Talk BP 3.1 Mon 14:00 C 243

How to Take a Quick Look—Rapid Neural Coding of Visual Information in the Retina — •Tim Gollisch — Max Planck Institute of Neurobiology, München-Martinsried

The neural processing and computation that underlies our visual perception begins in the retina, a neural network at the back of the eyeball. Here, all visual information available to the central brain is encoded into patterns of electrical pulses ("spikes"). Elucidating the nature of this neural code forms a central goal in visual neuroscience. A particular challenge for natural visual processing arises from frequent eye movements ("saccades"), which bring a new image onto the retina and initiate a short episode of visual processing. In this talk, I will discuss recent findings that specific retinal neurons encode the structure of a suddenly appearing image in the relative timing of their spikes. The characteristics of this neural code and its underlying circuitry are studied with a combination of experimental recordings of retinal spikes under visual stimulation and mathematical modeling. These retinal signals may serve as a channel for rapid and robust information transmission from the eye to the brain.

BP 3.2 Mon 14:30 C 243

Reorganization of neural circuitry during growth of cat visual cortex — •Wolfgang Keil[1,2,3], Fred Wolf[2,3], Siegrid Löwel[4], and Matthias Kaschube[1] — [1]Princeton University, Princeton, NJ USA — [2]MPIDS, Göttingen, Germany — [3]BCCN, Göttingen, Germany — [4]Friedrich-Schiller-University, Jena, Germany

In cat visual cortex, the period of postnatal cortical growth largely overlaps with the period of enhanced plasticity, but little is known about the interrelation between these two phenomena. We analyzed the two-dimensional spatial organization of ocular dominance (OD) columns during postnatal cortical growth. Despite a size increase of 50% of area 17 between postnatal week 3 and 10, the mean spacing between adjacent OD columns increased only slightly. Consequently, the number of hypercolumns increased considerably during this expansion period. Furthermore, this process was paralleled by a strong tendency of columns to change appearance from stripe-like to disordered patterns. Theoretically, this process resembles a behavior known as the zigzag instability in dynamical systems. This is a generic behavior in expanding self-organizing systems dominated by Mexican-hat like interactions and is therefore predicted by a large class of models for activity dependent visual cortical development. We analyzed the effect of cortical expansion on columnar layouts in an Elastic Net model and compared it to the degree of reorganization observed experimentally. We find that the observed reorganization indeed exhibits signatures of this type of instability. Thus, these models indicate that the observed mode of columnar reorganization results from cortical expansion.

BP 3.3 Mon 14:45 C 243

Fasciculation dynamics of sensory neurons — •Debasish Chaudhuri[1], Peter Borowski[2], Pradeep K. Mohanty[3], and Martin Zapotocky[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — [2]University of British Colombia, Vancouver, BC, Canada — [3]Saha Institute of Nuclear Physics, Kolkata - 700064, India

Sensory neurons are typically spread out in the periphery, but their axons connect to precisely determined locations in the brain. In addition to graded guidance cues, axon-axon interactions can strongly influence this connectivity. To understand these effects in the intrinsically dynamic neural connectivity of, e.g., the mammalian olfactory system, we model the axons as a set of interacting directed random walkers with turnover. The growing axons form fascicles. In the steady state we obtain scaling, and the exact functional form of the fascicle size distribution. The auto-correlation time of the number of axons in a fascicle shows a crossover from a short time-scale which is the inverse of axonal death rates to a long time scale as the fascicle size grows. A set of effective rate equations in terms of dynamical variables characterizing fascicles (rather than individual axons) explains the time-scales qualitatively.

15 min. break

BP 3.4 Mon 15:15 C 243

Broadband coding with dynamic synapses — •Benjamin Lindner[1], John Lewis[2], and Andre Longtin[3] — [1]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Biology, University of Ottawa, Ottawa, Canada — [3]Department of Physics, University of Ottawa, Ottawa, Canada

Short-term synaptic plasticity (STP) is commonly thought to provide a basis for low-pass or high-pass filtering of information transmission across the synapse depending on whether depression or facilitation, respectively, is dominant. To evaluate this assumption, we consider a general case of information transmission from a population of independent synaptic inputs to a model neuron. We show using standard information theoretic approaches that the changes in synaptic response amplitude produced by STP interact with associated membrane fluctuations, such that information transmission is frequency-independent

(no high-pass or low-pass filtering), regardless of whether synaptic depression or facilitation dominates. Interestingly, the baseline firing rate of the post-synaptic neuron is a critical factor in determining whether or not this frequency-independence is reflected in the output spike train: high-firing rates maintain broadband transmission, whereas low-firing rates recover the expected filtering. This suggests that neurons in a rate-coding regime will not be influenced by STP.

BP 3.5 Mon 15:30 C 243

Gating charge effects as an intrinsic mechanism for channel noise reduction — Gerhard Schmid, Igor Goychuk, and •Peter Hänggi — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Within generalizations of the archetypical Hodgkin-Huxley modelling we investigate the influence of intrinsic properties of ion channel gating on the spiking activity of neuronal membrane patches. Channel noise which stems from the randomness of ion channel gating causes spontaneous spiking and synchronization effects as Stochastic Resonance or Coherence Resonance. The random switching of voltage-gated ion channels between open and closed configurational channel states is connected with gating charge movement within the cell membrane. The latter results in a drastically reduced spontaneous spiking activity [1]. Consequently, this demonstrates a prominent intrinsic mechanism for channel noise reduction. Within the effect of Stochastic Resonance the effective reduction of intrinsic noise level manifests itself.
[1] G. Schmid, I. Goychuk, P. Hänggi, Phys. Biol. **3** (2006) 248

BP 3.6 Mon 15:45 C 243

Neuronal Avalanches in Networks with Short-Term Synaptic Plasticity — •Anna Levina[1,2,3], J. Michael Herrmann[1,4], and Theo Geisel[1,3,4] — [1]BCCN Göttingen — [2]GK "Identification in Mathematical Models" — [3]MPI for Dynamics and Self-Organization — [4]Göttingen University, Dept. of Physics, Bunsenstr. 10, Göttingen

Critical avalanches of neural activity have been identified analytically in globally coupled networks of spiking neurons and were observed subsequently in neurophysiological recordings in cortical slices. While in previous models a fine-tuning of the connectivity parameters was required, we recently showed that the biologically well-established activity-dependent dynamics of the synaptic efficacies provides a possible mechanism for the self-organized criticalization of the neuronal dynamics.

The present work is based on a realistic model of short-term plasticity that includes both facilitation and depression of the synaptic efficacies. In a simplified model that uses depression only, the critical regime is reached by a second-order phase transition, where the critical phase is characterized by a stable balance of neural activity and synaptic depression. We show here that the incorporation of synaptic facilitation entails a first-order transition from the sub-critical regime into the extended critical parameter range. The results are obtained by a stochastic mean-field analysis and are related to numerical experiments by finite-size scaling of the critical distribution. Furthermore, we discuss effects of non-trivial connectivity structure, and neural properties such as leakage and long-term potentiation of the synaptic strengths.

BP 3.7 Mon 16:00 C 243

Exact mean, variance, and autocorrelation function of neural subthreshold voltage — •Lars Wolff and Benjamin Lindner — Max-Planck-Institut für Physik komplexer Systeme

Neurons are subject to a vast number of synaptic inputs from many other cells. These inputs consist of spikes changing the conductivity of the target cell, i.e. they enter the neural dynamics as multiplicative shot noise. Up to now, only for simplified models like current-based (additive-noise) point neurons or models with Gaussian white noise input, exact solutions are available. We will present a method to calculate the exact time-dependent moments and the autocorrelation function for the voltage of a point neuron with conductance-based Poissonian shot noise and a passive membrane. The exact solutions show novel features (for instance, maxima of the moments vs time) and are in excellent agreement with numerical simulations. The theoretical analysis of subthreshold membrane fluctuations may contribute to a better comprehension of neural noise in general. It may also help devising schemes for the extraction of synaptic parameters or network parameters from voltage recordings.

BP 3.8 Mon 16:15 C 243

Chaotic dynamics in the balanced state — •Michael Kreissl[1], Siegrid Löwel[2], and Fred Wolf[1] — [1]Max Planck Institute for Dynamics and Self-Organization, BCCN in Göttingen, Germany, — [2]Friedrich Schiller University in Jena, Germany

We study the dynamics of sparse, neural networks in the balanced state. In our networks N Theta-neurons (phase representation of the Quadratic Integrate&Fire model) [Gutkin1998] are pulse-coupled to other neurons with the probability K/N. Using closed expressions for the time evolution of the individual neurons, we perform numerically exact, event based simulations of the network dynamics. Furthermore, we derive the Jacobian of the mapping between spikes analytically, which is used to calculate the long term Lyapunov spectrum through the evolution of a tangential orthonormal system.

Our simulations show that the Lyapunov spectrum in general contains a considerable fraction of positive Lyapunov exponents, indicating chaotic behavior of the network dynamics. The dimension of the attractor is in general large (approx. N/3). The mean Lyapunov exponent is found to be negative, expressing the networks dynamics to be dissipative. In a random matrix approximation, we find an analytic expression of the mean Lyapunov exponent, which is verified by the numerical simulations. We conclude that the balanced state in networks of neurons with active spike generation exhibits conventional and most-probably extensive chaos. This distinguishes such models from binary networks, exhibiting hyperchaos [Vreeswijk1996], and Leaky Integrate&Fire networks, exhibiting stable chaos [Zillmer2006, Jahnke2007].

BP 3.9 Mon 16:30 C 243

Statistical framework incorporating temporal and mutual correlations in a neural network ensemble. — •Tatjana Tchumatchenko[1,2], Theo Geisel[1,2], Stefan Treue[3], and Fred Wolf[1,2] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen — [2]Bernstein Center for Computational Neuroscience (BCCN), Göttingen — [3]Kognitive Neurowissenschaften, Deutsches Primaten Zentrum, Göttingen

We present a new class of parametric models for multiple impulse sequences correlated in time and between channels, which we call Gaussian Pseudo Potential Models (GPPMs). In our approach, correlated impulse sequences are defined by threshold crossings of temporally continuous random functions, called the Pseudo Potentials (PPs). Assuming Gaussian statistics of PPs, a correlated spike train ensemble is uniquely specified by the Matrix of cross- and auto-covariance functions of the PPs. Many spike train statistics, as e.g. firing rates, auto and cross conditional firing rates, can then be expressed in closed form [1]. In an ensemble of spike trains from a pair of neurons, we analyse the mapping between PP correlations and spike correlations. We show, that that for weak coupling strength the cross conditional rate is connected to the PP cross correlation function by a linear differential equation. The applicability of these differential equations is numerically confirmed for a simple set of model PP correlation functions. These and other exact results suggest that GPPMs provide a analytically very tractable parametric model of multiple correlated neuronal impulse sequences. [1] B. Naundorf et al. Nature, 440:1060–1063, 2006

BP 3.10 Mon 16:45 C 243

Optimal active network topologies for information transmission — •murilo da silva baptista — Max-Planck-Institut fuer Physik Komplexer Systeme, Noethnitzerstr. 38, D-01187 Dresden

The relation between neural circuits and behavior is a fundamental matter in neuroscience. In this talk, I will present a theoretical approach that has the potential to unravel such a relationship in terms of network topology, information, and synchronization, in active networks, networks formed by elements that are dynamical systems (such as neurons, chaotic or periodic oscillators). As a direct application of the proposed approaches, I will show how one can construct optimal neural networks that not only transmit large amounts of information from one element to another in the network, but also are robust under alterations in the coupling configuration.

This theoretical approach is general and do not depend on the particular dynamic of the elements forming the network, since the network topology can be determined by finding a Laplacian matrix (the matrix that describes the connections and the coupling strengths among the elements) whose eigenvalues satisfy some special conditions.

Since information might not always be easy to be measured or quantified in experiments, I will also better clarify the non-trivial relation between information and synchronization, a phenomenom which is often not only possible to observe but also relatively easy to characterize.

I will illustrate the theoretical approaches mainly using neural networks of electrically connected chaotic Hindmarsh-Rose neurons.

BP 3.11 Mon 17:00 C 243

Mechanical properties of coupled hair bundles — •Kai Dierkes, Frank Jülicher, and Benjamin Lindner — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

In all vertebrates the hair bundle is the mechano-electrical transducer in both the auditory and the vestibular system. In contrast to being purely passive resonators hair bundles from the sacculus of the bullfrog have been shown to possess the ability to amplify weak periodic stimuli by means of an active process. Spontaneous and evoked oscillations of single hair bundles in lower vertebrates have been studied in order to probe the underlying mechanism. Recently Nadrowski at al. (PNAS 2004) have proposed a model for active hair bundle motility that very well captures the experimental findings. In vivo hair bundles in the sacculus of the bullfrog are attached to an overlying structure that effectively mediates a coupling between them: the otolithic membrane. The same holds true for the hair bundles of outer hair cells in the mammalian cochlea whose tips are connected to the overlying tectorial membrane. We report on results that suggest that collective effects in arrays of coupled hair bundles could indeed play a significant role for signal detection in inner ear organs.

BP 4: Novel Methods

Time: Monday 14:30–16:00 Location: PC 203

BP 4.1 Mon 14:30 PC 203

A novel magneto-optical contrast mechanism in microscopy — •Gopalakrishnan Balasubramanian[1], Iu-Yam Chan[1], Roman Kolesov[1], Philip Hemmer[2], Fedor Jelezko[1], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart — [2]Electrical Engineering, Texas A&M University, College Station, TX, USA

A novel non-contact optical imaging technique is presented that can achieve atomic scale resolution at standoff distances large enough to eventually permit molecular imaging at ambient conditions. The pioneering aspect of this technique is the use of single paramagnetic optically active centers in diamond as the probe. The feasibility of proposed scheme is based on recent key discoveries related to detection and manipulation of single Nitrogen-Vacancy (NV) centers in diamond. A spatially varying magnetic potential shifts the frequency of a ESR resonance of the probe system, so that the resonance frequency is position dependent. Proposed technique will enable nm resolution at long standoff distances.

BP 4.2 Mon 14:45 PC 203

SERS Microscopy: Selective and Sensitive Localization of Proteins in Tissue Specimens — •Magdalena Gellner[1], Max Schütz[1], Carina Jehn[1], Florian Baum[1], Bernd Küstner[1], Carsten Schmuck[2], Alexander Marx[3], Philipp Ströbel[3], and Sebastian Schlücker[1] — [1]Physikalische Chemie, Julius-Maximilians-Universität, 97074 Würzburg — [2]Organische Chemie, Julius-Maximilians-Universität, 97074 Würzburg — [3]Pathologisches Institut, Universitätsklinikum, 68167 Mannheim

We have introduced surface–enhanced Raman scattering microscopy (μSERS) as a novel approach to immunohistochemistry. Specifically, the localization of prostate–specific antigen (PSA) in formalin–fixed and paraffin–embedded prostate tissue specimens from patients undergoing prostatectomy for prostate cancer has been demonstrated. In contrast to the use of either dyes or fluorophores as labels, organic molecules as Raman markers on the surface of metal nanoparticles offer unique capabilities for a highly multiplexed detection, because the line width of vibrational transitions is significantly smaller in comparison to electronic transitions. The SERS distance dependence, the SERS selection rules and the specific electronic resonance conditions lead to the fact that only a very few Raman bands from the marker moiety close to the nanoparticle surface are detected. In our case the characteristic Raman signals of the marker were measured in the PSA–(+) epithelial tissue. For negative controls, Raman spectra in the PSA–(-) stroma and lumen were recorded. Further applications for this innovative Raman technique in cell and tumor biology are discussed.

BP 4.3 Mon 15:00 PC 203

Immobilization of semiconductor nanocrystals on nanopatterned interfaces — •Eva Bock[1], Stefan Kudera[1], Angela Fiore[2], Liberato Manna[2], and Joachim P. Spatz[1] — [1]Max-Planck-Institute for Metals Research, Dept. of New Materials & Biosystems & University of Heidelberg, Dept. of Biophysical Chemistry, Heisenbergstr. 3, D - 70569 Stuttgart — [2]National Nanotechnology Labs of CNR, Via Arnesano, I * 73100 Lecce

Here we describe different approaches for the functionalization of nanopatterned substrates with semiconductor nanocrystals which are exceptional materials for their unique optical flexibility. Gold nanoclusters with diameters between 2 and 30 nm and lateral distances of 20 to 250 nm are arranged onto silicon wafers with a uniform diameter and a defined interparticle spacing. The patterning technique is based on self-assembly of metal loaded diblockcopolymer micelles (polystyrene-b-poly[2-vinylpyridine(HAuCl4)]) which form a quasi-hexagonal closed packed monolayer. The individual gold nanoparticles are potential candidates for immobilizing single molecules or nanoscopic objects. Several approaches proved useful for the immobilization of different semiconductor nanocrystals, such as tetrapods, dimers and dumbbells. One method of assembling nanoparticles on the surface is based on thiol-chemistry, another one is based on the hybridization of DNA. A third approach involves the direct attachment of the nanocrystals on the gold dots without organic linker molecules.

BP 4.4 Mon 15:15 PC 203

Microscopical visualization of Gold-Nanoparticles for biological and medical applications — •Andrea Isabel Matschulat, Franz-Josef Schmitt, Max Schoengen, and Hans Joachim Eichler — Institut für Optik und Atomare Physik, Technische Universität Berlin, Strasse des 17.Juni 135, 10623 Berlin

The application of novel nanotechnologies, especially in biotechnology and nanomedicine looks very promising. Improved and partly new physical, chemical and biological properties of nanostructures make them to powerful tools in diagnostics and therapy. Gold-Nanoparticles in contact with living HCT-116 colon carcinoma cells were visualized with several microscopical techniques such as Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), Scanning Near-Field Optical Microscopy (SNOM) and conventional Light Microscopy (LM). VIS-Spectroscopy was applied for studying long-time-stability and optical properties of the Gold-Nanoparticles. The goal is the *in vivo* visualization of the nanoparticles in living cells. This project is treated in collaboration with Surgical Research Unit OP 2000, Max-Delbrück-Centrum für Molekulare Medizin, Charité - Berlin *in vitro*. Especially in the field of conventional optical Far-Field Microscopy, measurements with colloids in living cells using a dark-field configuration showed that resolution was limited in the size range of 1 μm due to Abbe's limit of resolution and scattering effects, however, the particles were identifiable through their red colour as a result of the plasmon resonance effect which was calculated with classical Drude-Lorentz-model.

BP 4.5 Mon 15:30 PC 203

Combination of atomic force microscopy with timecorrelated fluorescence-spectrocopy — •Max Schoengen, Franz-Josef Schmitt, Andrea Matschulat, and Hans Joachim Eichler — Institut für Optik und Atomare Physik, Technische Universität Berlin

The combination of different microscopic techniques delivers completely new possibilities of analysing nanostructures. The topographic analysis performed with Atomic force microscopy can be complemented with time resolved fluorescence spectroscopy and fluorescence microscopy to deliver additional spectroscopic properties of the investigated sample with time and space resolution. With fluorescence microscopy even nanometer scaled structures can be visualised and localized inside the sample. Near field optical techniques like the combination of Foerster Resonance energy transfer (FRET) with AFM can help to investigate simultaneously the topographic and electronic properties of the nanoscaled structures (e.g. membrane proteins). Especially in liquids this kind of AFM combined with FRET technology

opens complete new possibilities of analysing (biological) nanostructures like cell membranes.

BP 4.6 Mon 15:45 PC 203

Adressing cells via immobilized magnetite particles on magnetically variable substrates — •Juliane Issle and Uwe Hartmann — Universität des Saarlandes, Institut für Experimentalphysik, Campus C6 3, D-66123 Saarbrücken

It is well known that magnetite nanoparticles in the range of 200 nm are biocompatible and they are used in drug delivery, hyperthermia etc. A new approach of immobilizing these beads by means of magnetic interaction on certain substrates gives rise to the opportunity to adress cells via transmembrane pathways without particle internalization. Magnetometry and Magnetic Force Microscopy deliver insight to the structural and magnetic properties of the nanoparticles. Magnetic garnet layers with perpendicular anisotropy, which enables magnetic bead deposition, have been used. They turned out to be biocompatible and furthermore the domain structure can be varied by application of external magnetic fields. The calculation of the interaction between particles and surface stray field shows that the forces are in the 100 pN range, so that cells can not take up the beads once they are immobilized. A climate chamber and coils to produce magnetic fields were integrated into an inverted microscope. This allows the investigation of cell behavior over days with respect to structural substrate changes in the range of some seconds to several days.

BP 5: Photobiophysics

Time: Monday 16:15–17:15 Location: PC 203

BP 5.1 Mon 16:15 PC 203

Optically "Dark" States of Carotenoids in the Major Plant Light-Harvesting Complex Investigated by Femtosecond Two-Photon Fluorescence Excitation Spectroscopy — •Alexander Betke[1], Bernd Voigt[1], Heiko Lokstein[2], and Ralf Menzel[1] — [1]Institut für Physik/Photonik, Universität Potsdam, Germany — [2]Institut für Biologie, Universität Potsdam, Germany

Carotenoids play several important roles in photosynthetic organisms: as structural components of pigment-protein-complexes, as accessory light-harvesting pigments, and in photoprotection. To understand the latter two functions and the underlying mechanism(s) it is vital to know the energetic positions of the first exited singlet state S_1 (2^1Ag^-) of relevant xanthophylls (carotenoids). Because single photon absorption is symmetry-forbidden for the S_0 (1^1Ag^-) $\rightarrow$ S_1 (2^1Ag^-) transition, the carotenoid 2^1Ag^- state cannot be readily investigated by conventional spectroscopy. This transition, however, is two-photon allowed. Moreover, the carotenoid S_1 state is assumed to lie close to the lowest excited chlorophyll singlet state. Thus, simultaneous two-photon absorption of tuneable fs-NIR-pulses being monitored by chlorophyll fluorescence is a useful approach to study the role of the "dark" states in excitation energy transfer and dissipation in light-harvesting complexes. Two-photon excitation spectra of the plant major light-harvesting complex (LHC II) with different xanthophyll-cycle pigment complements (violaxanthin, zeaxanthin) will be presented and implications for the photoprotective mechanism will be discussed. This research is supported by the DFG (SFB 429, TP A2).

BP 5.2 Mon 16:30 PC 203

Metal - enhanced fluorescence of chlorophylls in single light - harvesting complexes — •Sebastian Mackowski[1,2], Stephan Wörmke[1], Andreas Maier[1], Tatas Brotosudarmo[3], Hayk Harutyunyan[1], Achim Hartschuh[1], Alexander Govorov[4], Hugo Scheer[3], and Christoph Bräuchle[1] — [1]Department of Chemistry and Biochemistry, Ludwig-Maximilian-University, Munich, GERMANY — [2]Insitute of Physics, Nicolaus Copernicus University, Torun, POLAND — [3]Department of Biology, Ludwig-Maximilian-University, Munich, GERMANY — [4]Department of Physics and Astronomy, Ohio University, Athens OH, USA

Ensemble and single-molecule spectroscopy demonstrates that both emission and absorption of peridinin-chlorophyll-protein photosynthetic antennae can be largely enhanced through plasmonic interactions. We find up to 18-fold increase of the chlorophyll fluorescence for complexes placed near a silver metal layer. This enhancement, which leaves no measurable effects on the protein structure, is observed when exciting either chlorophyll or carotenoid and is attributed predominantly to an increase of the excitation rate in the antenna. The enhancement mechanism comes from plasmon-induced amplification of electromagnetic fields inside the complex. This result is an important step toward applying plasmonic nanostructures for controlling the optical response of complex biomolecules and improving the design and functioning of artificial light-harvesting systems.

BP 5.3 Mon 16:45 PC 203

Chlorophyll binding protein complexes: Nanostructure and optical properties — •Franz-Josef Schmitt[1], Christoph Theiss[1], Gernot Renger[2], and Hans Joachim Eichler[1] — [1]Institut für Optik und Atomare Physik — [2]Max Volmer Laboratorium TU Berlin, Strasse des 17. Juni 135, 10623 Berlin

The photophysical and biochemical properties of pigments change due to surrounding protein environments. This principle has been perfectly in the biosphere. Photosynthetic organisms developed pigment-protein complexes for efficient light collection, transfer of electronically excited states and transformation into electrochemical free energy. In addition to the photosynthetic apparatus plants contain also water soluble chlorophyll (Chl) binding proteins (WSCPs) which most likely exert not yet clarified regulatory functions. A striking feature -among several interesting properties-is the retardation of the formation of highly reactive singlet oxygen in WSCP. Although the origin of this effect is not yet clarified, it seems likely that the protein matrix is able to diminish the sensitized reaction of bound chlorophyll with the surrounding oxygen.

A wide range of linear and non-linear optical techniques have been used to determine successfully the properties of these pigment protein complexes providing a deeper understanding of the influence of protein interactions on the electronic structure of the pigments. Time resolved fluorescence spectroscopy combined with two photon excitation will help to investigate the pigment interactions directly in biological tissues.

BP 5.4 Mon 17:00 PC 203

Resonanz-Ramanspektroskopie an ß-Karotin und polarisationsabhängige Messungen an Photosystem II - Kristallen — •Katharina Brose[1], Norman Tschirner[1], Christian Thomsen[1], Matthias Schenderlein[2], Peter Hildebrandt[2] und Athina Zouni[2] — [1]Institut für Festkoerperphysik, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin — [2]Institut für Chemie, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin

Pflanzen wandeln Photonenenergie mit Hilfe der Photosysteme I und II (PS I und PS II) in chemische Energie um. An diesem Prozess ist unter anderem das Pigment ß-Karotin beteiligt, von dem sich im Reaktionszentrum des PS II zwei befinden, die zueinander senkrecht angeordnet sind.

Telfer et al. beobachteten wellenlängenabhängige Unterschiede in Resonanz-Ramanspektren des PS II, welche den unterschiedlich angeordneten Karotinen zugeordnet wurden [1]. Messungen an dem reinen Pigment ß-Karotin zeigen jedoch dasselbe Verhalten. Unsere Messergebnisse deuten auf zwei nahe beieinander liegende, nicht auflösbare Peaks hin, deren Resonanzverhalten für verschiedene Anregungswellenlängen variiert. Um die ß-Karotine im PS II dennoch unterscheiden zu können, wurden polarisationsabhängige Messungen an Photosystemkristallen [2] durchgeführt.

[1] A. Telfer, D. Frolov, J. Barber, B. Robert und A. Pascal, Biochemistry 2003, 42, 1008-1015

[2] A. Zouni, H.-T. Witt, J. Kern, P. Fromme, N. Krauß, W. Saenger und P. Orth, NATURE, Vol. 409, 739 (2001)

BP 6: Statistical Physics in Biological Systems (joint session DY/BP)

Time: Monday 14:30–16:45 Location: MA 001

see program DY 5

BP 7: Posters I

Time: Monday 17:00–19:30 Location: Poster A

BP 7.1 Mon 17:00 Poster A

Counterion Dynamics in DNA Electrophoresis — •Sebastian Fischer[1], Ali Naji[2], and Roland Netz[1] — [1]Physik Department, Technische Universität München, 85748 Garching, Germany — [2]Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106-9510, USA

We present Brownian Dynamics simulations of a coarse grained model for DNA in aqueous NaCl solution, moving under the influence of an externally applied electric field. The electrophoretic DNA mobility obtained is shown to agree almost quantitatively with experimental data. As theoretically predicted, the DNA mobility is found to decrease logarithmically with increasing salt concentration due to partial screening of hydrodynamic interactions caused by the adverse motion of oppositely charged ions.

Apart from the DNA mobility we focus on the mobility of the counterions in the immediate vicinity of the polymer which we find to be negative, *i.e.* the Na^+ ions are dragged along by the DNA, albeit at diffent speed. This result contrasts with a common theoretical concept where counterions in close proximity to the DNA polymer are assumed to move at the same velocity [2]. In contrast to the DNA mobility the Na^+ mobility increases with increasing salt concentration. At some point, the direction of motion changes from aligned to adverse with respect to the polymer. For weakly charged polymers the salt concentration dependence of the counterion mobility can be calculated using Green's function methods.

[1] G. S. Manning, J. Phys. Chem. **85**, 1506 (1981)

BP 7.2 Mon 17:00 Poster A

Fullerenes Can Induce Toxic Physical Changes of DNA — •Fabian Czerwinski and Lene B. Oddershede — Niels Bohr Institute, Blegdamsvej 17, Copenhagen

Fullerenes are fascinating symmetric carbon nanostructures. Nowadays, they are widely used because of their characteristic physical and chemical properties. Until now research has been mainly focused on commercial applications of fullerenes. Only a few investigations have addressed the potential biological hazards, one of which is that fullerenes are believed to alter the elastic properties of DNA upon binding.

In our experiments we use optical tweezers with sub-piconewton and nanometer resolution to probe the structural changes and the potential damages which fullerenes might induce on single DNA molecules. Therefore, force-extension relations can be obtained under physiological conditions while varying the concentration of different types of fullerenes.

It has theoretically been predicted [1], that certain fullerenes can function as a minor-groove binder to double-stranded DNA, thus altering its elastic properties significantly. Fullerenes are capable of causing severe damage inside living organisms by forming DNA regions which are not accessible for proper enzymatic functions. A further goal of the study is to establish fullerenes as a tool for a more detailed investigation of DNA-protein interactions, such as the trafficing of polymerases or the packing by procaryotic proteins.

[1] Zhao, Striolo and Cummings: BiophysJ (89):3856-62, 2005.

BP 7.3 Mon 17:00 Poster A

Exact Models for Denaturation Transitions of Nucleic Acids — •Thomas Rudolf Einert and Roland Netz — Technische Universität München, Garching, Germany

Stretching of double-stranded DNA leads to the denaturation of the molecule. A stretching force $F \approx 65\,\mathrm{pN}$ leads to a structural transition where DNA changes from its native state (B-DNA) to a stretched state (S-DNA). At even higher forces DNA denatures and the two DNA strands are separated from each other. We present a model with which force-extension curves can be calculated.

Thermodynamics of loops – especially multi-branched loops – in RNA are still not very well understood. We show that the melting curves and the melting temperatures are very sensitive to the modeling of the statistical weight of a loop employing recursion relations to calculate the partition function. Using the asymptotic form for the statistical weight $y^m m^{-c}$ of a loop of length m known from polymer theory we are able to solve the equations exactly and find a delicate dependence of the critical behavior on the loop exponent c.

BP 7.4 Mon 17:00 Poster A

Impact of alternative genetic codes on the stability of proteins — •Stefanie Sammet[1], Andreas Buhr[1], Ugo Bastolla[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Centro de Biologia Molecular, "Severo Ochoa", Campus UAM, Cantoblanco, 28049 Madrid, Spain

While nearly all free-living species use the same genetic code for the translation of genes into amino acid sequences, slightly different genetic codes are used in mitochondria and in some intracellular bacteria. In addition, the mitochondria genome mainly codes for membrane proteins, which have peculiar thermodynamic properties since they have to deal with a lipidic environment. While there has been a lot of work concerned with the optimality of the standard genetic code, it remains unclear whether alternative codes provide any advantage to the proteins they code for. We present a model based on mutations and purifying selection on thermodynamic properties, which takes into account that mitochodrial genome present a distinctive mutation bias. On the basis of point mutations in the DNA, the effects of different genetic codes on stability against unfolding and misfolding are examined. Furthermore, the robustness of proteins against mistranslations is considered.

BP 7.5 Mon 17:00 Poster A

Isothermal DNA Nanotube Self Assembly Using Chemical Dilution — •Thomas Sobey[1,2], Stephan Renner[1,2], Ralf Jungmann[1,2], and Friedrich Simmel[1,2] — [1]Center for NanoScience and Department of Physics, Geschwister-Scholl-Platz 1, 80539 Munich, Germany — [2]Physics Department E14, Technical University Munich, James-Franck-Straße, 85748 Garching, Germany

DNA-based supramolecular nanostructures are rapidly advancing in complexity and reproducibility, and are exciting because of their ability to act as scaffolds for other nano- and micro- sized objects, as molecular devices, and in molecular computation.

Those structures used for scaffolding and molecular computation are (generally) formed through a slow temperature annealing process in buffer, allowing the assembly to occur correctly. We have developed a successful isothermal room temperature procedure that reproduces this. It is based on slowly decreasing the concentration of a denaturing agent(formamide), which 'simulates' the thermal annealing step. With this process we have reproduced DNA nanotube structures previously realized by Mao et. al. using conventional annealing.

We are currently working to develop this technique with tile-based structures, algorithmic self-assembly, and also DNA origami. In addition, we attempt to create these DNA-based nanofilaments inside vesicles to act as an artificial cytoskeleton.

BP 7.6 Mon 17:00 Poster A

Orientation - Defined Stretching and Fixing of DNA by AC Voltage Induced Electro-Osmotic Flow — •Venkatesh Alagarswamy Govindaraj[1], Simone Herth[1], Anke Becker[2], Andreas Hütten[1], and Günter Reiss[1] — [1]Thin Films and Nano Structures, Department of Physics, Bielefeld University, Bielefeld, Germany — [2]Institute for Genome Research and Systems Biology, CeBiTec, Bielefeld University, Bielefeld, Germany

Application of DNA stretching at a single molecule level has become an attractive domain of research in the field of bioelectronics, genomics and nanobiotechnology. It was already reported that DNA could be stretched in an orientation-defined way between two electrodes with a gap of several micrometers using masks. In this work a new electrode design was fabricated to facilitate an orientation-defined stretching of dsDNA across a channel of submicron width. Tagged DNA strands of

defined length were synthesized by Polymerase Chain Reaction using pUC19 as template. The forward and reverse primers were 5'-tagged with thiol and biotin, respectively. The tagged DNA strands were then dielectrophorized on modified interdigitated electrodes with oppositely placed castellation at an intermediate frequency in order to induce electro-osmotic flow. The stretched DNA was observed through laser confocal microscopy using intercalating dye such as acridine orange. This method enables characterization of single molecule dynamics and its consequent application in DNA based electronics, DNA templated nano structures, mutation detection and DNA-protein interaction studies.

BP 7.7 Mon 17:00 Poster A

Exposure of transcription factor binding sites in single nucleosomes and nucleosome arrays — •Wolfram Möbius[1,2] and Ulrich Gerland[2] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), LMU München — [2]Institute for Theoretical Physics, Universität zu Köln

Nucleosomes do compactify eukaryotic DNA, as a consequence burying long stretches of DNA. Nevertheless, transcription factors can bind to the DNA which may be achieved by temporarily unwrapping stretches of DNA from the histone complex (site exposure mechanism). Recently, we theoretically studied the dynamics of this mechanism in single nucleosomes, motivated by analogous experiments. Now, the thermodynamics of nucleosome arrays becomes experimentally accessible. We present first results of corresponding Monte Carlo simulations and compare it with the situation in single nucleosomes.

BP 7.8 Mon 17:00 Poster A

Surface-Enhanced Fluorescence for microarray sensitivity improvement — •Eric Le Moal[1], Emmanuel Fort[2], and Sandrine Lévêque-Fort[3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn — [2]Laboratoire Matériaux et Phénomènes Quantiques, Université Paris Diderot-Paris7, Bât. Condorcet, 10 rue A. Domon et L. Duquet, F-75205 Paris cedex 13 — [3]Laboratoire de PhotoPhysique Moléculaire, Université Paris Sud, Bât. 210, F-91405 Orsay cedex

Fluorescence is the prevailing labeling technique in biosensors and microarrays. However, the detection of very low molecular concentrations and the precise localization of biomarkers are often limited by the weakness of the fluorescence signal. We present a new method based on sample substrates that improve in sensitivity the fluorescence detection. These active substrates consist in glass slides covered with silver and alumina films and can directly be used with common detection setups. Fluorescence enhancement affects both excitation and decay rates and is strongly dependant on the distance to the metal surface. Additional improvements are achieved by structuring the metallic layer. Surface roughness indeed allows converting into light the energy that is non-radiatively transferred by the fluorescent molecules to the substrate. We measured a signal enhancement by more than 40-fold on a DNA microarray with a commercial scanning device. Reaching a highly sensitive detection on a DNA microarray allows operating with less genetic material, which may be of major interest when this quantity is limited, e.g., in biomedical diagnosis.

BP 7.9 Mon 17:00 Poster A

Modeling Background Intensity in Affymetrix GeneChips — •K. Myriam Kroll[1], Gerard Barkema[2,3], and Enrico Carlon[1] — [1]Institute of Theoretical Physics, KU Leuven, Celestijnenlaan 200D, 3001 Leuven, Belgium — [2]Institute for Theoretical Physics, Universiteit Utrecht, Leuvenlaan 4, 3584 CE, Utrecht, The Netherlands — [3]Institute-Lorentz for Theoretical Physics, University of Leiden, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands

A new physical model for the calculation of the background intensity in Affymetrix GeneChips is introduced. We identify two major sources of background noise; the first is related to the sequence composition (CG-rich sequences are expected to have higher affinities for non-specific hybridization than e.g. AT-rich sequences). The second is due to local dependence of intensities from locations which are the physical neighbors of a specific spot on the chip. Both effects are incorporated in a background functional whose free parameters are fixed via minimization on a training data set. In all data analyzed, the sequence specific parameters strongly correlate with empirically determined stacking free energies in solution. Moreover, we find an overall agreement with experimental background data. We show that our physics/physical-chemistry model globally performs better in calculating background intensities than approaches which are only based upon statistics. Thus, our model provides an interesting alternative method for background subtraction schemes in Affymetrix GeneChips.

BP 7.10 Mon 17:00 Poster A

Nanoengineered Polymer Capsules: Tools for Controlled delivery and Site Specific Manipulation — •Raghavendra Palankar[1], Oliver Kreft[1], Andre Skirtach[1], Yannic Ramaye[1], Margorzata Garstka[2], Gleb B. Sukhorukov[2], Sebastian Springer[2], and Mathias Winterhalter[1] — [1]Jacobs University Bremen — [2]Max-Planck Institut Golm

Hollow nanometer-sized containers are of increasing interest in nanotechnology, since they can protect proteins, enzymes or drugs from hostile surroundings and provide an optimal microenvironment. Here we report on functionalized nanocapsules as intracellular reporters providing a new tool in cell biology. Cell active molecules, hormones, enzymes or reporter molecules may be hidden from the outside, protected against chemical and biological degradation, targeted to specific compartments inside a cell and released in a controlled manner. For example we loaded capsules with antigenic peptides and inject the capsule with electroporation. We describe here the laser-triggered release of peptides into the interior of a cell which is followed by their binding to MHC class I molecules, and the subsequent movement of the peptide-class I complex to the plasma membrane.

Sukhorukov GB et al. Multifunctionalized Polymer Microcapsules: Novel Tools for Biological and Pharmacological Applications. Small 3 (2007) 944-55.

BP 7.11 Mon 17:00 Poster A

Motility and membrane protein dynamics of trypanosomes in a microfluidic environment. — •Eric Stellamanns[1], Niko Heddergott[2], Thomas Pfohl[1], and Markus Engstler[2] — [1]Max PIanck Institute for Dynamics and Self-Organization, Bunsenstr.10, 37037 Göttingen, Germany — [2]Technical University of Darmstadt,Department of Cellular Dynamics, Schnittspahnstr. 10, 64287 Darmstadt, Germany

The bloodstream parasite, Trypanosoma brucei, causative organism of the sleeping sickness in human and domestic livestock, is highly adapted to its fluidic environment. Placed in serum, trypanosomes swim in an auger-like motion with velocities up to 20 microns per second - much slower than the host's bloodstream. The resulting drag forces are strong enough to move surface bound antibodies towards the posterior cell pole, where they are rapidly internalized and digested. This strategy of escaping the immune system is possible as long as the cell is able to propel with a net direction.

In order to analyze such protein sorting with respect to cell motility, we combine microfluidics with optical tweezers and state of the art fluorescence microscopy. We study the influence of confinement, fluid viscosity and obstacles on the cell movement and therefor on their immune escape.

BP 7.12 Mon 17:00 Poster A

Investigation of erythrocytes cell-cell adhesion forces using holographic optical tweezers — •Achim Jung[1], Matthias Brust[1], Patrick Steffen[1], Christian Wagner[1], Ingolf Bernhardt[2], Ljubomira Ivanova[2], Lars Kaestner[3], and Peter Lipp[3] — [1]Department of Physics, Saarland University, 66041 Saarbrücken, Germany — [2]Central Isotope Laboratory/Laboratory of Biophysics, Saarland University, 66041 Saarbrücken, Germany — [3]Institute for Molecular Cell Biology, Saarland University, 66424 Homburg, Germany

Prostaglandin E_2 (PGE_2) and lysophosphatidic acid (LPA) are released from activated platelets. Using fluorescence imaging, spectral imaging and the patch-clamp technique, we recently provided evidence that these lipid-mediators at physiological concentrations activate a non-selective cation-channel in human red blood cells (RBCs). This results in a Ca^{2+} influx and the consecutive intracellular Ca^{2+} concentration increase. Ca^{2+} increases elicits the Ca^{2+}-activated K^+ channel (Gardos channel) in the RBC membrane resulting in K^+ efflux and shrinkage of the cells. By means of holographic optical tweezers we investigate the inter-cellular adhesion forces between individual RBC arising after mediator stimulated increase of the intracellular Ca^{2+} concentration. We are going to compare this force to depletion controlled cell-cell adhesion forces in polymer solutions. Based on our results we conclude that the PGE_2 and LPA responses of RBCs reveal a direct and active participation of these cells in blood clot formation.

BP 7.13 Mon 17:00 Poster A

Three-dimensional Fluorescence Lifetime Imaging with a light sheet based microscope (SPIM-FLIM) provides an excellent signal-to-noise ratio — •Manuel J. Neetz, Klaus Greger, Emmanuel G. Reynaud, and Ernst H.K. Stelzer — European Molecular Biology Laboratory (EMBL), Meyerhofstrasse 1, D-69117 Heidelberg, Germany

Fluorescence Lifetime Imaging (FLIM) (Gadella, 1993) in combination with modern microscopes allows one to determine the spatial distribution of specific molecular interactions. A FLIM setup operating on three dimensional (3D) live specimens requires optical sectioning capabilities, a low sample exposure and a physiologically relevant environment (Pampaloni, 2007). The optical sectioning capabilities of scanning approaches are limited due to high photobleaching rates and long acquisition times while widefield based setups do not provide optical sectioning at a reasonable noise level. The combination of EMBL's Single Plane Illumination Microscopy (SPIM) (Huisken, 2004; Greger, 2007) with frequency domain FLIM overcomes these limitations by decreasing photobleaching rates as well as increasing the signal-to-noise ratio significantly. It thus utilizes the fluorophores more efficiently. Hence, our approach is particularly well suited for investigating cellular interactions in 3D. We use our setup to acquire fluorescence lifetimes of EGFP labelled E-Cadherin in complex multi-cellular MDCK cysts to study cell-cell adhesion under relevant conditions. E.g., the ratio between cell surfaces in contact with each other and their volumes is manyfold as compared to conventional assays.

BP 7.14 Mon 17:00 Poster A

Endothelzellen und Glatte-Muskel-Zellen auf strukturieren Oberflächen — •Sarah Biela, Su Yi, Stefanie Korte, Britta Striegl, Ralf Kemkemer und Joachim P. Spatz — MPI für Metallforschung, Stuttgart

Bei der Behandlung von Aderverengung bei Herzkreislauferkrankungen setzt die moderne Medizin auf intravaskuläre Stent-Implantate. Stents weiten die Ader und verhindern den völligen Verschluss und somit Infarkte. Häufige Folgeprobleme dieser Behandlung sind Entzündungen, Thrombose und Wiederverschluss durch unkontrolliertes Wachstum von Glatten Muskel-Zellen, genannt Restenose. Ein neuer Ansatz in der Forschung ist der Versuch, neue Materialien und Beschichtungen für Stents zu finden, um Restenose zu verhindern und das Einwachsen in die Endothelzellschicht zu fördern.

Ziel meiner Arbeit ist es, verschiedene Reaktionen der zwei Zelltypen (Endothel- und Glatte Muskel-Zellen) gegenüber äußeren stimulierenden Faktoren zu finden. Mein Interesse gilt dabei besonders Oberflächenchemie, Topographie, elektrischen Feldern und externen mechanischen Kräften. Die Zellen werden auf flachen und dreidimensionalen Substraten (Stents) beobachtet, sowohl unter statischen, als auch unter Scherfluss-Bedingungen.

Auf nicht transparenten Substraten werden die Zellen mit einem aufrechten Mikroskop und mit Hilfe von Fluoreszenz-Markern beobachtet. Auf PDMS-Mikro-Strukturen zeigen Endothel- und Glatte Muskel-Zellen eine weniger signifikante Ausrichtung nach der Struktur als Fibroblasten.

BP 7.15 Mon 17:00 Poster A

Close Packed μm-Wells as Culture System for hMSCs — •Julia Schölermann, Ralf Kemkemer, and Joachim P. Spatz — Max-Planck-Institute for Metals Research, Dept. of New Materials & Biosystems & University of Heidelberg, Dept. of Biophysical Chemistry, Heisenbergstr. 3, D - 70569 Stuttgart

Current culture and differentiation systems for human mesenchymal stem cells (hMSCs) lack control of the microenvironmental niche of single cells since local cell densities and therefore distribution of cell secreted or bound signalling molecules and the individual cell's mechanical environment differ within a population. A common method in inducing chondrogenesis is hMSC pellet culture. Distribution of matrix proteins within these pellets has been shown to be rather heterogeneous (Murdoch, 2007) highlighting different cell fates gathered in one population. Therefore, a culture system for hMSCs was designed that allows for controlled cell densities in spatially separated containers exhibiting a homogeneous geometric environment. Microsphere lithography was applied covalently attaching glass beads sized between 8 and 170 μm to Si wafers using silane chemistry. These structures were used as blueprints for casting polydimethylsiloxane (PDMS) yielding close packed arrays of hemispheres. Microstructured PDMS samples were used as hMSC culture substrates and differentiation was monitored using real time PCR. Necessity of PDMS functionalisation was assessed on non-structured samples showing that plasma treatment was sufficient in promoting hMSC survival whereas fibronectin seemed to unspecifically elevate osteogenesis related transcription factors.

BP 7.16 Mon 17:00 Poster A

Optical force based investigations of cell mechanical concepts during phagocytosis — •Felix Kohler[1], Holger Kress[2], and Alexander Rohrbach[1] — [1]University Freiburg, Freiburg, Germany — [2]Yale University, New Haven, USA

Macrophages internalize bacteria during phagocytosis, which is a central mechanism in the immune system. Still, only little is known about the mechanical properties of phagocytosis, in particular when mediated by cellular tentacles, i.e. filopodia. We used optical tweezers-based microscopy to investigate different mechanical concepts of the cell to take up 1 micron beads, which serve as synthetic bacteria. The motion of an optically trapped bead was tracked interferometrically in 3D with nanometer precision at a microsecond timescale. On the one hand, the measurement of the thermal bead fluctuations during the binding to the cell membrane enabled the observation of individual receptor-ligand bond formation. On the other hand, the measurement of the mean bead displacements allowed determining retraction forces of filopodia at various retraction speeds. We measured F-actin dependent 36-nanometer steps inside living cells during filopodia retraction likely belonging to actin-based molecular motors[1]. Steps remained clearly visible even at force regimes clearly beyond the stall force of a single myosin motor. This seems to indicate a kind of inter-motor coupling, a phenomenon which we try to explain by a stochastic multistate model.

[1] Kress, H., E.H.K. Stelzer, D. Holzer, F. Buss, G. Griffiths, and A. Rohrbach, PNAS, Vol.104, 2007, 11633 - 11638

BP 7.17 Mon 17:00 Poster A

Rigidity percolation in networks of stiff fibers — •Boris Schaefer[1], Claus Heussinger[1,2], and Erwin Frey[1] — [1]Arnold Sommerfeld Center for Theoretical Physics, LMU München, Theresienstraße 37, 80333 München — [2]Université Lyon I, LPMCN, Villeurbanne, France

We study the elasticity in random networks of stiff fibers. It is well known that by decreasing the density of fibers, these networks lose their stability and undergo a rigidity percolation transition that is distinct from the usual connectivity percolation. We present a self-consistent theory on Cayley-tree level that allows to determine both the percolation threshold as well as the critical exponent for the elastic modulus. The theory is based on the recognition that for stiff fibers stretching excitations are suppressed and the elastic energy is dominated by the bending mode ("floppy modes"). By suitably averaging over the quenched random structure we pin-point the role of architectural features, such as network anisotropy, on the critical properties of the system.

BP 7.18 Mon 17:00 Poster A

Characterizing circular semiflexible polymers — •Karen Alim and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics and CeNS, Department of Physics, Ludwig-Maximilians-Universtät München, Theresienstr. 37, 80333 München

Circular polymers such as viral DNA, plasmids or cytoskeletal bundles play a crucial role in various biological processes. We examine the shape of circular semiflexible polymers over their whole range of flexibility observing two distinct shape regimes depending on the flexibility of the polymer [1]. For small perimeter to persistence length the fluctuating rings exhibit only planar, elliptical configurations. At higher flexibilities three dimensional, crumpled structures arise. Analytic calculations confirm the qualitative behavior of the shape parameters and the elliptical shape in the stiff regime.

Further characteristic measures for circular semiflexible polymers are derived based on an elastic rod model with anisotropic bending stiffness and twist stiffness [2]. In this polymer ribbon model the geometric constraint causes an effective stiffning of bending modes and a coupling of bending and twisting modes. Furthermore, our model predicts the mean square diameter of a ribbonlike ring thus giving a novel parameter to determine bending and twist stiffnesses of polymers and especially bundles in experiments.

[1] K. Alim and E. Frey, *Shapes of semiflexible polymer rings*, Phys. Rev. Lett. **99**, 198102 (2007)

[2] K. Alim and E. Frey, *Fluctuating semiflexible polymer ribbon constrained to a ring*, Eur. Phys. J. E, in press

BP 7.19 Mon 17:00 Poster A

Nonlinear dynamic response of semiflexible polymers — •Benedikt Obermayer[1], Wolfram Möbius[1,2], Oskar Hallatschek[3], Klaus Kroy[4], and Erwin Frey[1] — [1]Arnold Sommerfeld Center and Center of NanoScience, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München — [2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln — [3]Lyman Laboratory of Physics, Harvard University, Cambridge, MA 02138, USA — [4]Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, 04009 Leipzig

We have theoretically analyzed the anisotropic nonlinear dynamic response of semiflexible polymers to external driving fields. Crossover scaling laws are extracted from a coarse-grained equation of motion that governs the propagation and relaxation of backbone tension and follows from a rigorous perturbation theory. Our analytical results are compared to simulation data for a variety of force protocols. We address explicitly the dependence on boundary conditions and other implications relevant for experiments and computer simulations, such as the influence of finite extensibility and microstructure.

BP 7.20 Mon 17:00 Poster A

Orientational correlations in a wormlike chain — •Semjon Stepanow — Universität Halle, Institut für Physik, 06099 Halle

We present results of the study of the distribution function of a wormlike chain with fixed orientation of one chain end, and as well as tangent correlation functions of segments along the chain with and without a global constraint on the chain.

BP 7.21 Mon 17:00 Poster A

Conformation of a semiflexible polymer in a disordered environment — •Sebastian Schoebl[1], Abigail Klopper[2], and Klaus Kroy[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Leipzig — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden

Biological cells are affected by the structural and mechanical properties of polymers and polymeric networks in an essential way. A particularly interesting question is how the conformations of a polymer in the cytoplasm is affected by molecular crowding. Despite the prolific attention paid to the analogous problem in flexible polymer networks in recent years, little is understood about how their stiffer counterparts respond to a disordered environment. We investigate the equilibrium and non-equilibrium conformations of semiflexible polymers in a variety of potential landscapes by Monte Carlo simulations. The polymer is represented as a Heisenberg chain, i.e. a discretised wormlike chain. Relevant observables such as the end-to-end distribution function and the tangent-tangent correlation function are evaluated.

BP 7.22 Mon 17:00 Poster A

Theory of Mechano-Transduction in Cells — •Sebastian Sturm[1], Jens Glaser[1], and Klaus Kroy[1,2] — [1]Institut für theoretische Physik, Universität Leipzig, Vor dem Hospitaltore 1, 04103 Leipzig — [2]Hahn-Meitner Institut, Glienicker Straße 100, 14109 Berlin

No higher forms of life could exist without the ability of biological cells to quickly sense and react to changes in their environment. In general, stimuli excite the cell membrane and have to be transmitted to the nucleus. Mechano-transduction through the cytoskeleton may arguably provide the fastest pathway for mechanical stimuli. Understanding the dynamics of tension propagation through biopolymer networks is thus an important task.

Our approach combines two highly successful recent theoretical developments: (i) a systematic theory of tension propagation in single semiflexible polymers [1]; (ii) the glassy wormlike chain (GWLC) model [2], which accounts for the influence of a crowded environment on polymer dynamics. We discuss asymptotic solutions of the theory for different force protocols to derive experimentally relevant predictions.

[1] O. Hallatschek, E. Frey and K. Kroy, Phys. Rev. Lett. 94, 077804 (2005)
[2] K. Kroy and J. Glaser, arXiv:0705.0490

BP 7.23 Mon 17:00 Poster A

Microtubule dynamics depart from wormlike chain model — Katja M Taute[1], •Francesco Pampaloni[2], Erwin Frey[3], and Ernst-Ludwig Florin[1] — [1]Center for Nonlinear Dynamics, University of Texas at Austin, 1 University Station C1610, Austin TX 78712, U.S.A. — [2]Cell Biology and Biophysics Unit, European Molecular Biology Laboratory, Meyerhofstraße 1, 69117 Heidelberg, Germany — [3]Arnold Sommerfeld Center for Theoretical Physics and CeNS, Department of Physics, Ludwig-Maximilians-University at München, Theresienstraße 37, D-80333 München, Germany

We study the dynamics of the tip's thermal fluctuations of grafted microtubules in the length range of 2-30 um, by employing high precision particle tracking on attached fluorescent beads. First mode relaxation times were extracted from the mean square displacement in the transverse coordinate. For short microtubules, the relaxation times were found to follow an L^2 dependence instead of L^4 as expected from the standard wormlike chain model. As these time scales are determined by an interplay of filament stiffness and friction, persistence lengths and drag coefficients were examined. The persistence lengths show a complex dependence on overall filament length and indicate a plateau value of ~600 um for microtubules shorter than ~ 5 um. This behavior is consistent with the elastic properties of bundles of wormlike filaments and hence suggests modeling microtubules as bundles of their constituent protofilaments. Our results emphasize that microtubule mechanics can be understood as a consequence of their complex protofilament architecture.

BP 7.24 Mon 17:00 Poster A

Optimization of a thermal Brownian Motor — •Florian Berger, Tim Schmiedl, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart

Since the introduction by Feynman, thermal Brownian ratchets have served as a model for a microscopic engine in a thermal environment. Following this route, we consider the motion of an overdamped Brownian particle in a periodic potential, which is divided into two regions with different temperatures T_1 and T_2. Within these two thermal environments the stochastic movement of the particle is influenced by different noise. This fact can be used to obtain a net flux in one direction for a properly chosen potential. By attaching a load to the particle we construct a heat engine that operates between the two heat baths. The dependency of the flux on the potential evokes the question: What is the optimal shape of the potential that maximizes the flux and thus the power of the engine for a given load? We calculate optimal shapes of the potential for different choices of model parameters like ratio of the two temperatures, length of the two regions and load.

BP 7.25 Mon 17:00 Poster A

Contraction waves in chains of spontaneous oscillating sarcomeres. — •Stefan Günther and Karsten Kruse — Saarland University, Theoretical Physics Department, Saarbrücken

Sarcomeres are the elementary force generating elements of skeletal muscle and consist of a regular arrangement of myosin motors and actin filaments. Under appropriate conditions, sarcomeres have been found to oscillate spontaneously [1]. Chains of sarcomeres show spontaneous contraction waves [2] displaying complex dynamics. We have proposed a microscopic model of sarcomere dynamics, which generates spontaneous oscillations resulting from force-dependent motor detachment rates [3]. By rigidly coupling several sarcomeric elements into a linear chain, non-trivial wave solutions emerge. With parameters deduced from single molecule experiments, we find wave solutions in quantitative agreement with experiments. Furthermore, we find spontaneous nucleation and annihilation of waves as reported, for example, in [2].

[1] Yasuda, Shindo, and Ishiwata, Biophys. J. 70 (1996)
[2] Sasaki et al, J. Muscle Res. Cell Motil. 26 (2005)
[3] Guenther, and Kruse, NJP in press

BP 7.26 Mon 17:00 Poster A

Manipulation of biological filaments by electric fields — •Christoph Wigge[1], Horst Hinssen[2], and Simone Herth[1] — [1]Thin Films and Nanostructures, Faculty of Physics, Bielefeld University — [2]Biochemical Cell Biology, Faculty of Biology, Bielefeld University

The induced alignment of biological filaments on surfaces has the potential to provide controllable geometries for lab on a chip like structures. Actin with a diameter of 7-8 nm and microtubules with a diameter of 25 nm were chosen to study filamentous structures of different size ranges. Both types of supramolecular aggregates show polarity and can be manipulated with electric fields. Many of the earlier experiments were performed as gliding assays, where the surfaces were structured and coated with the motor proteins. In this work, the so called bead geometry is used in which filaments are structured on dif-

ferent surfaces and motor proteins glide on these filaments transporting cargos. This approach has the advantage that not only biological filaments but also inorganic cargos, such as magnetic nanoparticles can be transported and manipulated. In this project biological filaments are manipulated on a chip by applied electrical fields. The alignment process is controlled by light microscopy, scanning electronmicroscopy (SEM) and atomic force microscopy (AFM). The goal of this project is to create a "Y"-structure made of biological filaments, which allows magnetic nanoparticles loaded with motor proteins to be separated using magnetic fields.

BP 7.27 Mon 17:00 Poster A

Superdiffusive motion with fractional power-law exponents in cytoskeleton-bound microbeads — •Max Sajitz-Hermstein, Claus Metzner, Raupach Carina, and Fabry Ben — Department Of Physics, University of Erlangen, Germany

The spontaneous random motion of microbeads bound to the cytoskeletal (CSK) network of living cells is a non-Brownian process [1]. The mean-squared-displacement (MSD) of the bead as a function of lag time shows a sub-to-superdiffusive transition that arises from the interplay of uncorrelated noise, dominating at short time scales, and persistent traction forces, dominating at longer times scales [2]. However, the fractional powerlaw exponent of the superdiffusive bead motion in the range from 1-2 is unexplained. We propose an analytical model for the CSK dynamics that accounts for superdiffusive behavior with fractional power-law exponents. The CSK is described as a network of elastic springs (stress fibers) undergoing gradual changes of rest length and stiffness due to ATP-driven processes. In addition, new fibers emerge spontaneously, generating an increasing and finally saturating prestress, which is coupled to the reinforcement of focal adhesions. The fiber growth is catalyzed by enzymes which constitute a limited, shared resource of the cell. We demonstrate that superdiffusion with a fractional powerlaw exponent arises naturally by a multiplicative noise process. Our model accounts quantitatively for the MSD data. [1] C. Raupach et al., Phys. Rev. E 76, 011918 (2007) [2] C. Metzner et al., Phys. Rev. E 76, 021925 (2007)

BP 7.28 Mon 17:00 Poster A

Mechanosensitive pattern formation in active cytoskeletal networks — •Volker Schaller[1], Ronny Peter[1], Falko Ziebert[2], and Walter Zimmermann[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Materials Science Division, Argonne National Laboratory, 9700 S Cass Avenue, Argonne, IL 60439, USA

We present a one-dimensional model combining two of the main features of active biopolymer solutions, namely the molecular motor driven active transport of filaments and the (visco-)elastic properties of filament networks held together by crosslinkers or entanglement effects.

It is shown that the pattern forming mechanisms, associated to the motor-mediated transport of filaments, are substantially altered if coupled to a filament network: in case of a permanent network, the long-range clustering of filaments changes either to stationary periodic filament density patterning or to propagating pulses. However if the network is viscoelastic, molecular motor activity can lead to traveling or standing filament density waves[1].

Moreover we investigate the mechanosensivity of pattern formation and the contractive behavior of the network.

[1]R. Peter and V. Schaller and F. Ziebert and W. Zimmermann; *Pattern formation in active cytoskeletal networks*, Submitted to: New J. Phys.

BP 7.29 Mon 17:00 Poster A

Functional and structural characterisation of plasmodium falciparum actin-I — •Stefan Schmitz, Munira Grainger, Iwan A.T. Schaap, Simone Harder, Irene T. Ling, Antony A. Holder, and Claudia Veigel — National Institute for Medical Research, London, UK

A novel form of acto-myosin regulation has recently been proposed in which the polymerization of actin filaments regulates various types of apicomplexan motility, including parasite invasion of malaria merozoites into red blood cells of the mammalian host. Although it is difficult to visualize filamentous actin within the parasite, we found that actin is one of the most abundant proteins in the merozoite stage of the Plasmodium falciparum life cycle and that monomeric actin extracted from merozoites could be polymerized in the presence of F-actin stabilizing drugs rhodamine-phalloidin or jasplakinolide. In in-vitro motility assays, the average filament velocity of malaria F-actin over rabbit myosin subfragment HMM was indistinguishable from that of rabbit skeletal actin. However, malaria actin filaments polymerized in presence of rhodamine-phalloidin appeared spot-like in fluorescence microscopy, while rabbit skeletal actin prepared under similar conditions had the usual length of several micrometers. Using electron microscopy we found that Malaria actin filaments were on average only about 100 nm long. In order to resolve structural differences between mammalian and malaria F-actin we investigated both forms using atomic force microscopy and negative stain electron microscopy.

BP 7.30 Mon 17:00 Poster A

In vitro assembly and characterization of keratin intermediate filaments — •Anke Leitner[1], Katrin Hübner[1], Othmar Marti[1], Harald Herrmann[2], and Tatjana Wedig[2] — [1]Ulm University, Institute Of Experimental Physics, Germany — [2]Division of Molecular Genetics, German Cancer Research Center Heidelberg, Germany

The aim of this work is to compare the properties of in vitro assembled keratin intermediate filaments with those of authentic keratin cytoskeletons. We will show the details of the assembly process of the keratin filaments. In a first step the recombinant keratin 8/18 dimers assemble into tetramers. In the second step the tetramers form unit length filaments (ULF). In a third step, the ULFs longitudinally anneal into loosely packed filaments and radially compact into mature intermediate filaments. The properties of the assembled filaments are investigated by means of atomic force microscope (AFM) and photonic force microscope (PFM) and are compared to those of cytoskeletons prepared from cultured human pancreatic cancer cells (line Panc 1).

BP 7.31 Mon 17:00 Poster A

Linear and nonlinear laser-trapping microrheology — Daisuke Mizuno[1] and •Christoph F. Schmidt[2] — [1]Kyushu University, Fukuoka, Japan — [2]Georg-August-Universität, Göttingen, Germany

We have developed a high-bandwidth technique for active 2-particle microrheology (AMR) with which we can probe linear and nonlinear responses of soft materials. Micron-sized colloidal probe particles are driven by an oscillating optical trap, and the resulting correlated motions of neighboring particles are detected by laser interferometry. Lock-in detection at the driving frequency and at its second harmonic makes it possible to measure the linear and the non-linear response of the embedding medium at the same time. We demonstrate the sensitivity of the method by detecting a second-harmonic response in water which is of purely geometric origin and which can be fully understood within linear hydrodynamics.

BP 7.32 Mon 17:00 Poster A

High-resolution probing of active cellular traction forces — Daisuke Mizuno[1], Rommel Bacabac[2], Catherine Tardin[2], David Head[3], and •Christoph F. Schmidt[4] — [1]Kyushu University, Fukuoka, Japan — [2]Vrije Universiteit, Amsterdam, The Netherlands — [3]University of Tokyo, Tokyo, Japan — [4]Georg-August-Universität, Göttingen, Germany

Living cells mechanically probe their environment, which can consist of an extracellular matrix to which they adhere or of other cells. The response of the environment directly affects internal regulatory processes. In this study, we have quantitated the active traction force of mechano-sensitive osteocyte-like cells (MLO-Y4) in a simple suspended geometry with a pair of optical traps of adjustable stiffness. By alternatingly actively probing the cells with an oscillating force and passively observing shape fluctuations, we could detect forces generated by the cells and at the same time follow the change of their mechanical properties. We found that intracellularly generated force was more efficiently transmitted to the sites of adhesion between the cell and the probes when the traps were stiffer than the cell. We propose that cells sense the elastic response of their surroundings by using their own stiffness as a reference.

BP 7.33 Mon 17:00 Poster A

Transport through OmpF channels simulated using molecular dynamics — •Soroosh Pezeshki, Catalin Chimerel, Mathias Winterhalter, and Ulrich Kleinekathöfer — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Ion transport through the outer membrane porin (OmpF) of E. Coli is simulated using all atom molecular dynamic simulations. The temperature dependence of the conductance is determined at different salt

concentrations and the results are compared to experimental measurements. The agreement between experiment and simulations is very reasonable. Using the atomistic details obtained from the simulations, it is possible to analyze the behavior of the pore and ions during the simulations. Here special attention was put on ion pairing. Furthermore, constraining part of the pore in the simulations can change the conductivity drastically. This allows to draw conclusions about the influence of different parts of the pore (e.g. the beta barrels, the loops, etc.) on the current.

BP 7.34 Mon 17:00 Poster A

Localized heating effects in optical tweezers investigated using ionic currents through nanopores — •Jan Henning Peters and Ulrich Felix Keyser — Institut für Experimentelle Physik I, Universität Leipzig

Optical tweezers are a powerful and widely used experimental tool in biological physics including single molecule investigations. The strongly focused laser-beam in such a setup can reach power densities in the order of $10^8 W/cm^2$ that cause significant heating exceeding 10K per Watt of incident laser power for a 1064nm-Laser ([1],[2]). As the reaction constants of biomolecules are temperature dependent, heating effects should be considered in biophysical experiments.

The ionic current through a nanopore depends on the local temperature in a well-defined manner and hence can be used for temperature measurements with high spatial resolution [1]. We compare experiments using nanopores with numerical finite element calculations and investigate the dependence of heating effects on parameters like geometry and thermal conductivity of water and nanopore material. We were able to confirm earlier findings as the logarithmic dependence of the maximal temperature on the size of the system [2] and also gain a more detailed insight into the temperature distribution found in optical tweezers.

[1] U. Keyser, et al., Nano Letters Vol. 5 No. 11 2253-2256
[2] E. Peterman, et al., Biophys. Journal Vol. 84, 1308-1316

BP 7.35 Mon 17:00 Poster A

Simulating an Efflux Pump: Opening the Exit Duct TolC — •Robert Schulz and Ulrich Kleinekathöfer — Jacobs University Bremen, Campus Ring 1, 28759 Bremen,Germany

Bacteria, such as E. coli, use efflux pumps to regulate the permeation of water soluble substances through cell membranes. To allow transport through the outer membrane part of the efflux pump, the so-called TolC, its periplasmic coiled-coil has to be opened [1]. Using all-atom molecular dynamics simulations, including about 200 000 atoms, one is faced with the problem that the conformational changes take place on a timescale far larger than computationally affordable even on today's supercomputers. Hence, it was investigated whether the opening of TolC and several mutants can be forced by applying an electric field and thereby inducing an extra force by the ions that are solvated in the surrounding water. The rate of opening can easily be traced by calculating the distances of the monomers' tails from the trimer's planar center of mass. From the obtained data, ion density, potential maps, and ion currents have been calculated. It is planned to investigate the other constituents of the efflux pump as well.

[1] J. Eswaran, E. Koronakis, M.K. Higgins, C. Hughes, and V. Koronakis, Curr. Op. Struct. Biol. **14**, 741 (2004).

BP 7.36 Mon 17:00 Poster A

Quantum dots as substrates for nuclear-cytoplasmic transport. — •Ulrike Schmitz-Ziffels, Birgit Klaiberg, Jan-Peter Siebrasse, and Ulrich Kubitscheck — Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, 53115 Bonn

Nuclear-cytoplasmic transport of macromolecules is accomplished by the nuclear pore complex (NPC) - a transport machine imbedded in the nuclear envelope (NE). The NPC enables high selective translocation across the NE, known to be facilitated by the interaction of soluble transport receptors with the NPC's nucleoporins. However, detailed mechanisms and kinetics of the translocation still remain unknown. Single molecule fluorescence microscopy provides a direct observation of processes at the NPC with excellent spatial and time resolution. We use functionalized biocompatible quantum dots as transport substrates to investigate nuclear import in permeabilized cells at the single particle level. As bright and photostable probes, quantum dots yield an excellent localization precision (< 10nm). This is of great importance when tracking the import complex through the approximately 100 nm long NPC. Experiments with NTF2-functionalized quantum dots demonstrated that a specific interaction with the NPC can be achieved. We detected nuclear import of the smallest, green fluorescent quantum dots, yet their fluorescence is not bright enough to yield the required localization precision. The brighter red fluorescent quantum dots on the other hand could not pass the NPC, due to their larger stokes radius. Currently we are focussing on the preparation of smaller red fluorescent substrate-conjugated nanoprobes.

BP 7.37 Mon 17:00 Poster A

Stochastic model for mitochondria transport along the cytoskeleton — •Thomas Sokolowski and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

Inside an eukaryotic cell mitochondria master a variety of vital tasks: They keep up the production of ATP, thus providing the energetic base for cellular processes, regulate the programmed cell death and act as strongly dynamic Ca^{2+} buffers, just to name a few of its functions. In the last years it became evident that the mitochondria distribution and the Ca^{2+} concentration influence themselves mutually. Based on previous approaches, we develop a stochastic model for the intracellular organelle transport processes including the dynamics of the cytoskeleton and various patterns of transport. We investigate the impact of different cell geometries and the variation of cytoskeleton parameters on the distribution of the mitochondria.

BP 7.38 Mon 17:00 Poster A

Influence of Receptor Mobility and Micropatterning upon Biomembrane Adhesion — •Susanne Fenz[1], Cornelia Monzel[1], Sabine Dieluweit[1], Kheya Sengupta[2], and Rudolf Merkel[1] — [1]Institute of Bio- and Nanosystems 4: Biomechanics, Research Centre Jülich, Germany — [2]CRMC-N (UPR CNRS 7251), Luminy, Marseille, France

The adhesion of cells is a complex process essential for life. It is caused by specific binding between biomolecules that form supramolecular structures at late times. However, the initial steps of cell adhesion, where physical forces dominate, are barely understood. Therefore we developed and quantitatively analyzed a simplified model system. Cell adhesion was mimicked by vesicles, with the specific binding being mediated by the biotin neutravidin complex. Micropatterns of adhesion-competent and repulsive areas were produced by microcontact printing. The adhered vesicle exhibited areas of fluctuating and frozen membrane, corresponding to the underlying pattern. From Reflection Interference Contrast Microscopy (RICM) analysis we obtained the distribution of height fluctuations yielding the potential of interaction. Printed pattern and receptor density were varied systematically. To further investigate the correlation between vesicle adhesion and receptor mobility a supported lipid bilayer was used as substrate. Thus, the lipid coupled receptors were able to diffuse freely. The process of vesicle adhesion was monitored in RICM as well as fluorescence microscopy. We found vesicle adhesion induced distinct protein enrichment in the adhesion disc accompanied by a decrease in diffusivity.

BP 7.39 Mon 17:00 Poster A

Model Membranes under Tension — •Jörg Neder[1], Beate West[2], Friederike Schmid[2], and Peter Nielaba[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz — [2]Department of Physics, University of Bielefeld, 33615 Bielefeld

Recently O. Lenz and F. Schmid [1] introduced a simple coarse-grained model to study lipid layers and their phase transitions. Using an extension of this model we are investigating the influence of an applied surface tension to a bilayer membrane by Monte Carlo simulations. We recorded pressure profiles and calculated the area per lipid as a function of tension for temperatures ranging from the gel phase to the liquid phase of the system. Another aim of our work is the investigation of lipid-mediated interactions between two anchored cylindrically shaped model proteins. We compared the tensionless state to states with non-vanishing surface tension. Our results indicate that the agglomeration behavior of the model proteins is only weakly influenced by an additional tension. We are also working on semi-grand-canonical simulations [2] of lipid bilayers forming tubular objects and the influence of incorporated model proteins on their properties.

[1] O. Lenz and F. Schmid, *Phys. Rev. Lett.* **98**, 058104 (2007)
[2] F. Schmid, et al., *Comp. Phys. Comm.* **177**, 168 (2007)

BP 7.40 Mon 17:00 Poster A

Lateral diffusion of receptor-ligand bonds in membrane adhesion zones: Effect of thermal membrane roughness — •Heinrich Krobath[1], Gerhard Schütz[2], Reinhard Lipowsky[1],

and Thomas Weikl[1] — [1]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Wissenschaftspark, D-14476 Potsdam-Golm — [2]Johannes-Kepler-Universität Linz, Institut für Biophysik, A-4040 Linz

The adhesion of cells is mediated by membrane receptors that bind to complementary ligands in apposing cell membranes. It is generally assumed that the lateral diffusion of mobile receptor-ligand bonds in membrane-membrane adhesion zones is slower than the diffusion of unbound receptors and ligands. We find that this slowing-down is not only caused by the larger size of the bound receptor-ligand complexes, but also by thermal fluctuations of the membrane shape. We model two adhering membranes as elastic sheets pinned together by receptor-ligand bonds and study the diffusion of the bonds using Monte Carlo simulations. In our model, the fluctuations reduce the bond diffusion constant in planar membranes by a factor close to 2 in the biologically relevant regime of small bond concentrations.

BP 7.41 Mon 17:00 Poster A

Monte-Carlo simulations of a coarse-grained model for lipid membranes — •Beate West and Friederike Schmid — Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

A simple coarse-grained model for self-assembling lipid membranes is presented. The "lipids" are represented by short linear spring-bead chains, which self-assemble to membranes due to the presence of a computationally cheap "phantom" solvent environment. These membranes may contain "transmembrane proteins", represented by cylinders with diameters corresponding to the diameter of an alpha-helix. The system is studied by Monte Carlo simulations at constant pressure using a parallel code with a newly devised domain decomposition scheme. Pure fluid membranes are characterized in some detail. The pressure profiles and the fluctuation spectra are calculated, and the elastic constants are extracted. Then, the membrane distortions caused by single embedded proteins are determined as a function of the lipid-protein interaction strength. These distortions influence the effective interactions between proteins, which are obtained by determining the protein-protein pair-correlation function with umbrella sampling techniques.

BP 7.42 Mon 17:00 Poster A

Diffusion of single actin filaments bound to cationic model membranes — •Lydia Woiterski, Florian Rückerl, Josef Käs, and Carsten Selle — Universität Leipzig, Physik Weicher Materie, Linnéstr. 5, 04103 Leipzig

Actin is one of major components of the cytoskeleton in eukaryotic cells. The filaments form a quasi-two-dimensional network - the so-called actin cortex that plays an important role for motility and adhesion. It is associated with the inner leaflet of the cell membrane via protein anchors and was suggested to control protein motion. Thus, it is of great interest to elucidate the nature of interaction of polymerized actin and lipid membrane models. In previous work it was reported that binding of filamentous actin to cationic lipid membranes is governed by Coulomb interactions [Sengupta et al. 2006]. Under certain conditions, these liquid membranes show coexistence of ordered and disordered phases. We propose that actin binding can be regulated by the phase state and that preferential binding to one of the coexistent phases occurs due to varied surface charge density. First, the binding process of F-actin is studied using giant vesicles prepared from mixtures of phosphatidylcholine, the cationic lipid DOTAP, and cholesterol that adsorb actin filaments which is monitored by fluorescence microscopy. Secondly, the diffusion of single actin filaments adsorbed to supported bilayers is investigated by single polymer tracking in order to study how the domains confine the lateral motion of the polymer.

[1] Sengupta, K., E.Sackmann, et al. (2006), Langmuir 22(13): 5776.

BP 7.43 Mon 17:00 Poster A

Interactions of nanoparticles and semiflexible polymers with inhomogeneous membranes — Florian Rückerl, Lydia Woiterski, Josef A. Käs, and •Carsten Selle — University of Leipzig, Institute for Experimental Physics I, Linnestraße 5, 04103 Leipzig, Germany

Lateral diffusion within membranes plays a major role in biologically important processes as signal transduction. We present experimental studies on diffusion of proteins within or at a variety of inhomogeneous model membranes where two differently ordered phases coexist. We use Langmuir monolayers, planar supported bilayers and giant unilamellar vesicles as membranes in order to rule out effects of surrounding medium and geometry. The diffusants range from fluorescent spheric nanoparticles to linear semiflexible polymers (f-actin) whose motion is monitored by single-particle or single-polymer tracking. Associated to ordered domains, dimensionally reduced motion was observed for nanoparticle diffusion in monolayers and bilayers. Monte-Carlo simulations demonstrate that model protein diffusion can be strongly affected by both the strength of these interactions and the domain size. We conclude that cellular membranes might use similar mechanisms to adjust two-dimensional diffusion for the control of biochemical reactions within the membrane. Furthermore, we expect that our experiments might contribute to a better understanding of actin-membrane interactions.

BP 7.44 Mon 17:00 Poster A

Characterization of polymer-supported native membranes by X-ray and neutron reflectivity — •Fernanda Rossetti[1], Emanuel Schneck[1], Stefan Kaufmann[1], Murat Tutus[1], Oleg Konovalev[2], Giovanna Fragneto[3], and Motomu Tanaka[1] — [1]Biophysical Chemistry Laboratory II, University of Heidelberg, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Institut Laue Langevin, Grenoble, France

Polymer-supported artificial and/or native membranes attract increasing interest as planar models of cell membranes. Immuno-fluorescence labeling experiments have demonstrated that native cells and microsomes can be spread on polymer "cushions" based on ultrathin films of regenerated cellulose. However, structures of such "two-dimensional biological membranes" on the molecular level are still unknown. This poster will present a quantitative study–performed by X-ray and neutron reflectivity measurements at the solid-liquid interface–of structures of bio-membranes on cellulose cushions that mimic the extracellular matrix (ECM). The films are prepared by Langmuir-Blodgett transfer, so that the thickness can be controlled within nm accuracy in the range of ˜ 5-50 nm. It will be shown that the deposition of several types of natural bio-membrane extracts (sarcoplasmic reticulum membranes, human erythrocyte ghosts, HeLa cell membrane extracts) results in a clear change in the global shape of the reflectivity curves for cellulose supports of different thickness. The observed changes coincide with the formation of homogeneous polymer-supported lipid membranes over a macroscopically large area.

BP 7.45 Mon 17:00 Poster A

Micromachined apertures for x-ray structure analysis of free-standing lipid membranes — •André Beerlink and Tim Salditt — Institut für Röntgenphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

A wealth of functional and physiological properties of membranes has been derived from patch clamp and other electrophysiological methods carried out on small membrane patches. At the same time, a wealth of structural information of single and multi-component membranes has been provided by x-ray and neutron scattering techniques, mostly on isotropic suspensions or on planar model bilayers, composed of a controlled lipid/protein composition. The combination of functional and structural studies has to date been rarely achieved. We want to put forward a model system which well developed in membrane electrophysiology, but which was previously not amenable to structural studies, i.e. single freely suspended bilayers spanned in between two separate fluid compartments. To this end, stability and size of the freely suspended membranes must be addressed, and requires new technological tools of sample and aperture preparation. We propose an experimental setup allowing for freely suspended bilayers in aqueous solution spanning a controlled aperture between two compartments (differing in pH, ion concentrations etc.), and amenable to a collimated and focused synchrotron reflectivity experiment beam, as well as to a highly collimated and partially coherent beam for x-ray phase contrast imaging. Such a setup can open the door to a wide range of experiments, probing structure and conductivity simultaneously.

BP 7.46 Mon 17:00 Poster A

Effect of Cholesterol on the Collective Dynamics of Phospholipid Membranes — •Beate Brüning[1,2], Tim Salditt[2], and Maikel C. Rheinstädter[3] — [1]Institut Laue-Langevin, Grenoble, France — [2]Institut für Röntgenphysik, Georg-August Universität Göttingen, Germany — [3]Department of Physics and Astronomy, University of Missouri-Columbia, USA

Phospholipid membranes often serve as simple model systems to understand basic properties of their far more complex biological coun-

terparts. Only recently, the collective short wavelength dynamics in a model membrane system (DMPC), i.e., the corresponding dispersion relation, were investigated by inelastic neutron scattering techniques [1]. The insertion of the membrane-active molecule cholesterol, which is known to regulate membrane fluidity, membrane permeability and the lateral mobility of proteins, is now a first step towards the understanding of coherent dynamics in physiologically relevant membrane systems. While the structure of phospholipid/cholesterol systems is well studied, their short scale dynamics are so far largely unknown. We have studied the influence of cholesterol to the collective short wavelength fluctuations of the phospholipid acyl chains using inelastic neutron scattering. The measurements were carried out with thermal as well as cold neutrons on the three-axis spectrometers IN12 and IN8 at the high flux reactor of the ILL in Grenoble, France. We were able to determine the dispersion relations within the plane of the membranes in the fluid and in the liquid ordered phase.

[1] M.C. Rheinstädter et al., Phys. Rev. Lett. 93, 108107 (2004).

BP 7.47 Mon 17:00 Poster A

Translational Brownian motion and rotational shape deformations of freely suspended micron-sized phospholipid vesicles — •Christoph Herold, Eugene P. Petrov, and Petra Schwille — Biophysics / BIOTEC, TU Dresden, Tatzberg 47-51, 01307 Dresden

Do shape fluctuations of a body suspended in a viscous fluid affect its translational diffusion coefficient? Theoretical studies [1, 2] predict the effect as large as ∼20%. However, to the best of our knowledge, this prediction has never been challenged experimentally. We carry out video microscopy studies on freely suspended fluorescently labeled giant unilamellar vesicles (GUVs) with radii in the range of $R = 2 - 7\mu$m, both in the tensed state and showing pronounced shape fluctuations ($|\Delta R| / \langle R \rangle \sim 0.1$). In contrast to the predictions [1, 2], we find that vesicles, irrespectively of the presence or absence of shape fluctuations, follow the Einstein−Stokes relation within our experimental uncertainty (2% for the GUV radius and 3% for the diffusion coefficient). In addition, we study the apparent rotational diffusion of undulating vesicles. We find that the rotational diffusion of the principal axis of the gyration tensor of the vesicle image is about two orders of magnitude faster than that of a rigid spherical body and is closely related to the slowest shape relaxation rate of the vesicle.

[1] E. van der Linden *et al.*, Physica A **162**, 99 (1989).
[2] M. Schwartz, G. Frenkel, Phys. Rev. E **65**, 041104 (2002).

BP 7.48 Mon 17:00 Poster A

Specular and Off-Specular Neutron Scattering from Solid-Supported Multilayers of Cell-Surface Model Membranes under Bulk Buffers — •Emanuel Schneck[1], Bruno Demé[2], Christian Gege[3], Richard Schmidt[3], and Motomu Tanaka[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, INF 253, 69120 Heidelberg, Germany — [2]Institut Laue-Langevin, B.P. 156, F-38042 Grenoble Cedex 9, France — [3]Fachbereich Chemie, Universität Konstanz, Fach M 725, D-78457 Konstanz, Germany

Oriented, solid-supported phospholipid membrane multilayers, containing synthetic glycolipids (membrane-anchored Lewis-X oligosaccharides) at various well defined concentrations were studied by specular and off-specular neutron scattering. The samples act as model systems for the study of saccharide mediated inter-membrane interactions, which play key roles in the mechanism of cellular adhesion, a process of outstanding biological importance. Recent in-vitro experiments suggest that membrane-anchored Lewis-X, a basic component of blood group antigens, induces cellular adhesion in the presence of calcium ions. Furthermore, several 2D-NMR studies evidenced that Lewis-X forms homophilic dimers in the presence of calcium ions. A new self-developed liquid cell is used for measurements with bulk buffers at various ion concentrations. The planar sample geometry allows for the identification of out-of-plane and in-plane scattering vector components and offers the possibility to study quantitatively the influence of ions on oligosaccharide-mediated inter-membrane interactions and on membrane bending rigidities.

BP 7.49 Mon 17:00 Poster A

Specular and Off-Specular Neutron Scattering from Solid-Supported Glycolipid Membrane Multilayers — •Emanuel Schneck[1], Florian Rehfeldt[2], Bruno Demé[3], Christian Gege[4], Richard Schmidt[4], and Motomu Tanaka[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, INF 253, 69120 Heidelberg, Germany — [2]Lehrstuhl für Biophysik E22, Technische Universität München, D-85748 Garching, Germany — [3]Institut Laue-Langevin, B.P. 156, F-38042 Grenoble Cedex 9, France — [4]Fachbereich Chemie, Universität Konstanz, Fach M 725, D-78457 Konstanz, Germany

Solid-supported glycolipid membrane multilayers, acting as well-defined model systems for the study of saccharide-mediated inter-membrane interactions, were studied by specular and off-specular neutron scattering. Experiments were carried out at controlled temperatures and humidities, as well as under bulk water using a self-developed liquid cell. Force-distance relationships were recorded by measuring at various osmotic pressures. Mechanical properties of the studied membranes (i.e. bending moduli and inter-membrane compression moduli) were extracted by comparing scattering signals to reciprocal space maps simulated in the framework of smectic crystal theory. The results demonstrate that distinct variations in the oligosaccharide headgroup structures of the glycolipid molecules can result in significant changes in bending modulus and inter-membrane interactions.

BP 7.50 Mon 17:00 Poster A

Pattern formation in membranes due to electrostatic protein-lipid interacion — •Sergio Alonso[1], Karin John[2], and Markus Baer[1] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Université J. Fourier, Grenoble, France

We study the formation of protein patterns near membranes of living cells by mathematical modelling. The formation of protein domains by electrostatic lipid-protein interactions and the nonequilibrium biochemical reaction cycle of proteins near the membrane give rise to complex dynamics. On the other hand, Calcium is a intracellular signal which controls numerous processes, including the activity of the proteins attached to the membrane. We incorporate the effects of the calcium in a previous model for the dynamics of such proteins in the membrane.

BP 7.51 Mon 17:00 Poster A

X-Ray Investigations on Langmuir and LB Films — •Volker Schön and Patrick Huber — Saarland University, 66123 Saarbrücken, Germany

We present the set up Butterfly X-Ray Reflectometer suitable for the investigation of liquid samples.

We demonstrate it's potential with measurements of OTS/DTS on a silicon substrate and Langmuir films (phospholipid DPhPC and Block Copolymer PFMA-PEO-PFMA (with variable molecular lengths and ratios) as well as mixtures of these components) on an aqueous subphase alongside with a proper subtraction of the subphase bulk scattering background and an accessibiltiy of 7-8 orders of magnitude in reflected intensity.

BP 7.52 Mon 17:00 Poster A

The effect of antibiotic binding to bacterial membrane proteins on drug accummulation — •Tivadar Mach[1], K R Mahendran[1], Andrey Bessonov[1], Enrico Spiga[2], Isabel Sousa[3], Helge Weingart[1], Paula Gameiro dos Santos[3], Matteo Ceccarelli[2], and Mathias Winterhalter[1] — [1]Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]Università di Cagliari, 09042 Monserrato (CA), Italy — [3]Universidade do Porto, Rua do Campo Alegre, 4169-007 Porto, Portugal

One of the main mechanisms through which bacteria exhibit resistance to antimicrobials is reduced drug accummulation. A change in permeability of the bacterial membrane for highly effective hydrophilic drugs can be effected by resistant bacteria through the modification or abscence of certain transmembrane proteins. We investigate the permeation pathways of several b-lactam and fluoroquinolone antibiotics into the bacterial cell by the reconstitution of a single bacterial porin into an artificial planar lipid bilayer, measuring the binding of antibiotic molecules through the time-resolved modulation of a small-ion current. Combining these conductance results with fluorescence spectroscopy, molecular dynamics simulations and Minimum Inhibitory Concentration assays, we conclude that efficiency of permeation for antimicrobials depends strongly on their association constant with bacterial pores, with the binding energy counteracting the loss of free entropy of the antibiotic confinement in the channel - potentially leading the way to new antibiotic design.

BP 7.53 Mon 17:00 Poster A

Artificial Organelles from Giant Unilamellar Vesicles — •Jakob Schweizer and Petra Schwille — Biotec/TU Dresden,

Tatzberg 47, 01307 Dresden, Germany

Giant Unilamellar Vesicles (GUV) constituted from lipid bilayers serve as a model system for the minimal cell. However, they are also an ideal tool to synthesize sub-cellular structures in order to mimic intracellular processes. Here we present a way to construct a rudimentary artificial chloroplast from purely biological raw materials using merely three main components: lipids, bacteriorhodopsin and F0F1-ATP synthase. Powered by photon absorption bacteriorhodopsin pumps protons into the vesicle, whereas the F0F1-ATP synthase utilizes the emerging proton gradient to produce ATP. The most crucial step is therefore the reconstitution of the functional proteins into the GUVs in the correct orientation. Establishing an artificial chloroplast can provide further insight into the evolution of biological chloroplasts. Moreover, these photo-sensitive systems will also serve as miniature power plants, providing the ATP essential for more complicated cellular model systems. Besides protein reconstitution and proteo-GUV formation we want to present methods to proof the protein activity of BR and the ATP-synthase in GUVs.

BP 7.54 Mon 17:00 Poster A

Diffusion of glycosylphosphatidylinositol (GPI)-anchored bovine prion protein (PrPc) in supported lipid membranes studied by single-molecule and complementary ensemble methods. — •Thomas Schubert[1,2], Michael Bärmann[2], Monika Rusp[2], Walter Gränzer[3], and Motomu Tanaka[1,2] — [1]Biophysikalische Chemie II und BIOQUANT, Universität Heidelberg, 69120 Heidelberg, Germany — [2]E22, Technische Universität München, James-Frank-Str, 85748 Garching, Germany — [3]Institut für Tierhygiene, TU München, Weihenstephaner Berg 3, 85354 Freising-Weihenstephan, Germany

In this work bovine cellular bovine prion protein (PrPc) was incorporated in supported lipid membranes and its lateral diffusion was studied by single-dye tracking (SDT) and a complementary ensemble method, fluorescence recovery after photobleaching (FRAP). FRAP results demonstrated very high mobile fractions of up to 94 %, confirming that most of the GPI-anchored PrPc are freely diffusive in the fluid supported membrane matrix. Moreover, the lateral diffusivity of PrPc significantly depends on the pH of the buffer. To complement the ensemble results obtained by FRAP, the statistical variation of lateral diffusion coefficients of individual PrPc molecules in the supported membranes were measured with SDT. Simulation-based statistical analysis indicated that in addition to the expected statistical scatter there is a significant spread of diffusion coefficients. In further experiments, 2D membrane electrophoresis also indicated non-uniform PrPc molecules.

BP 8: Active Filament Networks

Time: Tuesday 9:30–13:00 Location: C 243

Invited Talk BP 8.1 Tue 9:30 C 243

Active stress fluctuations in biopolymer networks driven by molecular motors — •Gijsje H. Koenderink[1], Marina Soares e Silva[1], and Frederick C. MacKintosh[2] — [1]FOM Institute AMOLF, Amsterdam, Netherlands — [2]Vrije Universiteit, Amsterdam, Netherlands

Living cells are active soft materials in which non-equilibrium driving forces lead to shape changes, contractility, and migration. To elucidate the physical origin of these active material properties, we reconstitute simple model systems from purified cytoskeletal proteins. I will show that model systems of filamentous actin exhibit active internal stress fluctuations and active stiffening upon addition of myosin II motors. The myosin motors use chemical energy to generate directional forces on the actin filaments to slide filaments past one another. In un-crosslinked networks, this leads to transient contractile stresses. These are apparent when microtubules, cytoskeletal filaments with a persistence length of 1 mm, are embedded in the actin network. In the presence of processive myosin thick filaments, the microtubules display large, non-thermal bending fluctuations. These reveal transverse forces of 10-20 pN originating from local network contractions. Even though the myosin motors are processive, they generate random stress fluctuations because they transiently bind and then collectively release. When the actin filaments are cross-linked with an actin-binding protein such as filamin A, myosin contractile forces generate an internal stress that drives the network into a non-linear, stress-stiffened regime. These findings shed light on physical design principles of cells.

Invited Talk BP 8.2 Tue 10:00 C 243

Regulation of microtubule sliding by antagonizing microtubule motors and crosslinkers — •Marcel Janson — Wageningen University, Wageningen, The Netherlands

Polarized microtubule networks, like the mitotic spindle, are organized in part by molecular motors that actively slide microtubules along each other. Proteins like ase1, on the other hand, create static crosslinks between these biofilaments. How cells tune both antagonizing activities to make sure that microtubules attain their correct position and polarity is largely unknown. We quantified the relative sliding of microtubules in live fission yeast cells. Here, motor proteins bind to the ends of microtubules while ase1-crosslinks are established between overlapping microtubules. The corresponding distribution of forces generates a length-dependent sliding velocity. Computer simulations were used to demonstrate that the resulting velocities are sufficient to organize randomly nucleated microtubules into an array of antiparallel microtubules that is morphological similar to arrays in yeast. The localization of ase1 in these arrays is of special interest. Ase1 selectively binds to pairs of antiparallel microtubules and in doing so sets up spatial signals in cells. Single molecule fluorescence imaging and controlled in vitro assays demonstrated that dimers of ase1 diffuse along the lattice of microtubules. These dimers multimerized into higher-order structures that were stably docked to microtubules. Multimerization preferentially occurred between overlapping microtubules showing that cells exploit the local geometry and abundance of ase1 binding sites to achieve selective ase1 localization.

15 min. break

BP 8.3 Tue 10:45 C 243

Adhesion Patches in Early Cell Spreading — •Hans-Günther Döbereiner, Marcus Prass, Meike Gummich, and Jac-Simon Kühn — Institut für Biophysik, Universität Bremen

Cell motility is controlled by an active polymer gel enclosed by a complex membrane relaying extracellular signals and forces. We report on the dynamics of spreading mouse embryonic fibroblasts. Advancing membrane edges and adhesions patterns on two-dimensional substrates can be well characterized by total internal reflection fluorescence and reflection interference contrast microscopy. One finds various dynamic phases [1] and collective modes [2]. We discuss characteristic spatial-temporal correlations and relate our findings to theoretical calculations [3]. Especially, we present recent results on adhesion patches in early spreading events.

[1] H.-G. Döbereiner et al., Phys. Rev. Lett. 93, 108105 (2004).
[2] H.-G. Döbereiner et al., Phys. Rev. Lett. 97, 38102 (2006).
[3] R. Shlomovitz and N. S. Gov, Phys. Rev. Lett 98, 168103 (2007).

BP 8.4 Tue 11:00 C 243

Cytoskeleton nanosurgery Part I : Force sensing mechanism within actin stress fibers — •Julien Colombelli[1], Achim Besser[2], Emmanuel Reynaud[1], Holger Kress[3], Philippe Girard[1], Ulrich Schwarz[2], Victor Small[4], and Ernst Stelzer[1] — [1]EMBL. Meyerhofst. 1, D-69117 Heidelberg — [2]University Heidelberg, Bioquant, BQ0013 BIOMS, D-69120, Heidelberg — [3]Mech. Eng. Dept., Yale University, New Haven CT 06511, USA — [4]Institute for Molecular Biotechnology (IMBA), Bohr Gasse, A-1030 Vienna

Mechanotransduction defines the ensemble of mechanisms by which cells convert mechanical stimuli into biochemical activity. The cytoskeleton plays a central role in propagating mechanical signals, however the molecular sensors that potentially recognize mechanical movements, forces and tensions are widely missing. We focus here on perturbing the mechanical equilibrium of the actin cytoskeleton. We study the mechanical relaxation of actin stress fibers (SFs) after combined FRAP and laser nanosurgery in living cells. Quantitative analysis provides support for a theoretical viscoelastic model of SFs dynamics,

which predicts the dynamics of contractile forces throughout the SFs. We then analyze the localization by live fluorescence and correlative EM of zyxin, an alpha-actinin partner in SFs. Non-equilibrium dynamics of zyxin after force perturbation by drug treatment, nanosurgery, or external micromanipulation show a high correlation between the modeled forces within the SFs and the localization of zyxin. We propose that SFs sense the molecular forces generated through actomyosin contractility with the mechanosensitive protein zyxin.

BP 8.5 Tue 11:15 C 243

Cytoskeleton nanosurgery Part II: Modeling the retraction dynamics of stress fibers after laser cutting — •Achim Besser[1], Julien Colombelli[2], Holger Kress[3], Ernst Stelzer[2], and Ulrich Schwarz[1] — [1]University of Heidelberg, Bioquant, BQ 0013 BIOMS Schwarz, INF 267, D-69120, Heidelberg, Germany — [2]European Molecular Biology Laboratory (EMBL), Meyerhofstrasse 1, D-69117 Heidelberg, Germany — [3]Department of Mechanical Engineering, Yale University, New Haven, CT06511, USA

Cellular stress fibers are bundles of actin filaments that are cross-linked by α-actinin and non-muscle myosin II molecular motors. Due to myosin motor activity, stress fibers are under tension and retract over several microns when being cut with a pulsed laser. The time-dependent displacement field along the fiber is recorded with fluorescence microscopy and thus provides quantitative time course data. Here, we present a continuum stress fiber model that takes into account the internal visco-elastic and contractile properties of the fiber as well as visco-elastic interactions with the surrounding cytoplasm. Through detailed comparison of theory and experiment we are able to quantify physical properties of stress fibers: we extract the average contraction length of sarcomeric units, the degree of cross links of the fibers and we find that external friction due to the retraction within the cytosol can be neglected compared to internal friction resulting from relative filament sliding and myosin motor activity.

BP 8.6 Tue 11:30 C 243

A Mechanism of Filament Length Regulation — •Christoph Erlenkämper and Karsten Kruse — Universität des Saarlandes, Theoretische Physik, 66041 Saarbrücken, Germany

The cytoskeleton is a network of filamentous polymers, notably actin filaments and microtubules. It determines the mechanical properties of a cell and is involved in various vital cellular processes. An important characteristic of the cytoskeleton is the distribution of filament lenghts. *In vitro* filaments typically show an exponential length distribution, which can be explained by the intrinsic filament dynamics [1][2]. In cells, however, filament lengths are regulated by additional proteins. Here, we investigate a mechanism of length regulation by proteins which influence depolymerization at the ends of treadmilling filaments. It applies, for example, to ADF/cofilin which promotes subunit removal from the ends of actin filaments. We present stochastic simulations as well as an analytic calculation of the steady state distribution. In contrast to the *in vitro* situation, we find a distribution that is peaked around the average filament length.

[1] F. Oosawa and S. Asakura, "Thermodynamics of the Polymerization of Protein", Academic Press, New York, 1975

[2] M. Dogterom and S. Leibler, PRL, **70** (1347), 1993

BP 8.7 Tue 11:45 C 243

Microtubule-driven multimerization recruits ase1 onto overlapping microtubules — Lukas C. Kapitein[1], Marcel E. Janson[1], •Christoph F. Schmidt[2], and Erwin J.G. Peterman[1] — [1]Vrije Universiteit, Amsterdam, The Netherlands — [2]Georg-August-Universität, Göttingen, Germany

Microtubule cross-linking proteins of the ase1/PRC1/Map65 family play a major role in the construction of microtubule networks such as the mitotic spindle. Most homologues have been shown to localize with a remarkable specificity to sets of antiparallel overlapping microtubules. Using in vitro experiments in combination with single-molecule fluorescence microscopy, we obtained evidence for a mechanism of localized protein multimerization underpinning this specific targeting. Dimers of the fission yeast homologue, ase1, diffused along the lattice of single microtubules and assembled into stable multimeric structures at concentrations above a threshold. This threshold was significantly lower between overlapping microtubules. These findings show that cells use a finely tuned cooperative localization mechanism that exploits differences in the geometry and concentration of ase1 binding sites along single and overlapping MTs.

BP 8.8 Tue 12:00 C 243

Viscoelastic Actin Bundles — •Dan Strehle[1], José Alvarado[1], Brian Gentry[1], Lukas Hild[1], Mark Bathe[2,3], Erwin Frey[2], and Josef Käs[1] — [1]Universität Leipzig — [2]LMU München — [3]C.N.R.S. Gif-sur-Yvette

Bundles of actin perform a number of important functions in cells. As stress fibers they play a crucial role in biopolymer networks constituting the cytoskeleton, in filopodia they probe the extracellular environment, in acrosomal processes of sperm cells they perforate the membrane of the egg, whereas in stereocilia they serve as signal transducing organelles of hair cells.

For these various tasks cells are able to finely tune the mechanical properties of bundles by determining their thickness and choosing from a variety of actin bundling proteins. Dynamic crosslinkers, for instance, create the possibility for a viscoelastic-like response to different stresses encountered in cellular conditions.

We are actively probing the mechanical properties of actin bundles using optical tweezers. Upon applying stress, a timescale-dependent novel behavior, plastic deformation, is observed, shedding light on the internal structure and kinetics of the bundles. Using this method, properties of bundles formed with different bundling proteins can be compared.

Elucidating the mechanical behavior of bundles might also provide additional insight into the viscoelastic response of biopolymer networks.

BP 8.9 Tue 12:15 C 243

Three-dimensional preparation and imaging reveal intrinsic microtubule properties — Philipp J Keller, •Francesco Pampaloni, and Ernst H K Stelzer — Cell Biology and Biophysics Unit, European Molecular Biology Laboratory (EMBL), Meyerhofstrasse 1, D-69117 Heidelberg, Germany

Microtubule dynamic instability has been studied for over two decades, employing two-dimensional experimental approaches and focusing on two dynamic states, microtubule growth and shrinkage. The role of a "third state", the microtubule pause, has not yet been investigated in detail, although microtubule pausing is often observed in interphase cells. We present a study of microtubule dynamic instability in three dimensions, performed with laser light sheet-based fluorescence microscopy (SPIM). In order to prevent any experimental bias due to surface proximity effects, we developed a three-dimensional (3D) assay employing transparent Teflon-based cylinders. Close-to-life conditions were ensured by the use of Xenopus laevis egg extract. We performed a three-dimensional quantification of all known states of microtubule dynamic instability, including a thorough investigation of microtubule pausing. The three-dimensional approach gives experimental access to the intrinsic microtubule dynamic properties and to microtubule population statistics in single asters. We obtain evidence for the stochastic nature of microtubule pausing and discovered a strong influence of microtubule pausing on the microtubule's dynamic properties. Moreover, our data rule out a simple GTP-cap model of microtubule stabilization for interphase Xenopus laevis extracts.

BP 8.10 Tue 12:30 C 243

Instabilities of active gels with stress-dependent depolymerization — •Davood Nourozi and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

The cytoskeleton is a network of filamentous proteins which is responsible for many cellular processes such as crawling on a substrate, division and for organising intracellular transport. It is internally driven by the hydrolysis of ATP, which fuels molecular motors as well as the polymerization and depolymerization of filaments [1]. The physics of such active gels is largely unexplored. Here we study the effect of mechanical stresses on the depolymerization rate. To this end we use a multi-component hydrodynamic description of an active gel [2]. A linear stability analysis of the isotropic homogeneous state reveals various instabilities. Furthermore, we numerically analyse the system behaviour beyond the linear regime. Finall we discuss possible implications of our work for the formation of cellular structures.

[1] Alberts, B. et. al., Molecular Biology of the Cell, 4th edition (Garland, New York, 2002).

[2] Joanny, J. F., Jülicher, F., Kruse, K., Prost, J., New J. Phys., in press.

BP 8.11 Tue 12:45 C 243

Modeling the lamellipodial protrusion in motile cells —

•Mihaela Enculescu and Martin Falcke — Hahn-Meitner-Institut, Berlin

A variety of eukaryotic cells has the ability to crawl on a substrate by extending a thin plane cytoskeletal structure, called the lamellipodium. The force that pushes the cell membrane forward emerges from the growth of a cross-linked actin network through polymerization at the leading edge. We model the lamellipodial protrusion by coupling the mechanics of the membrane to the dynamics of the length distribution of the polymer ends, and by computing the entropic forces exerted by single actin filaments on the membrane. Our approach takes into consideration actin polymerization, attachment and detachment of filaments to the membrane and cross-linking of the actin network.

BP 9: Membranes and Interfaces

Time: Tuesday 10:30–13:00 Location: PC 203

BP 9.1 Tue 10:30 PC 203

Size distribution and radial density profile of synaptic vesicles by SAXS and light scattering — •Simon Castorph[1], Matthew Holt[2], Michael Sztucki[3], Reinhard Jahn[2], and Tim Salditt[1] — [1]Institute for X-ray Physics, Göttingen, Germany — [2]Max Plank Institute for Biophysical Chemistry, Göttingen, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France

Synaptic vesicles are small membraneous organelles within the nerve terminal, encapsulating neurotransmitters by a lipid bilayer. The transport of the neurotransmitter, the fusion at the plasma membrane, and the release of the stored neurotransmitters into the synaptic cleft are since long know as essential step in nerve conduction of the chemical synapse. A detailed structural view of these molecular mechanisms is still lacking, not withstanding the enormous progress in the field during recent years [1, 2].

From measurements and quantitative fitting of small angle x-ray scattering curves and dynamic light scattering the averaged structural properties of synaptic vesicles can be determined.

We present SAXS measurements and fits revealing the width of the size distribution function and details of the radial scattering length profile of synaptic vesicles from rat brain. Representative values for the inner and outer radius and the size polydispersity as well as the density and width of the outer protein layer are obtained.

References: [1] Südhof, T. (2004) *Annu. Rev. Neurosci.* **27**, 509 - 547 [2] Takamori, S., et al. (2006) *Cell* **127**, 831 - 846

BP 9.2 Tue 10:45 PC 203

Local Heating of Phospholipid Bilayers with Gold Nanoparticles — •Alexander S. Urban[1], Margaret R. Horton[2], Srujan K. Dondapati[1], Tapan K. Sau[1], Thomas A. Klar[1], Joachim O. Rädler[2], and Jochen Feldmann[1] — [1]Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München — [2]Soft Condensed Matter Group , Ludwig-Maximilians-Universität München

We examine the possibility of increasing the membrane permeability for drugs and large bio-molecules by exploiting light-induced local heating of phospholipid bilayers containing gold nanoparticles. Giant unilamellar vesicles (GUVs) provide model systems for cellular membranes. They were prepared from 1,2-Dioleoyl-sn-Glycero-3-Phosphocholine via the electroformation method. Nanoparticles were made in various shapes (rods, spheres, cubes), sizes (20-100 nm) and with different surfactants, the latter playing an important role in the vesicle adhesion efficiency. Cetyl trimethylammonium bromide forms bilayers around the gold and was readily incorporated into GUV membranes. Too high a concentration of gold nanoparticles resulted in vesicle rupture due to osmotic stress. Furthermore, we investigated the heating of the GUV-gold complexes by illumination with laser light near the plasmon resonance. Increasing the laser intensity led to rupturing of the bilayers. The intensity required for rupture was highly dependent on nanoparticle size and the number of gold nanoparticles in close proximity. This model system is also being used to quantitatively study the transport of biologically active molecules across the lipid membrane through specific and local cell heating.

BP 9.3 Tue 11:00 PC 203

Transport at nanoscale revealed by the temperature dependence of ion conductance — •Catalin Chimerel[1], Liviu Movileanu[2], Ulrich Kleinekathöfer[1], and Mathias Winterhalter[1] — [1]Jacobs University Bremen, Bremen, Germany — [2]Syracuse University, Syracuse, New York, USA

Temperature dependent ion conductance in nanopores is measured in a wide range of electrolyte concentration and compared with molecular modeling. Single outer membrane protein F (OmpF) channels from E. coli are reconstituted into planar lipid bilayers. In a qualitative agreement with the experimental data, applied field molecular dynamics revealed atomistic details of the charge transport in the studied nanopore. Comparing the temperature dependence of the channel conductance with that of the bulk electrolyte conductivity in the range from 0°C to 72°C revealed that at low salt concentration the charge transport is mainly driven along the pore surface. Increasing the salt concentration saturates the surface charge transport and induces charge transport in the center of the nanopore. Opposite to the surface transport, the transport in the nanopore center favors the formation of ion pairs. Increasing the salt concentration increases the ion pair formation in the nanopore faster than in the bulk, therefore an increase in salt concentration leads to a slower increase in the nanopore conductance compared to the bulk conductivity. Increasing the temperature reduces the life time of the ion pairs and leads to a faster increase in channel conductance compared to the bulk conductivity.

BP 9.4 Tue 11:15 PC 203

Specular and Off-Specular Neutron Scattering from Solid-Supported Glycolipid Membrane Multilayers — •Emanuel Schneck[1], Florian Rehfeldt[2], Bruno Demé[3], Christian Gege[4], Richard Schmidt[4], and Motomu Tanaka[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, INF 253, 69120 Heidelberg, Germany — [2]Lehrstuhl für Biophysik E22, Technische Universität München, D-85748 Garching, Germany — [3]Institut Laue-Langevin, B.P. 156, F-38042 Grenoble Cedex 9, France — [4]Fachbereich Chemie, Universität Konstanz, Fach M 725, D-78457 Konstanz, Germany

Solid-supported glycolipid membrane multilayers, acting as well-defined model systems for the study of saccharide-mediated intermembrane interactions, were studied by specular and off-specular neutron scattering. Experiments were carried out at controlled temperatures and humidities, as well as under bulk water using a self-developed liquid cell. Force-distance relationships were recorded by measuring at various osmotic pressures. Mechanical properties of the studied membranes (i.e. bending moduli and inter-membrane compression moduli) were extracted by comparing scattering signals to reciprocal space maps simulated in the framework of smectic crystal theory. The results demonstrate that distinct variations in the oligosaccharide headgroup structures of the glycolipid molecules can result in significant changes in bending modulus and inter-membrane interactions.

15 min. break

BP 9.5 Tue 11:45 PC 203

Diffusion of nano-particles bound to model membranes — •Florian Rückerl, Lydia Woiterski, Josef Käs, and Carsten Selle — Universität Leipzig, Linnéstr. 5, 04103 Leipzig

The diffusive transport in membranes is an important process in cells, especially for signaling at the cell surface. In our investigations we compare the diffusive motion of different nano-particles (latex beads, quantum dots and quantum dots bound to lipids) in a variety of model membranes (monolayers, tethered bilayers and giant unilamellar vesicles). The model membranes,composed of ternary mixtures of lipids (DOPC, cholesterol and DPPC or Sphingomyelin), form liquid membranes and exhibit an ordered-disordered phase coexistence. Our aim is to elucidate the interactions of the membrane with the particles close to the border of such phase coexistence regions. The comparison of the systems enables to differentiate between the mechanisms that influence the diffusion, mainly electrostatic and hydrodynamic interactions. In monolayers the dipolar interaction is dominant leading to a confinement of the partially charged particle at the border of the domain. This transition from two- to one-dimensional diffusion is also dependent on the domain size, being most effective for small domains

($R < 1\mu m$). A similar change can be observed for latex beads adsorbed to lipid vesicle, where dipolar interactions are considered only weak and short-ranged.

Thus, domain associated dimensional reduction might play a significant role in more physiological bilayer systems. This might be utilized by cellular systems in order to control membrane protein diffusion.

BP 9.6 Tue 12:00 PC 203

Fluorescence correlation spectroscopy measurement of anomalous diffusion and crowding of lipid-bound proteins — •Margaret Horton[1], Felix Höfling[1,2], Joachim Rädler[1], and Thomas Franosch[1,2] — [1]Center for Nanoscience, Ludwigs-Maximilians-Universität, München, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics, Ludwigs-Maximilians-Universität, München, Germany

In cell membranes, proteins and lipids diffuse in a highly heterogeneous landscape. Aggregates and dense domains of proteins or lipids can modify the path of diffusing molecules, giving rise to anomalous transport. We study two-dimensional diffusion in membranes that are heterogeneous due to protein crowding. Using fluorescence correlation spectroscopy (FCS), we measure the diffusion of the protein avidin bound to biotinylated lipids in a supported bilayer. The density of avidin is controlled by varying the concentration of the lipid anchors. A clear distinction between anomalous and normal diffusion can be achieved with long measurement times (200s) and analysis of the mean squared displacement (MSD). This approach offers an alternative to standard methods of fitting autocorrelated FCS data to probe the dynamic arrangement of molecules in heterogeneous membranes. At low protein surface coverage, normal diffusion is observed. As more protein covers the membrane, there is a transition to anomalous diffusion that becomes more anomalous as the membrane becomes more crowded. These results suggest mechanisms by which cell membrane-associated molecules remain mobile in crowded environments.

BP 9.7 Tue 12:15 PC 203

A simulation approach to membrane protein aggregation via hydrophobic mismatch — •Gernot Guigas, Ulrich Schmidt, and Matthias Weiss — Cellular Biophysics Group, Deutsches Krebsforschungszentrum, Bioquant Center, Im Neuenheimer Feld 267, 69120 Heidelberg

The oligomerization of membrane proteins is a vital and ubiquitous phenomenon in living cells, e.g. when receptor proteins at the cell's plasma membrane oligomerize after ligand binding to trigger downstream signaling cascades. While a pairwise attractive interaction may account for many oligomerization phenomena, several lines of evidence also implicate membrane-mediated forces as important driving forces for membrane protein aggregation. Using dissipative particle dynamics (DPD), we have studied the aggregation of membrane proteins in a simple yet generic setup. Depending on the strength of the hydrophobic mismatch of the transmembrane domain and the surrounding lipid bilayer we observed a strong aggregation of membrane proteins. Moreover, the diffusive properties of the membrane proteins were strongly altered when the hydrophobic mismatch was varied.

BP 9.8 Tue 12:30 PC 203

Adhesion of Fluid Vesicles at Chemically Structured Substrates — Gunnar Linke, Reinhard Lipowsky, and •Thomas Gruhn — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany

Spatial immobilization of vesicles is important for many vesicle applications like the usage as chemical reactor in nano laboratories or as modules in membrane sensors. A controlled fixation of a vesicle can be achieved by adhering it to a finite adhesive domain on an otherwise repulsive substrate surface. We have studied this scenario with the help of mesoscopic Monte Carlo simulations. If the vesicle is larger than the attractive domain, the spreading of the vesicle onto the substrate is restricted by the size of this surface domain. Once the contact line of the adhering vesicle has reached the boundaries of the domain, further deflation of the vesicle leads to a regime of low membrane tension with pronounced shape fluctuations, which are now governed by the bending rigidity. For a circular domain and a small bending rigidity, the membrane oscillates strongly around an average spherical cap shape. If such a vesicle is deflated, the contact area increases or decreases with increasing osmotic pressure, depending on the relative size of the vesicle and the circular domain. The lateral localization of the vesicle's center-of-mass by such a domain is optimal for a certain domain radius, which is found to be rather independent of adhesion strength and bending rigidity. For vesicles adhering to stripe-shaped surface domains, the width of the contact area perpendicular to the stripe varies non-monotonically with the adhesion strength.

BP 9.9 Tue 12:45 PC 203

Effective potential for a fluctuating membrane between two walls — •Ana-Suncana Smith — II. Institut für Theoretische Physik, Universiät Stuttgart

Lipid membranes, due to their weak curvature elasticity, typically exhibit large out of plane fluctuations. In the vicinity of the substrate, it is the balancing of the attractive van der Waals potential against the bending deformations of the membrane and the steric repulsion arising from fluctuations, which determines the effective potential between the substrate and the membrane. The difficulty is that the effective potential is coupled to the fluctuation amplitude, which thus must be determined self-consistently. Exact solution of this problem has so far been found only in the vicinity of the unbinding transition (Lipowsky, R.; Leibler, S. Phys. Rev. Lett. 1986, 56, 2541). However, the shape of this potential away from the transition has not been calculated yet. We here present an approximate analytic model for the effective potential. We concentrate particularly on the case when the membrane is placed between two walls, and explore the shape of effective potential for a variety of direct interaction potentials.

BP 10: Self Propulsion

Time: Tuesday 14:00–15:00 Location: C 243

BP 10.1 Tue 14:00 C 243

Cilia Dynamics — •Jens Elgeti and Gerhard Gompper — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

Cilia are hair-like extensions of some cells that propel fluid over its surface by performing a whip-like motion. Cilia appear in many places in nature, e.g. to remove mucus from the human respiratory system, or on the surface of *Paramecium*.

We present simulation results for a two-dimensional array of autonomously beating cilia, solely coupled by hydrodynamic interactions. These hydrodynamic interactions are sufficient to lead to synchronization of cilia motion in the form of a "metachronal wave". We show that the metachronal wave enhances velocity and efficiency of solute transport compared to synchronously beating cilia. The transport velocity increases up to a factor of 3, when the cilia are packed more densely, while transport efficiency increases almost an order of magnitude.

Furthermore, we characterize transport and wave properties as functions of the viscosity, effective stroke direction and cilia spacing. For example, we show that the main correlation direction roughly coincides with the effective stroke direction, and that the beat frequency decreases through metachronal coordination while the energy consumption per beat is largely independent of cilia spacing, effective stroke direction, and metachronal coordination.

We believe, that for the fitness of the cell, both the efficiency and especially the transport velocity are essential. The metachronal wave pattern is thus of great functional significance for ciliated cells.

BP 10.2 Tue 14:15 C 243

Theory and simulation of artificial cilia — •Matthew Downton and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

We present simulations that explore the possibility of creating magnetically actuated artificial cilia. Motivated by experiments on an artificial swimmer[1,2], we analyse a model that consists of a simple bead-spring chain interacting with an external magnetic field able to induce a magnetic moment in the beads. Low Reynolds number hydrodynamic interactions are introduced at the Rotne-Prager level and different beating kinematics of the filament are studied by varying

the time dependence of the applied field. We examine separate cases of the beating pattern of individual filaments and use a measure of propulsion to study their ability to transport fluid. The behavior of multiple interacting filaments is also studied. By choosing the phases of the actuating magnetic fields separately for each filament, we are able to study how phase shifts between neighboring filaments influence the dissipated energy and the propulsive performance of several filaments. This might be important for the understanding of the so-called metachronal waves that occur in fields of biological cilia.

[1] Dreyfus et al., Nature, 437, 862 (2005)
[2] Gauger and Stark, Phys. Rev. E, 74, 021907 (2006)

BP 10.3 Tue 14:30 C 243

Orientational ordering and clustering in a simple model of self-propelled particles — Fernando Peruani[1,2,3], Andreas Deutsch[2], and •Markus Bär[3] — [1]MPIPKS Dresden — [2]TU Dresden — [3]PTB Berlin

We study the emergence of collective effects in a two-dimensional stochastic systems of self-propelled particles interacting locally through an apolar, liquid crystal-based alignment mechanism. In the model particles are driven at constant speed and align their direction of motion to the local director. We show through extensive simulations hat the behavior of the system at high and low densities is remarkably different. At high density orientational order emerges upon decrease of the noise strength. The phase transition appears to be of mean-field type. In contrast at low density, an instability leading to inhomogeneous particle density and clustering is found upon decrease of the noise strength. A comparison between active and diffusive particles reveals that diffusive particles can exhibit orientational order for high densities in a similar fashion as self-propelled particles, while clustering at low densities and related orientational order is absent low densities.

BP 10.4 Tue 14:45 C 243

Diffusion in different models of active Brownian particles of relevance in biological self-propelled motion — •Ernesto M. Nicola and Benjamin Lindner — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

Self-propelled motion is one of the most fascinating aspects of biological systems. This motion can appear in many different biological contexts either inside cells or on the multi-cellular level. Simple phenomenological models can help to understand the dynamics of self-propelled entities and their statistics (including their transport properties). One class of models successfully studied during the last 15 years are active Brownian particles (ABP). Here we study, both theoretically and numerically, the effective diffusion coefficient of one-dimensional ABP models. We show that, depending on the choice of the friction function, the diffusion coefficient does or does not attain a minimum as a function of noise intensity. We furthermore discuss the case of an additional bias breaking the left-right symmetry of the system. We show that this bias induces a drift and that it generally reduces the diffusion coefficient. For a finite range of values of the bias, the models can exhibit a maximum in the diffusion coefficient vs. noise intensity.

BP 11: Transport Processes

Time: Tuesday 15:15–17:15 Location: C 243

BP 11.1 Tue 15:15 C 243

Subdiffusion as an efficient intracellular sampling strategy — •Matthias Weiss and Gernot Guigas — Cellular Biophysics Group, Deutsches Krebsforschungszentrum, Bioquant Center, Im Neuenheimer Feld 267, 69120 Heidelberg

Diffusion-mediated searching for interaction partners is an ubiquitous process in cell biology. Transcription factors, for example, search specific DNA sequences, signaling proteins aim at interacting with specific co-factors, and peripheral membrane proteins try to dock to membrane domains. Brownian motion, however, is affected by molecular crowding that induces subdiffusion of proteins and larger structures, thereby compromising diffusive transport and the associated sampling processes. Contrary to the naive expectation that subdiffusion obstructs cellular processes we show here by computer simulations that subdiffusion rather increases the probability of finding a nearby target. Consequently, important events like protein complex formation and signal propagation are enhanced as compared to normal diffusion. Hence, cells indeed benefit from their crowded internal state and the associated anomalous diffusion.

BP 11.2 Tue 15:30 C 243

How Nature beats the central limit theorem: non-Brownian search from gene control to animal foraging — •Ralf Metzler and Michael Lomholt — Technical University of Munich, Physics Department T30g, James Franck Strasse, D-85747 Garching

Simple chemical reactands search for each other by three-dimensional diffusion until encounter. At low concentrations of reactands, pure 3D search is quite inefficient. Nature has come up with various active and passive solutions to speed up search. I will discuss two examples.

Facilitated diffusion of regulatory proteins in search for their specific binding site on a DNA combines 3D volume diffusion with 1D motion along the DNA. The combination of these two mechanisms significantly speeds up the search. In addition, intersegmental transfers that occur at contact points of chemically remote segments of the DNA due to looping gives rise to Levy flights along the DNA that further optimise the search. While this model holds for diluted solutions, in the cell molecular crowding occurs, leading to the subdiffusion of larger molecules. Consequences of this effect include a weak ergodicity breaking, that could allow low regulatory protein concentrations (Phys Rev Lett 95, 260603 (2005); Phys Rev Lett 98, 200603 (2007)).

Bacteria or higher animals perform an active search for food. It turns out that long-tailed distributions, that help avoiding the spell of the central limit theorem, lead to significantly higher search efficiency and significantly reduced sensitivity to a changing environment (E-print arXiv:0709.2352; compare also Phys Rev Lett 99, 160602 (2007)).

BP 11.3 Tue 15:45 C 243

Target Search on a Dynamic Polymer — •Thomas Schötz[1], Richard Neher[2], and Ulrich Gerland[3] — [1]Arnold Sommerfeld Center (ASC), LMU München, Germany — [2]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, USA — [3]Institute for Theoretical Physics, University of Cologne, Germany

The diffusive search of a particle (protein) for a specific site on a heterogeneous polymer (DNA) is an interesting physics problem posed by the molecular biology of gene regulation. In the relevant limit where the DNA is in a compact conformation and the generic (electrostatic) attraction between the protein and DNA is strong, this search proceeds predominantly by local 1D sliding along the DNA and "hopping"to a different segment of the DNA, which is closeby in 3D space but may be distant along the contour. If the time between two hopping events is sufficiently long, such that the DNA conformations at subsequent events are uncorrelated, the dynamics of this search process can be described with the fractional Fokker-Planck-equation approach [Lomholt et al. PRL (2005)]. However, outside of this "annealed limit", the search dynamics changes drastically, as has been demonstrated in a study of the "quenched limit", i.e. the frozen polymer case [Sokolov et al. PRL (1997)]. In biological systems, typically neither of these limits is realized. Here, we study the full problem of the target search on a dynamic polymer. We observe a non-trivial crossover between the two limits, which is due to the breakdown of the correlations in the polymer conformations. We characterize these correlations and their effect on the transport in detail.

BP 11.4 Tue 16:00 C 243

Stochastic models for bidirectional transport on biological networks — •Maximilian Ebbinghaus[1], Rosemary Harris[2], and Ludger Santen[1] — [1]Department of Theoretical Physics, Saarland University, 66041 Saarbruecken, Germany — [2]School of Mathematical Sciences, Queen Mary, University of London, Mile End Road, London E1 4NS, United Kingdom

The intracellular transport on the cytosceletal filament network is driven by molecular motors. They carry different kinds of cargo through the cell by performing a directed stochastic along the polarized filaments. Although the motion of a given molecular motor is unidirectional, it is possible to transport cargo in opposite direction along a filament, e.g., dyneins and kinesins move in opposite directions

along microtubule filaments. We model the bidirectional transport by means of a one-dimensional stochastic lattice models. The model motor proteins interact by exclusion such that effective transport on a single track is possible only by detaching and reattaching moves from the microtubule. Simulations have been carried to investigate the influence of different hopping rates and densities on mean current, path lengths and cluster sizes on the filament. In addition, the influence of tau proteins that decorate the filament will be presented. These proteins intervene in the system by altering the attachment rate of kinesins only. Thus, spatial disorder is found in the system and the impact on measurable quantities have been studied. The results of these simulations can be used in order to elucidate general transport phenomena in elongated cells as, e.g., axons.

BP 11.5 Tue 16:15 C 243

Driven transport on parallel lanes with particle exclusion and obstruction — •Anna Melbinger, Tobias Reichenbach, Thomas Franosch, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität, München, Germany

Traffic phenomena emerge in intracellular transport, where molecular motors move along parallel one-dimensional filaments, serving as biological engines. Recently, we have proposed a prototypical model for transport on parallel lanes [1]. Here, we consider the situation where motors on the same lane exclude each other, while a certain obstruction, stemming e.g. from the interaction of the bigger cargo particles, occurs between motors adjacent on parallel lanes. Depending on the strength of the obstruction, a rich phase behavior emerges, with density separation between the lanes as well as domain walls in the density profiles of the individual lanes being feasible. We rationalize our observations in an analytic approach, and show an intimate relation between the current-density relation and the systems' phase diagrams.

[1] T. Reichenbach, T. Franosch, E. Frey, Phys. Rev. Lett. 97, 050603 (2006)

BP 11.6 Tue 16:30 C 243

A Natural Molecule Trap — Dieter Braun[1], Franz Weinert[1], Stefan Duhr[1], Kono Lemke[2], Michael Russell[3], and •Dieter Braun[1] — [1]Biophysics, CENS, LMU München, Amalienstr. 54, 80799 München, Germany — [2]Institute for Mineralogy, ETH-Zürich, Switzerland — [3]Jet Propulsion Laboratory, CalTech, California, USA

We simulate molecular transport in elongated pores of rock near warm hydrothermal vents. We find extreme accumulation of molecules in a wide variety of plugged pores. The mechanism is able to provide highly concentrated single nucleotides, suitable for operations of an RNA world at the origin of life. It is driven solely by the thermal gradient across a pore. On the one hand the fluid is shuttled by thermal convection along the pore, whereas on the other hand, the molecules drift across the pore, driven by thermodiffusion. As a result, millimeter-sized pores accumulate even single nucleotides more than 10^8-fold into micrometer-sized regions. Since the accumulation depends exponentially on the pore length and temperature difference, it is considerably robust with respect to changes in the cleft geometry and the molecular dimensions. Our results indicate that for life to evolve, complicated active membrane transport is not required for the initial steps.

References:
PNAS 104, 9346-9351 (2007)
PNAS 103, 19678-19682 (2006)

BP 11.7 Tue 16:45 C 243

Protein Diffusion and Hydodynamic Interactions in Red Blood Cells — Wolfgang Doster[1] und •Stephane Longeville[2] — [1]Technische Universität München Physik E 13 — [2]CEA Saclay Paris

Die Konzentration von Makromolekülen in biologischen Zellen ist weit weg vom Ideal der verdünnten Lösung. Volumfraktionen um 0.3 sind typisch. Das *molecular crowding* beeinflusst Reaktionsraten, Dissoziations-Gleichgewichte und diffusiven Transport. Kann die Beweglichkeit der unterschiedlichen Komponenten einer Zelle auf der Basis von intermolekularen Wechselwirkungen verstanden werden? Der Transport von Sauerstoff in Muskelzellen und Erythrozyten wird durch Proteindiffusion unterstützt. In diesem Beitrag diskutieren wir Wechselwirkungen und Diffusion in konzentrierten Myoglobinlösungen und von Hämoglobin in Erythrozyten mit Neutronenspektroskopie [1]. Mit der Kombination von Kleinwinkestreuung und Spin-Echotechnik kann man die Diffusion auf der Skala der intermolekularen Kräfte untersuchen. Vor allem hydrodynamische Wechselwirkungen dominieren aus diesen Längenskalen. [1] W. Doster and S. Longeville Biophy.J. 93 1360 (2007).

BP 11.8 Tue 17:00 C 243

Anomalous diffusion of transmembrane proteins due to oligomerization — •Ulrich Schmidt[1], Markus Elsner[2], Maria Smedh[3], Tommy Nilsson[3], and Matthias Weiss[1] — [1]Cellular Biophysics Group, Deutsches Krebsforschungszentrum, Bioquant Center, Im Neuenheimer Feld 267, 69120 Heidelberg — [2]Cell Biology and Metabolism Branch, National Institutes of Health, USA — [3]Dept. of Medical and Clinical Genetics, Inst. of BioMedicine, Sahlgrenska Academy, Gothenburg University, Sweden

Membrane proteins frequently form higher-order structures, e.g. oligomers, to facilitate their function and to assume proper subcellular localization. Oligomerization, however, alters the diffusion properties of participating individual proteins. Here, we have tested this aspect for membrane proteins undergoing a dynamic oligomerization process by means of computer simulations. We find that the diffusion of individual proteins becomes anomalous on short time scales with the anomality depending on the underlying binding kinetics and the number of binding sites per protein. In support of these theoretical results, we find via fluorescence correlation spectroscopy that a fluorescently tagged transmembrane Golgi enzyme is highly anomalous in vivo. This observation is consistent with the notion that Golgi-resident proteins oligomerize, presumably to maintain correct cisternal localization and to enhance enzymatic reactions.

BP 12: Cellular Force Generation

Time: Tuesday 17:30–18:45 Location: C 243

BP 12.1 Tue 17:30 C 243

Force and Motorprotein Concentration Determine Dynamics of Bacterial Pili — •Martin Clausen and Berenike Maier — WWU Münster, Institut für Allgemeine Zoologie und Genetik, Schloßplatz 5, 48149 Münster, Germany

Type IV pili are major bacterial virulence factors required for adhesion, surface motility and gene transfer. In the human pathogen Neisseria gonorrhoeae, these flexible polymeric filaments extend several micrometers from the cell surface and generate force in the range of 100pN by retraction. Two antagonistic ATPases, PilF and PilT, support elongation and retraction respectively. We investigated the dynamics of individual pili using laser tweezers and observed that the probability for polymerization increased with increasing force for forces up to 100pN. The length change of the pilus as a function of time was analyzed using the statistical randomness parameter as well as direct sectioning. The data reveals two distinct time scales: on a time scale of miliseconds backsteps and pauses were detected, while on the longer timescale directional reversal of the pilus movement was observed. This observation is inconsistent with simple Arrhenius kinetics. We therefore investigated the effect of the concentration of the pilus retraction ATPase PilT and found that the retraction probability decreased with decreasing PilT concentration indicating that binding of PilT strongly increases the retraction probability. Fine-tuning of pilus dynamics by force and motor concentration may be important for surface motility and interaction with mammalian cells.

BP 12.2 Tue 17:45 C 243

Efficiency of molecular motors at maximum power: "Power stroke" beats "Brownian ratchet" — •Tim Schmiedl and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart

Molecular motors transduce chemical energy from hydrolizing ATP into mechanical work exerted against an external force. The efficiency of such a motor usually increases when increasing the force, reaching

the maximum at the stall force. At this force, however, the velocity of the molecular motor and the power output vanishes. It is thus more meaningful to characterize such motors by the efficiency at maximum power. We calculate this efficiency for a simple model and show that the qualitative behaviour depends crucially on the position of the transition state or, equivalently, on whether the motor step occurs in a so called "power stroke" or in a "Brownian ratchet" manner. Specifically, we find a power stroke mechanism, as realized e.g. in myosin motors, to be most favourable with respect to both high power output and high efficiency at maximum power. In this regime, driving the motor farther out of equilibrium by applying higher chemical potential differences can, contra-intuitively, increase the efficiency.

BP 12.3 Tue 18:00 C 243

Transport of micrometer-sized vesicles by kinesin in vitro — •Christoph Herold[1], Cécile Leduc[2], Eugene P. Petrov[1], Stefan Diez[2], and Petra Schwille[1] — [1]Biophysics / BIOTEC, TU Dresden, Tatzberg 47-51, 01307 Dresden — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr.

Cytoskeletal motor proteins (e.g., kinesin) are responsible for directed transport in cells. Motor proteins can also be used in artificial bionanotechnological systems to provide a controlled cargo transport. We explore this possibility by using giant unilamellar vesicles (GUVs) as a micrometer-sized cargo model and establish an *in vitro* system to transport this cargo by kinesin (rK430) molecules along surface-attached microtubules (MTs). Kinesin was linked to GUVs (diameter 1−4 μm) via biotin−streptavidin interaction. MTs and moving GUVs were visualized using fluorescence wide-field imaging microscopy. We observe directed transport of GUVs along MTs with traveling distances of up to 100 μm and velocities of $\sim$0.7 μm/s being in a good agreement with the velocity of kinesin motion along MTs ($\sim$0.8 μm/s). The long walking distances, as well as the visualization of the GFP-labeled kinesin molecules by total internal reflection fluorescence imaging, suggest that a large number ($\gtrsim$10) of kinesin molecules is involved in the transport of a single GUV. Apart from its biotechnological importance, this system might additionally be useful to gain further understanding of vesicle transport processes in cells.

BP 12.4 Tue 18:15 C 243

Stochastic force generation by small ensembles of myosin II molecular motors — Thorsten Erdmann[1] and •Ulrich Schwarz[2] — [1]Amolf, Biochemical Networks Group, 1098 SJ Amsterdam, The Netherlands — [2]University of Heidelberg, Bioquant 0013, INF 267, 69120 Heidelberg, Germany

Myosin II molecular motors are non-processive and therefore have to work together in ensembles in order to generate appreciable levels of force. In contrast to the situation in muscle, in the actin cytoskeleton (including the actin cortex and stress fibers) myosin II molecular motors usually work in small groups and therefore stochastic effects are expected to be more pronounced. Taking advantage of the separation of time scales present in the myosin II hydrolysis cycle, we are able to reduce the complex network of stochastic transitions within a finite-sized ensemble of myosin II motors to a one-step master equation. We derive analytical expressions for the average time of attachement and the average walk length. We also derive force-velocity relations as a function of ensemble size and compare the average results with exact stochastic simulations of single realizations. Our results show that stochastic effects persist up to a system size of about 15 motors.

BP 12.5 Tue 18:30 C 243

Interaction with host cells influences bacterial pilus dynamics — •Dirk Opitz and Berenike Maier — WWU Münster, Institut für Allgemeine Zoologie und Genetik, Schloßplatz 5, 48149 Münster, Germany

The human pathogen *Neisseria gonorrhoeae* generates force in the range of 100pN. The force generating machine is the type IV pilus, a polymeric cell appendage that generates force by retracting into the cell body. Eucaryotic cells can sense mechanical force and respond by cytoskeletal rearrangements. We therefore hypothesize that force generated by pilus retraction is a signal to their epithelial host cell which may facilitate phagocytosis. Vice versa, products of activated signalling pathways upregulate the expression level of the putative pilus retraction motor PilT. Here, we investigated the dynamics and force generation by individual type IV pili using laser tweezers between 3h and 24h after infection of epithelial cells was initiated. We found that the velocity at forces below 50pN decreased from (1.1±0.1)μm/s in abiotic environment to (0.7±0.1)μm/s. Bacteria generated considerable force during infection but the maximum force was reduced from (125±36)pN in abiotic environment to (73±25)pN on epithelial cells independent of infection time. The type IV pilus dynamics in abiotic environment and on host cells is significantly different suggesting that the signalling between pathogen and host cell is bidirectional.

BP 13: Biopolymers

Time: Tuesday 17:15–18:45 Location: PC 203

BP 13.1 Tue 17:15 PC 203

Fibrin network dynamics in nanodroplets — •Heather M Evans[1], Enkhtuul Surenjav[1], Craig Priest[1], Ralf Seemann[1,2], Stephan Herminghaus[1], and Thomas Pfohl[1] — [1]Max Planck Institute for Dynamics and Self-organization, Göttingen, Germany — [2]Experimental Physics, Saarland University, Saarbrücken, Germany

This work explores complex dynamic phenomena of the blood clotting protein, fibrin. Protein "monomers" of fibrinogen assemble into fibers in the presence of the enzyme, thrombin, to ultimately form a three-dimensional fibrin network. Consequently, fibrin is a vital component of blood clots and provides an interesting yet relevant model system to study network properties. In order to study the development and manipulation of this robust network, we utilize new microfluidic designs that allow us to produce fibrin networks within nanodroplets. The droplets prohibit sticky surface interactions between the protein and the device walls. Furthermore, the incorporation of geometric structures on the microdevice enables the controlled deformation of individual droplets containing fibrin networks. The behavior of the networks is found to depend on parameters such as the network age and droplet velocity, as well as the relative protein concentrations. Using high resolution fluorescence microscopy, we analyze the elastic recovery of these networks through several cycles of mechanical deformation.

BP 13.2 Tue 17:30 PC 203

Morphological and Mechanical Characterization of Reconstituted Collagen Type I Networks — •Stefan Münster[1], Thorsten Koch[1], Philip Kollmannsberger[1], Louise Jawerth[2], David Vader[2], Gerd Schroeder-Turk[1], and Ben Fabry[1] — [1]Department of Physics, University of Erlangen-Nuremberg, Germany — [2]Department of Physics, Harvard University, Cambridge, USA

Collagen is the most abundant extracellular matrix (ECM) protein and serves as 3D culture environment for cell biology assays. Cell behavior in 3D sensitively depends on the mechanical properties of the ECM. Moreover, for computing cell tractions from the matrix deformations around invaded cells, knowledge of the matrix rheology is necessary.

Confocal images of collagen gels (2.4 mg/ml) show a narrowly distributed pore size of Ø1 μm. Macrorheology using a parallel-plate rheometer revealed predominantly elastic behavior that was approximately linear for strains <5%, with a shear modulus G' of 80 Pa, a loss modulus G" of 11 Pa, and a weak frequency dependency of both moduli according to a power-law with exponent 0.09. Microrheological behavior was measured by applying a 21 nN 'point' force to a ferrimagnetic Ø4.5 μm bead, and tracking the resulting 3D displacements of Ø1 μm fluorescent beads dispersed in the gel. Local strain fields were also determined by indenting the gel surface with a sphere and by shearing the bulk between two parallel glass plates. Under all conditions, the microscopic gel deformations for small strains closely followed that of an affine, predominantly elastic, isotropic and homogeneous continuum.

BP 13.3 Tue 17:45 PC 203

Microrheology of hyaluronan solutions: implications for the endothelial glycocalyx — •Nadja Nijenhuis[1], Daisuke Mizuno[2], Christoph F. Schmidt[3], Hans Vink[1], and Jos A.E. Spaan[1] — [1]University of Amsterdam, Amsterdam, The Netherlands — [2]Kyushu University, Fukuoka, Japan — [3]Georg-August-Universität, Göttingen,

Germany

The endothelial glycocalyx (EG) forms an anti-adhesive surface at the luminal side of a blood vessel, acting both as a molecular sieve and as a mechanotransducer of fluid shear stress to the underlying endothelial cell layer. One of the components involved in these processes is the highly hydrated glycosaminoglycan (GAG) hyaluronan (HA). HA is the largest of the GAGs present in the EG. We used an optical tweezers setup and laser interferometry to measure the high bandwidth storage (G') and loss (G") modulus of HA solutions. The HA networks, consisting of approximately physiological molecular weight chains and concentrations had a frequency regime up to about 1000 Hz in which the mechanical response was more elastic than viscous. The addition of hyaluronidase to the entangled HA solution rapidly changed its rheological behavior: G' decreased, the entangled network character disappeared, and viscosity became dominant over elasticity.

BP 13.4 Tue 18:00 PC 203

Modelling of individual Hyaluronan-Aggrecan Complexes in the Extracellular Matrix — •Marcel Hellmann[1,2], Matthias Weiss[2], and Dieter W. Heermann[1] — [1]Institut für Theoretische Physik, Philosophenweg 19, Universität Heidelberg, D-69120 Heidelberg, Germany — [2]Cellular Biophysics Group, German Cancer Research Center, Bioquant Center, Im Neuenheimer Feld 267, D-69120 Heidelberg, Germany

The extracellular matrix (ECM) forms a protective layer of varying thickness around mammalian cells that acts as a rampart against potentially hostile invaders. To a large extent, the ECM consists of flexible hyaluronan (HA) filaments anchored in the cell's plasma membrane with rather rigid aggrecan complexes radially attached. In order to elucidate the influence of aggrecans on the ECM thickness, we have studied the behavior of an end-grafted, flexible polymer backbone with a single rigid side chain by means of Monte Carlo simulations.

We have found that already an individual flexible backbone with a single rigid side chain shows appreciable conformational changes compared to an undisturbed flexible chain: Depending on the side chain length (S) and the branching site (b), the backbone (length N) stretches from a mushroom-like to a more brush-like configuration. For $b = N$, i.e., when attaching the side chain to the free end of the backbone, the effect is strongest. Our data indicate that the thickness of the ECM may be tuned by simply altering the attachment of aggrecans to the HA backbone.

BP 13.5 Tue 18:15 PC 203

Why ion-terminated, finite polyalanine helices are stable in the gas phase — •Volker Blum[1], Joel Ireta[1,2], Alexandre Tkatchenko[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Universidad Autonoma Metropolitana-Iztapalapa, Mexico DF, Mexico

The formation of helical secondary structure in peptides is often associated with a "hydrophobic effect", but a series of landmark experiments indicate an *intrinsic* helical stability of isolated gas-phase polyalanine peptides, when terminated, e.g., by simple alkali ions [1]. We here quantify the mechanisms that stabilize Li^+ ion-terminated helices from first principles, including (i) the direct stabilization by saturating missing H-bonds near the C-terminus, (ii) indirect (de-)stabilization by the absence of H-bond cooperativity in short chains, (iii) the electrostatic presence of the positive ion, which more than offsets the missing H-bond cooperativity, and (iv) the stabilizing effect of non-local correlation (van der Waals) between side chains with increasing helix length. (i), (ii), and (iii) are covered by density-functional theory (DFT) in the PBE generalized gradient approximation; regarding (i), we show how details of the termination affect the stability hierarchy of different helix types (α, 3_{10}) For short helices Ala_n (n=1-10), we capture (iv) by quantum-chemical MP2 perturbation theory; this is used to corroborate a set of semi-empirical C6 corrections to DFT, which are then used to describe the limit of even larger helices. [1] Kohtani, Kinnear, Jarrold, JACS **122**, 12377 (2000).

BP 13.6 Tue 18:30 PC 203

How Large are Cooperative Effects in Hydrogen Bonded Molecular Chains? — •Martin Fuchs[1], Joel Ireta[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Univ. Autonoma Metropolitana Iztapalpa, Mexico

Intermolecular hydrogen bonds play an eminent role in a wide range of materials. In particular, they are critical for the secondary structure stabilization of biopolymers like proteins and nucleic acids. Arrays of hydrogen bonds (hbs), such as in chains or helices, often display a cooperative strengthening of the individual hbs. This cooperativity is crucial for understanding the stability and properties of hydrogen bonded materials. Here we investigate the hb cooperativity in model chains of HCl, HF, HCN, formamide, and 4-pyridone, i.e. molecules forming weak to strong hbs. We calculate the hb strength of infinitely long chains using density-functional theory (DFT) with the Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA). We show that for large intermolecular separations, the hbs in the infinite chain strengthen by 20% over the respective molecular dimers, consistent with dipolar electrostatics [1]. At the equilibrium separation, the hbs strengthen significantly further (up to 260% for HF), with additional stabilization from induced dipolar interactions. Comparing with results from higher-level calculations (MP2 and quantum Monte Carlo) we find that DFT faithfully describes the cooperativity in these systems in which the hbs are close to linear. [1] P.B. Allen, J. Chem. Phys. **120**, 2951 (2004).

BP 14: Single Molecules (joint session CPP/BP)

Time: Tuesday 17:00–19:00 Location: C 230

see program CPP 15

BP 15: Single Molecules

Time: Wednesday 14:00–17:15 Location: C 243

BP 15.1 Wed 14:00 C 243

Single molecule detection of Myosin V in living cell — •Paolo Pierobon[1], Giovanni Cappello[1], Sarra Achouri[1], Sebastien Courty[2], Maxime Dahan[2], Alex Dunn[3], and James Spudich[3] — [1]Institut Curie, Physico-Chimie-Curie, 11 rue P. et M. Curie, 75005 Paris, France — [2]Laboratoire Kastler Brossel, Physics & Biology Department, Ecole Normale Supérieure 24, rue Lhomond 75005 Paris, — [3]Dept. of Biochemistry, Stanford University School of Medicine, Beckman Center B405, Stanford , CA 94305

Single molecule imaging and manipulation provide an irreplaceable tool to isolate each component of the cell and to quantitatively study its dynamics in a perfectly controlled environment. However, the experiments are usually performed out of the physiological context and a priori no indication on the behaviour of the molecule in the cell can be given. To show that this limitation can be overcome, we marked with a quantum dots single myosin V (a processive motor whose physical properties have been largely investigated in vitro). We observed the motion of the motors at sub-pixel resolution directly in living cells. We measured for the first time the processivity, the speed and the step size of the motor in its natural environment and compared the results with the one obtained from in vitro experiments.

BP 15.2 Wed 14:15 C 243

Walking the line: kinesin motors observed with submolecular resolution by atomic force microscopy — •Iwan A.T. Schaap[1], Carolina Carrasco[2], Pedro J. de Pablo[2], and Christoph F. Schmidt[3] — [1]National Institute for Medical Research, London, UK — [2]Universidad Autónoma de Madrid, Madrid, Spain — [3]Georg-August-Universität, Göttingen, Germany

Intracellular transport is largely driven by dyneins and kinesins moving on microtubules in complex, but highly coordinated patterns. How

exactly a single motor proceeds on the 13 narrow "lanes" or protofilaments of a microtubule remains unknown because the required resolution lies beyond the reach of light microscopy. We have here succeeded to image kinesin-1 dimers immobilized on microtubules with single-head resolution and in addition in their motion along microtubules with nanometer resolution by atomic-force-microscopy. We show that both heads of one dimer are microtubule-bound for the major part of the chemical cycle. Furthermore, we could unambiguously resolve that both heads bind to the same protofilament, instead of straddling two, and remain on this track during processive movement.

BP 15.3 Wed 14:30 C 243

Towards resolving single helicase steps on DNA using magnetic tweezers — •Daniel Klaue and Ralf Seidel — Biotechnology Center, Dresden University of Technology, Germany

Replicative helicases drive processive DNA unwinding during DNA replication, the process during which a copy of the genome is synthesized. They are large hexamers, which encircle DNA. ATP hydrolysis in each of the six monomers drives processive movement of the helicase along DNA, which is coupled to DNA unwinding. However, it still remains elusive, how the six ATPase units are coordinated to achieve directional movement. To address this question, we study Large T antigen, a viral replicative helicase, which serves as an important model system for eukaryotic replication. We apply magnetic tweezers in order to follow the DNA unwinding of a single DNA hairpin in real-time. DNA unwinding by T antigen is comparably slow with 1-2 $\mathrm{bp\,s^{-1}}$. Resolving the bp-sized steps of the helicase along DNA would provide important insight into the coordination of the ATPase units. We therefore tested and improved the resolution limits of the applied magnetic tweezers, where a magnetic microsphere is used to exert force on a single DNA molecule. We achieve sub-nm accuracy in detecting the position of immobilized microspheres. However, we find that DNA bound microspheres can exhibit significant rotational fluctuations thereby limiting the resolution in these experiments. Nonetheless, by carefully selecting the measured microspheres we can obtain nm resolution on a second time scale, which would be sufficient to resolve bp-sized helicase steps.

BP 15.4 Wed 14:45 C 243

Transcriptional pausing and proof reading — •Martin Depken, Stephan Grill, and Eric Galburt — Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

RNA polymerases are protein molecular machines that read the genetic information and transcribe it into messenger RNA. The process of adding new bases to the nascent RNA molecule is frequently interrupted by pauses. Here we consider the nature of these pauses, and show that they are well described by a diffusive process. This has implications for the pause time distribution, and the polymerase ability to transcribe through structural barriers such as nucleosomes and other DNA binding proteins. We further consider the possible relation between transcriptional pausing and proof reading, and examine the resulting interplay between fidelity and transcription speed.

BP 15.5 Wed 15:00 C 243

A unified model of transcription elongation — •Dáibhid Ó Maoiléidigh — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The copying of DNA into RNA is the first step required for the production of proteins and RNA with a direct function. This process of transcription is highly regulated and is carried out by RNA polymerase (RNAP), a complex multi-functional molecular motor. In this talk we present a model which explains most published single-molecule observations of the elongation of the RNA transcript by RNAP. The model is an extension of previous work where we successfully predicted the sequence dependent positions of pauses during the elongation process [1]. Pauses have many functions, for example, they are associated with the correction of errors during transcription and are required for the termination of transcription. We have proposed previously that the folding of the RNA transcript behind RNAP creates a barrier which restricts the backwards movement of RNAP along DNA during a pause [1]. We now provide an estimate for the barrier position distribution. Furthermore, we present new analytical expressions which describe the dependence of the elongation velocity on force applied in single-molecule experiments. The model resolves many of the inconsistencies in the interpretations of single-molecule experiments on transcription elongation and illuminates mechanisms for its control.

[1] Tadigotla V. R., Ó Maoiléidigh D., Sengupta A. M., Epshtein V., Ebright R. H., Nudler E., Ruckenstein A. E., Proc Natl Acad Sci U S A, 103:4439-44 (2006).

BP 15.6 Wed 15:15 C 243

Peptide adsorption, friction and unfolding: Theoretical approaches — •Roland Netz, Dominik Horinek, Andreas Serr, Hirofumi Wada, Alfredo Alexander-Katz, and Thorsten Hugel — Physik Department, TU München, 85748 Garching

Single-molecule behavior combines the fields of non-equilibrium thermodynamics, elasticity theory and hydrodynamics. Theoretical approaches thus rely on molecular simulations, continuum modeling and scaling approaches. This is demonstrated with a few examples: - Spider silk consists of polypeptides with highly repetitive motives and readily adsorbs on hydrophobic and hydrophilic surfaces. Single molecule AFM studies yield adsorption energies and point to an extremely high mobility on hydrophobic surfaces. The dominant hydrophobic attraction can be quantitatively explained with classical MD simulations including explicit water. Both water structural effects and dispersion interactions contribute to this solvation attraction. - The friction coefficient of bound polymers is very low on hydrophobic substrates, which is traced back to the presence of a vacuum layer between substrate and water, which forms a lubricating cushion on which a polymer can glide. Conversely, friction forces on hydrophilic substrates are large and make determining the equilibrium binding constant in computer simulations impossible. - Shear-flow induced unfolding of proteins plays an important role in starting the coagulation cascade in small blood vessels. In the theoretical modeling the unfolding is initiated by single-chain protrusion-like excitations and leads to a hydrodynamic unfolding transition, which is well captured by a scaling nucleation argument.

15 min. break

BP 15.7 Wed 15:45 C 243

Fluorescent Nanodiamonds for Biological Applications — •Felix Neugart[1], Andrea Zappe[1], Fedor Jelezko[1], Carsten Tietz[1], Jean Paul Boudou[2], Anke Krüger[3], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Stuttgart — [2]Université Pierre et Marie Curie, Paris VI — [3]Christian-Albrechts-Universität, Kiel

Nanodiamonds with nitrogene vacancy (NV) defects as colour centre are a promising candidate for a bright, not toxic, not blinking and not bleaching lable for biological aplications. The NV centre is excited in the green (514nm or 532nm wavelength) and emites around 700nm where living cells show a low autofluorescence. We inserted nandiamonds into living cells via microinjection and endocytosis. The diamonds could be detected by fluorescence as well refraction.

Functionalisation of the nanodiamonds surface is important for labelling as well as for the avoidance of aggregation under physiological conditions. The stability of hydrosols strongly depends on the surface potential of the particles, pH, and solvent salt concentration.

The fluorescence and motional dynamics of single diamond nanocrystals in buffer solution and in living cells is investigated. Stable hydrosols of nanodiamonds in buffer solutions are analysed by fluorescence correlation spectroscopy. [1]

[1] Neugart et al., Nano Letters, (2007)

BP 15.8 Wed 16:00 C 243

(Non-) linear deformation of viral shells — •Wouter H. Roos[1], Charlotte Uetrecht[2], Norman Watts[3], Paul Wingfield[3], Alasdair Steven[3], Albert Heck[2], and Gijs J. L. Wuite[1] — [1]Natuur- en Sterrenkunde, Vrije Universiteit, Amsterdam, Niederlande — [2]Bijvoet Instituut, Universiteit Utrecht, Niederlande — [3]NIH, Bethesda, USA

Nanoindentation techniques are increasingly being applied to study the mechanical properties of complex protein assemblies such as viral shells (capsids). Numerical simulations guided by the Föppl- von Kármán (FvK) number γ (a dimensionless number relating the "in-plane" elasticity of the shell to its "out-of-plane" bending rigidity) have been able to explain indentation results on capsids with $\gamma < 150$ (linear response) and $\gamma > 700$ (buckling transition). Yet for shells with a γ between those values a non-linear, but continuous response is expected. Here we report nanoindentation experiments with an atomic force microscope on capsids of the Hepatitis B Virus (HBV) to investigate this intermediate response regime. HBV was chosen as a model system because its capsids can form in a smaller T=3 and a bigger T=4 configuration that have FvK values within our region of interest.

We demonstrate that the HBV T=3 capsid shows a subtle non-linear behaviour while the T=4 capsid reacts strongly non-linear, but continuously to deformation. Both non-linear responses can be understood in relation to their FvK values. At large indentations HBV undergoes permanent plastic deformation indicating a rearrangement of capsid proteins. The presented results demonstrate the surprising strength of continuum elastic theory to describe these nanometre sized objects.

BP 15.9 Wed 16:15 C 243

Effect of low pH on the Influenza virus membrane — •Frederic Eghiaian, Iwan A.T. Schaap, John J. Skehel, and Claudia Veigel — National Institute for Medical Research, London, UK

The Influenza virus is an enveloped virus from the Orthomyxovirus family. The protein-rich membrane of the viral particle needs to persist in the often hostile extracellular environment when the virus transfers from host to host, but, to allow infection, it also needs to permit membrane fusion within the acidic compartments of the target cell. To investigate how the virus negotiates these apparently conflicting demands on its rigidity, we developed methods to image this relatively large virus (˜100 nm diameter) using an atomic force microscope, and to probe its mechanical properties under conditions mimicking the different stages of the viral life-cycle. We compared the complex response of the viral envelope with the behaviour of simplified model systems to understand the contribution of the various parts of the viral structure to its mechanical properties. In addition we investigated how the acid-induced conformational change of the Influenza Hemagglutinin protein (involved in membrane fusion) disturbs lipid membranes and we set out to identify the responsible parts of the protein (the fusion peptide or the transmembrane region).

BP 15.10 Wed 16:30 C 243

TIRFM evanescent field calibration using tilted microtubules — •Chris Gell, Michael Berndt, and Stefan Diez — MPI-CBG, Dresden, Germany

Total internal reflection fluorescence microscopy (TIRFM) has become a powerful tool to study the dynamics of subcellular structures and single molecules near substrate surfaces. However, the penetration depth of the evanescent field , i.e. the distance at which the excitation intensity has exponentially decayed to 1/e, is often left undetermined. This presents a limit on the spatial information about the imaged structures. Moreover, in multi-color TIRFM applications, e.g. to perform colocalization studies, it is crucial to ensure equal penetration depths for the different excitation wavelengths. Here, we present a novel method to quantitatively characterise the illumination in TIRFM using tilted, fluorescently labelled, microtubules. Importantly, the use of in vitro reconstituted microtubules as nanoscale rulers results in a minimal perturbation of the evanescent field. Excitation light scattering is essentially eliminated and the refractive index of the sample environment is virtually unchanged. Our method has the potential to provide a generic tool for in-situ calibration of the evanescent field.

BP 15.11 Wed 16:45 C 243

C-Ring conformational rotation of a single F0F1- ATP synthase motor using alternating laser excitation — •Stefan Ernst[1], Monika Düser[1], Nawid Zarrabi[1], Rolf Reuter[1], Stanley D. Dunn[2], Gary D. Glick[3], and Michael Börsch[1] — [1]3rd Institute of Physics, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Department of Biochemistry, University of Western Ontario, London, Ontario, Canada N6A 5C1 — [3]Department of Chemistry, University of Michigan, Ann Arbor, MI, USA 48109-1001

Formation of ATP from ADP and Phosphate (ATP synthese) is of great importance for any living cell. This chemical reaction is catalyzed by the enzyme F0F1- ATP synthase. By hydrolyzing ATP the enzyme can also work as an proton pump. Catalysis driven by a stepwise internal rotation of subunits of the lipid membrane embedded enzyme. To detect these substeps the single molecule fluorescence resonance energy trasfer (FRET) approach was used. We labeled one rotary c subunit with the FRET acceptor dye and the static a subunit with the FRET donor.

It was possible to determine the stepsize of rotation and dwell times. It was also possible to study the influence of different bacterial drugs, i.e. inhibitors of F0F1- ATP synthase like AMP-PNP and Aurovertin.

The different substep movements were identified with Hidden Markov Models (HMM). Duty cycle optimized alternating laser excitation provides an acceptor test to improve the accurancy of the single molecile FRET analysis.

BP 15.12 Wed 17:00 C 243

Data Analysis with Hidden Markov Models on a single Kdp-ATPase — •Nawid Zarrabi[1], Michael Börsch[1], Thomas Heitkamp[2], and Jörg Greie[2] — [1]3. Physikalisches Institut, Pfaffenwaldring 57, Universität Stuttgart, 70569 Stuttgart — [2]Universität Osnabrück, Fachbereich Biologie/Chemie, Arbeitsgruppe Mikrobiologie, Barbarastraße 11, 49069 Osnabrück

The membrane-embedded KdpFABC complex belongs to the group of P-type ATPases which transports potassium across a lipid bilayer using ATP hydrolysis. This enzyme contains a central catalytic subunit which mediates ion transport and ATP-hydrolysis.

We measured the stepwise conformational changes of this protein using confocal single-molecule fluorescence resonance energy transfer (FRET) and analyzed this data with Hidden Markov Models (HMM).

To prove the capability of the HMM approach we generated single molecule data of freely diffusing enzymes in liposomes by a Monte-Carlo-simulation. Thereby we included the intensity fluctuations due to Brownian motion. The conformational states of the ATPases were described by a Markov process with predefined rates for the transitions of the reaction cycle.

The aim of the data analysis method was to investigate the reaction cycle of the KdpFABC-complex and, furthermore, to elucidate the effectiveness of different inhibitors of the ion transport mechanisms.

BP 16: Pattern Formation and Developmental Processes

Time: Wednesday 17:30–19:00 Location: C 243

BP 16.1 Wed 17:30 C 243

Coupling vs. Noise: The Rise and Fall of Synchrony in the Segmentation Clock — •Ingmar Riedel-Kruse[1,2], Claudia Mueller[2], and Andrew Oates[2] — [1]California Institute of Technology, Pasadena, USA — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

The "segmentation clock" is thought to coordinate sequential segmentation of the body axis in vertebrate embryos. This clock comprises a multi-cellular genetic network of synchronized oscillators, coupled by intercellular Delta/Notch signaling. How this synchrony is established, and how its loss determines the position of segmentation defects in Delta/Notch mutants is unknown. We analyzed the clock's synchrony dynamics by varying strength and timing of Notch coupling in zebrafish embryos using techniques for quantitative perturbation of gene function. We developed a physical theory based on coupled phase oscillators explaining the observed onset and rescue of segmentation defects, the clock's robustness against developmental noise, and a critical point beyond which synchrony decays. We conclude that synchrony among these genetic oscillators can be established by simultaneous initiation and self-organization, and that the segmentation defect position is determined by the difference between coupling strength and noise.

Science 317: 1911 (2007).

BP 16.2 Wed 17:45 C 243

Firewalls in atrial myocytes — •Rüdiger Thul[1], Stephen Coombes[1], and Martin Bootman[2] — [1]School of Mathematical Sciences, University of Nottingham, Nottingham, NG7 2RD, UK — [2]Laboratory of Molecular Signalling, The Babraham Institute, Babraham, Cambridge, CB22 3AT, UK

Atrial myocytes play a prominent role in the generation of heart beats. Their contraction is controlled by Calcium signals that emerge at the cellular periphery and then proceed centripetally to engage the force-generating myofilaments. Experiments have demonstrated that these initial signals need to overcome a barrier just below the cell membrane before they move inward. Since atrial myoctes lack transverse tubules that transmit external signals to the cell interior as e.g. in ventricular myocytes, such a firewall represents a crucial determinant of atrial dynamics. For instances, it allows atrial myocytes to fine tune their

responses to a wide range of vital stimuli. Here, we present a computationally advantageous model to investigate the mechanisms that give rise to these graded centripetal signals. Our framework takes into account the three dimensional organisation of atrial myocytes, especially the spatially restricted release of Calcium from internal storage compartments. We employ a fire-diffuse-fire (FDF) model to examine the spatio-temporal patterns and to probe the dependence of wave propagation on physiologically relevant parameters. Mimicking an excitable medium, the FDF approach reflects the significance of noise in intracellullar Calcium dynamics. The explicit construction of the corresponding Green's function allows for a detailed analysis.

BP 16.3 Wed 18:00 C 243

A stochastic Boolean network model of receptor cross-talk in angiogenesis — •Thimo Rohlf[1,2] and Amy L. Bauer[3] — [1]Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA — [2]Max-Planck Institute for Mathematics in the Sciences, Inselstrasse 22, D-04103 Leipzig — [3]Los Alamos National Laboratory (T-14), MS B-262, Los Alamos, NM 87545, USA

How cells interpret and synthesize multiple biochemical signals initiated by key external stimuli during angiogenesis, namely growth factors, matrix molecules, and cell-cell communication via cadherins, is a challenging problem. From available databases, we construct a Boolean network model that highlights the cross-talk between growth factor, integrin, and cadherin receptors, and systematically analyze the dynamical stability of the network under continuous-time Boolean dynamics with a noisy production function.

We find that the signal transduction network exhibits robust and fast response to external signals, independent of the internal cell state. We derive an input-output table that maps external stimuli to cell phenotypes, which is extraordinarily stable against molecular noise, with one important exception: an oscillatory feedback-loop between the key signal molecules RhoA and Rac (as sometimes is postulated in the literature) is unstable under arbitrarily low noise, leading to erratic, dysfunctional cell motion. Finally, we show that the network exhibits an apoptotic response rate that increases with noise, suggesting that the probability of programmed cell death increases in response to conflicting or confusing signals.

BP 16.4 Wed 18:15 C 243

MarkovModelForBoneRemodelling — •Marco Rusconi[1,2], Richard Weinkamer[2], Angelo Valleriani[2], and Juergen Kurths[1] — [1]Non-linear dynamics group,institute of physics,faculty of mathematics and science, Potsdam University,D-14415 Potsdam — [2]Max Planck Institut of Colloids and Interface, Department of Biomaterials,Research Campus Golm, D-14424 Potsdam, Germany

Bone is a continuously regenerated living tissue. During this remodelling process, bone is cyclically resorbed and formed to allow it to achieve the optimal adaptation to the external mechanical environment. The investigation of the connection between external mechanical stimuli and bone remodelling is a not completely understood problem. In this contribution, we introduce a markov model for bone remodelling. We focus our attention on the remodelling of the inner spongy structure of bone, the trabecular structure. Assuming a connection between mechanical stimulus and trabecular cross-sectional area (A), we define phenomenological relations between the probability of formation and resorption and A. This is essentially a *translation* of the Wolff-Roux law in terms of an architectural parameter of the trabecular structure. We evaluate the evolution with time of the trabecular area distribution (TAD) for several different mechanical stimuli proposed in literature. The different assumptions lead to different TAD and we compare them with those obtained from micro tomographic scans of real bone.

BP 16.5 Wed 18:30 C 243

Collective processes set the clock in vertebrate segmentation — •Saul Ares[1], Luis Morelli[1], Leah Herrgen[2], Christian Schroeter[2], Andrew C. Oates[2], and Frank Julicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Somitogenesis, the first stage of the body axis segmentation in vertebrate development, is a complex process driven by the interplay of oscillations in gene expression and the elongation of the body axis. In order to understand it quantitatively at a tissue level, a theoretical framework based on discrete coupled phase oscillators with a time delay in their mutual communication has been proposed. Global properties as the time necessary for the formation of a somite can be calculated, finding a scenario of multiple solutions and multistability. To get analytic expressions from the theory, a continuum limit for arbitrary values of the time delay is formulated. This continuum formulation allows to determine the parameters of the theory from available data on the wavelength of the patterns of gene expression. The fit to the experimental data supports the main conclusion of the theory: the periodicity of somitogenesis arises as a collective process where the intercellular communication plays a key role in the setting of the frequency of the segmentation clock.

BP 16.6 Wed 18:45 C 243

Spatiotemporal patterns in signal transduction: effect of cytoskeleton structure and molecular crowding — •Michael Klann, Alexei Lapin, and Matthias Reuss — Institute of Biochemical Engineering, University of Stuttgart, Stuttgart, Germany

Cellular signaling depends on the efficient translocation of signals from the cell membrane to target proteins. The cytoskeleton network hinders diffusion but also offers express-ways for active transportation along the filaments. Amplification or regulation of the signal strength through a cascade of reactions depends on the local concentration of the molecules, which is strongly affected by molecular crowding. The low number of molecules in signaling pathways leads to a significant level of stochastic noise. Local fluctuations that do not cancel out on the cell level due to nonlinear interactions lead to deviations from continuum ODE-models. To analyze the spatiotemporal signaling patterns affected by the inhomogeneous background of cellular architecture we developed a stochastic simulation method that allows us to track the position of every molecule of interest including reactions, diffusion and active transport through the cell. Simulations show that in presence of the cytoskeleton, diffusion is slowed down but the reaction rate is increased due to the higher effective concentration of reactants. Overall this can reduce the travel time from the plasma membrane to the nucleus. Active transport along the cytoskeleton furthermore increases the efficiency of the signaling cascade.

BP 17: Physics of Cells

Time: Wednesday 14:00–15:45 Location: PC 203

BP 17.1 Wed 14:00 PC 203

Collective Dynamics of Endocytic Vesicles in Membrane Trafficking — •Mirko Birbaumer[1], Markus Kalisch[2], Frank Schweitzer[3], Peter Bühlmann[2], and Lucas Pelkmans[1] — [1]Institute of Systems Biology, Swiss Federal Institute of Technology, ETH Hönggerberg, CH-8093 Zurich — [2]Seminar for Statistics, Swiss Federal Institute of Technology, Leonhardstrasse 27, CH-8092 Zurich — [3]Chair of Systems Design, Swiss Federal Institute of Technology, Kreuzplatz 5, CH-8032 Zurich

Spatial organization and compartmentalization of intracellular organelles such as endocytic vesicles play an essential role for many cellular processes. A variety of different vesicle patterns can result from a systematic perturbation of the cell, as e.g. by RNA interference in mammalian cells. By silencing a large set of genes in a mammalian cell numerous well distinguishable patterns arise and we are therefore dealing with a clustering problem. In order to cluster vesicle patterns, we first need to extract as much relevant information about intracellular organelles as possible, such as intensity distribution, location with respect to the cell center, shape, their spatial distribution and quantity. A new clustering approach enables us to distinguish between different patterns and group these according to their properties. These patterns should also result as steady states from a macroscopic theory of intracellular transport. Here we present a modeling approach of intracellular trafficking based on Brownian Agents.

BP 17.2 Wed 14:15 PC 203

Particle tracking and microscopy of the intracellular trans-

port of polyethyleneimine based gene carriers — •Ralf Bausinger[1] and Andreas Zumbusch[2] — [1]Fachbereich Physik, Universität Konstanz, Fach M684, 78457 Konstanz — [2]Fachbereich Chemie, Universität Konstanz, Fach M722, 78457 Konstanz

Polyethyleneimine (PEI) based gene carriers are among the most efficient synthetic vectors for the delivery of DNA into the cell nucleus. We use highly sensitive fluorescence microscopy and single particle tracking methods for the investigation of the particles' paths from the plasma membrane to the nucleus. Active actin polymerization around the particle supports its cell entry and Rab protein accumulation initiates the fast vesicular transport on microtubules. Trajectories of this bidirectional transport process are segmented by a numerical algorithm separating different modes of motion. Diffusion analysis of these segments allows the unravelling of the distribution of intracellular transport velocities. We further investigated the role of mitosis on the particle distribution of the daughter cells and the subsequent expression of the transgene.

BP 17.3 Wed 14:30 PC 203

Actin-membrane interactions in a biomimetic systems studied by a novel, high precision optical method — •Timo Betz, Léa Laetitia Pontani, and Cécile Sykes — Institut Curie, UMR CNRS 168, 11 rue Pierre et Marie Curie, 75248 Paris, France

The lethal potential of cancer results from abnormal cell division and aggressive metastatic activity that turns resting cancer cells into motile structures which spread through an organism, resulting in numerous and often uncontrollable growing subpopulations. It is well known that both cell motility and cell division depend crucially on cell mechanics, namely on the actin cortex which is a dense biopolymer network that is steadily contracted by myosin motors. A key to understand the abnormal motility and proliferation of cancer cells is the quantification of the physical properties of the actin cortex. Of special interest is the activity of the acto-myosin network and its interaction with the plasma membrane that contributes to the physical properties of the cell. To investigate these interactions we combine a novel optical technique that detects the edge fluctuations of a biomimetic cell with high spatial and temporal resolution. The investigated system mimics the actin cortex by polymerizing an actin network under the membrane of a lipid vesicle. Analyzing the membrane fluctuation with and without the actin cortex allows the quantification of physical parameters like bending rigidity and viscoelastic properties of the actin membrane system.

BP 17.4 Wed 14:45 PC 203

Stem Cell Fate Directed by Matrix Elasticity and Ligands — •Florian Rehfeldt, Shenshen Cai, and Dennis E. Discher — University of Pennsylvania, Biophysical Engineering Lab, Philadelphia, USA

Mesenchymal stem cells (MSCs) from adult bone marrow have recently been found responsive to matrix elasticity in their differentiation. Collagen-I coated hydrogels induce MSCs to express neurogenic, myogenic, and osteogenic markers depending on the Young's modulus E (ranging from 1 to 34 kPa) of the substrate that is used to approximate the physiological elasticity of native tissue. While collagen is the most abundant protein in mammals, hyaluronic acid (HA) is the major non-protein factor in the marrow and is a widely distributed load-bearing matrix polysaccharide that promotes proliferation and migration during embryonic development and other processes. We show that MSCs dynamically express an HA-receptor, and we use the tunable elasticity of novel HA hydrogels to understand the morphology, motility, and fate choices of MSCs as they depend on matrix elasticity and adhesive ligands. Marrow-derived hematopoietic stem cells (HSCs) are also studied, and the results amplify the influence of matrix elasticity in stem cell fate choices.

BP 17.5 Wed 15:00 PC 203

Dynamics of different probe particles to study local microenvironments inside living cells — •Michael Duits, Yixuan Li, Siva Vanapalli, and Frieder Mugele — MESA+ institute, University of Twente, PO Box 217, 7500 AE The Netherlands

To understand the dynamics of particles inside living cells in relation to intracellular rheology, we examined living endothelial cells in untreated form, and after (chemical) interventions, aimed at revealing specific contributions to particle motions via driving forces or passive mechanical resistances. Endogenous granules (EG) and ballistically injected particles (BIP) were used as tracers. At 37 C the mean-squared displacement (MSD) showed different time dependence for the two probes. While EGs showed only a linear dependence, for BIPs also a transition to a plateau at small lagtimes was observed. Moreover, the (normalized) MSDs were much larger for the EGs. This suggests different local micro-environments for EGs and BIPs. Also the sets of individual trajectories were analyzed. Here, both the magnitude and the power-law exponent showed distributions that suggest heterogeneity in the environment for both probes. Depletion of intracellular ATP resulted in opposite effects on the MSDs of EGs and BIPs. While for EGs the MSD and the fraction of trajectories with superdiffusive exponents were reduced, for BIPs an increase in MSD was found. It thus seems that ATP depletion not only annihilates active processes, but also alters the cytoskeleton. These observations of cytoskeletal network heterogeneities have profound implications for the quantification of global mechanical behavior in living cells.

BP 17.6 Wed 15:15 PC 203

A new approach in Ca^{2+} modeling — •Alexander Skupin and Martin Falcke — Hahn Meitner Institut, Glienicker Straße 100, 14109 Berlin, Germany

Ca^{2+} is the most important second messenger in living cells serving as a critical link between a variety of physiological stimuli and their intra and intercellular response. In our recent study we have demonstrated the stochastic character of Ca^{2+} oscillations, which are caused by the stochastic opening of ion channels releasing Ca^{2+} from internal stores into the cytosol. This liberated Ca^{2+} can activate adjoining channels resulting in a global Ca^{2+} wave within the cell, i.e. that microscopic fluctuations determine the global behavior of cells.

Thus modeling has to take the spatial character of this phenomenon into account, since oscillation are orchestrated on that level. The describing system of coupled reaction diffusion equations exhibits huge gradients which slow down the simulation speed of straight forward methods. Therefor we linearized the equations and developed an analytical solution in terms of coupled Greens function which are driven by the stochastic behavior of the ion channels acting as source terms in the equations. We will compare the results of the interplay of our analytical solution and the stochastic driving modeled by a Gillespie algorithm with our experimental results.

BP 17.7 Wed 15:30 PC 203

Transmembrane Potential and Proton Buffering Capacity of a Small Vesicle — •Tihamér Geyer and Sarah Blass — Zentrum für Bioinformatik, Universität des Saarlandes, D 66041–Saarbrücken

The dynamic behavior of a metabolic network is determined both by the reaction rates and by the buffering capacities of the reservoirs. While a lot of effort goes into determining rate constants, much less emphasis is put on the capacities. Consequently, for setting up a dynamic simulation of a part of the metabolism of a cell, it is much easier to gather the necessary rates than to find reliable information on how to describe, e.g., a proton buffering capacity in a typical *in vivo* geometry like a small vesicle.

To shed some more light onto how to incorporate a specific biological setup into a simulation, we used stochastic molecular simulations of a photosynthetic vesicle of the purple bacterium *Rhodobacter sphaeroides* to investigate how the transmembrane potential $\Delta\Phi$ has to be described in order to reproduce the measured time course after a short flash of light. By treating the small vesicle as a spherical capacitor, both the biphasic rise and the exponential decay of $\Delta\Phi$ are reproduced, while a Nernst-like model based on the pH gradient leads to a different signature in time. The simulation also reproduces the simultaneously measured cytochrome c oxidation state.

We also discuss how the findings from the vesicle apply to other confined geometries as, e.g., the cristae of the mitochondria.

BP 18: Biomaterials

Time: Wednesday 16:00–17:15 Location: PC 203

BP 18.1 Wed 16:00 PC 203

The isopod exoskeleton: A model to study formation and function of amorphous calcium carbonate in calcified tissues — •Sabine Hild and Andreas Ziegler — Central Facility for Electron Microscopy; University of Ulm, Germany

The mineralized exoskeleton (cuticle) of crustaceans is subjected to periodic molting in which it is periodically decalcified and shed. A new larger cuticle, synthesized before shedding, is mineralized after every molt. These processes cause spatial and temporal variations of the mineral distribution. Thus, the cuticle is an excellent model to study mineralization processes of calcified tissues. The mineral composition of the cuticle of the land living crustacean Porcellio scaber (Isopoda) was examined using Micro-Raman spectroscopy. It was shown that Calcite is restricted to the outer area of the cuticle, whereas amorphous calcium carbonate (ACC) is localized in the middle having only little overlap with the calcite layer. In biological systems ACC is thought to be a precursor phase for crystalline modifications and, because of its high solubility, it is beneficial for temporary calcium carbonate storage. In order to better understand the formation and function of ACC, changes in the distribution and content of mineral phase were monitored during natural and in-vitro decalcification. It was shown that the protective outer calcite layer is shed away during each molt, while ACC is recycled to quickly re-establish the protective calcite layer in the new cuticle. The addition detection of magnesium and phosphate derivates suggests that they assist ACC stabilization.

BP 18.2 Wed 16:15 PC 203

Structural effects on enamel through fluoridization: an XPS and AFM study — •Christian Zeitz[1], Frank Müller[1], Matthias Hannig[2], Karin Huber[2], Stefan Hüfner[1], and Karin Jacobs[1] — [1]Saarland University - Department of Experimental Physics, 66123 Saarbrücken, Germany — [2]Saarland University Hospital - Department of Conservative Dentistry, Parodontology and Preventive Dentistry, 66421 Homburg/Saar, Germany

Enamel, the hardest material in the human body, has been a research topic for many years. The material shows outstanding resistance against abrasion, but it is relatively easy affected by agents of low pH value. The resistance against acids can be increased by fluoridization with an adequate fluoride containing solution. However, it is unknown up to now, what exactly happens during this process.

The aim of our study is to clarify the reactions during fluoridization and to reveal structural changes that can be referred to the treatment. To accomplish this, we perform AFM and XPS measurements on natural teeth. Moreover, to simplify the system, we also study chemical and structural changes on hydroxylapatite pellets.

BP 18.3 Wed 16:30 PC 203

Structure determination of spider silk from X-ray images — •Stephan Ulrich[1], Martin Meling[2], Anja Glisovic[3], Tim Salditt[3], and Annette Zippelius[1] — [1]Universität Göttingen, Institut für Theoretische Physik — [2]Max-Planck-Institut für biophysikalische Chemie, Göttingen — [3]Universität Göttingen, Institut für Röntgenphysik

Spider silk consists of interconnected crystallites, which are typically aligned along the fiber axis. We present a method to systematically determine the structure of these crystallites. Hereby we introduce a model that calculates the scattering function $G(\mathbf{q})$ which is fitted to the measured X-ray image (silk from nephila clavipes). With it, the crystallites' size, the constitution and dimensions of their unit cell, as well as their tilt with respect to the fiber axis is identified, and furthermore the effect of coherent scattering from different crystallites is investigated. The shown methods and the presented model can easily be generalized to a wide class of composite materials.

BP 18.4 Wed 16:45 PC 203

Elektronenmikroskopische Untersuchungen des Polymer/ Mineral-Verbundmaterials Perlmutt — •Katharina Gries[1,2], Roland Kröger[1], Christian Kübel[3], Monika Fritz[2] und Andreas Rosenauer[1] — [1]Institut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen — [2]Institut für Biophysik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen — [3]Fraunhofer Institut für Fertigungstechnik und Angewandte Materialforschung (IFAM), Wiener Straße 12, 28359 Bremen

Mittels Transmissionselektronenmikroskopie (TEM) wurde das Perlmutt der Meeresschnecke *Haliotis laevigata* untersucht. Perlmutt, die innere, schimmernde Schicht in den Schalen von Meeresschnecken, besteht aus Aragonitplättchen, die jeweils durch Schichten aus organischem Material voneinander getrennt sind. Durch hochauflösende TEM konnte gezeigt werden, dass zwischen übereinander liegenden Aragonitplättchen kristalline, durchgängige Verbindungen, so genannte Mineralbrücken, auftreten, die ebenfalls aus Aragonit bestehen. Zum ersten Mal konnte nachgewiesen werden, dass sich innerhalb der Aragonitplättchen facettierte Nanoporen befinden. Elektronentomographische Messungen und anschließende dreidimensionale Rekonstruktion der Nanoporen ermöglichten die Bestimmung der Form, Größe und räumlichen Verteilung der Poren. EDX und EELS Messungen zeigten, dass die Nanoporen einen erhöhten Kohlenstoffanteil und somit eventuell organisches Material enthalten.

BP 18.5 Wed 17:00 PC 203

Untersuchung von kolloidalen Protein-Mineral Partikeln mit Neutronenkleinstreuung — •Alexander Heiss[1], Vitaliy Pipich[1], Willi Jahnen-Dechent[2] und Dietmar Schwahn[1] — [1]IFF des Helmholtz Forschungszentrum Jülich — [2]IBMT der RWTH Aachen

Das Serumprotein Fetuin-A ist in vivo ein wichtiger Kalzifikationsinhibitor [1]. In vitro konnte gezeigt werden, dass in übersättigter Lösung Fetuin-A die Bildung kolloidaler Protein-Mineral Partikel (CPP) vermittelt [2]. Fetuin-A inhibiert die Mineralausscheidung transient, wie der zweistufige Prozess der Partikelreifung zeigt. Während die primären CPPs etwa 50 nm groß und kugelförmig sind, bestehen sekundäre CPPs aus lamellaren kristallinen Domänen und haben eine ellipsoidale Form von etwa 200x100 nm Größe. Außerdem konnte mit Neutronen Kleinwinkelstreuung (SANS) und Kontrastvariation gezeigt werden, dass die sekundären CPPs aus einem kompakten Octacalcium Phosphat Kern bestehen, der von einer Fetuin-A Monoschicht umhüllt ist [3]. Bei peritoneal dialysierten Patienten ist die kalzifizierende Peritonitis eine selten vorkommende Komplikation. Es stellte sich heraus, dass die dabei auftretenden kolloidalen Mineralpartikel eine bemerkenswerte Ähnlichkeit zu den in vitro synthetisierten sekundären CPPs besitzen [3]. Auch hier liefern Kontrastvariations-Experimente Informationen über Topologie und Zusammensetzung.

[1] Schäfer, C. et al. (2003) J Clin Invest. 112, 357 - 366 [2] Heiss, A. et al. (2003) J. Biol. Chem. 278,13333-41. [3] Heiss, A. et al. (2007) Biointerphases 2, 16 * 20

BP 19: Semiflexible Polymers and Networks

Time: Wednesday 17:30–19:30 Location: PC 203

BP 19.1 Wed 17:30 PC 203

Orientational order in two-dimensional random networks of semiflexible polymers — •Martin Kiemes[1], Panayotis Benetatos[2], and Annette Zippelius[2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany — [2]Institut für Theoretische Physik, Universität Göttingen, Germany

It has recently been shown that in a 3D melt of semiflexible polymers random permanent cross-links that fix the corresponding segments to align give rise to orientationally ordered gels [1]. In the current work, using a similar semimicroscopic replica field-theoretic approach, we focus on the 2D case which allows us to consider cross-links that prescribe a finite angle between the corresponding segments. We discuss the resulting phase diagram in terms of the cross-link density, the polymer stiffness, and the crosslinking geometry.

[1] P.Benetatos and A.Zippelius, PRL 99, 198301 (2007)

BP 19.2 Wed 17:45 PC 203

A Stiff Rod in Dense Environments: A Paradigm for Translation–Rotation Coupling — •Tobias Munk, Felix Höfling, Erwin Frey, and Thomas Franosch — Arnold Sommerfeld Center and CeNS, Ludwig-Maximilians-Universität München, Germany

Everybody who once observed a long lorry trying to turn in a small street knows of the consequences of the coupling of translational and rotational motion in the macroscopic world. On the micro scale, similar things happen to anisotropic objects diffusing in a crowded environment. This is found for example in biological cells: their interior is enormously crowded by huge amounts of proteins and other complexes, thus diffusing anisotropic objects are largely constricted by their surroundings. This happens e.g. to free actin filaments moving in the cytoskeleton.

We have set up a simple two-dimensional model in order to examine the Brownian motion of a stiff rod in a sterically hindered medium on all physically relevant timescales. A theoretical description of the unobstructed motion is developed by mapping the corresponding anisotropic diffusion equation to the Smoluchowski-equation. This, however, is not sufficient to grasp the translation–rotation coupling induced by the obstacles. By means of molecular dynamics simulations we point on these coupling effects and demonstrate that the motion is non-gaussian at intermediate times.

BP 19.3 Wed 18:00 PC 203

Stretching of buckled filaments by thermal fluctuations — •Krzysztof Baczynski, Reinhard Lipowsky, and Jan Kierfeld — Max Planck Institute of Colloids and Interfaces, Department of Theory & Bio - Systems, Science Park Golm, 14424 Potsdam, Germany

We study the buckling instability of filaments or elastic rods in two spatial dimensions in the presence of thermal fluctuations. We present an analytical solution based on a renormalization-like procedure where we integrate out short wavelength fluctuations in order to obtain an effective theory governing the buckling instability. We calculate the resulting shift of the critical force by fluctuation effects and the average projected filament length parallel to the force direction as a function of the applied force and of the contour length of the filament. We find that, in the buckled state, thermal fluctuations lead to an increase in the mean projected length of the filament in the force direction. As a function of the contour length, the mean projected length exhibits a cusp at the buckling instability, which becomes rounded by thermal fluctuations. Our analytic results are confirmed by Monte Carlo simulations.

BP 19.4 Wed 18:15 PC 203

Misfits never yield – A microscopic approach to the nonlinear rheology of biopolymer solutions — •Pablo Fernández[1] and Klaus Kroy[2,3] — [1]E22 Biophysik, Technische Universität München, James Franck Straße 1, D-85748 Garching, Germany — [2]Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, D-04009 Leipzig, Germany — [3]Hahn-Meitner Institut, Glienicker Straße 100, D-14109 Berlin, Germany

We propose a nonlinear extension of the standard tube model for semidilute solutions of semiflexible polymers. Non-affine filament deformations at the entanglement scale, the renormalisation of direct interactions by thermal fluctuations, and the geometry of large deformations are systematically taken into account. The analysis of the shear response of a simplified unit cell sheds light onto fundamental issues in cytoskeletal mechanics. The strong geometric stiffening predicted for purely enthalpic networks is found to be thermally suppressed. Instead, we obtain a broad linear response regime covering typical physiological mesh sizes. Surprisingly, we discover a destabilizing effect of large strains ($\sim$ 100%). The theory thus provides a novel perspective at the widely observed catastrophic collapse of *in-vitro* sheared biopolymer solutions, usually attributed to irreversible network damage. It moreover supports the interpretation of shear stiffening at finite frequencies as indicative of adhesive polymer interactions. In combination with such friction-type interactions, our analysis provides an analytically tractable framework to address the nonlinear viscoplasticity of biological tissue on a molecular basis.

BP 19.5 Wed 18:30 PC 203

Accessory contribution of actin binding proteins to the viscoelastic properties of composite actin-networks — •Kurt Schmoller, Oliver Lieleg, and Andreas Bausch — Lehrstuhl E22 für Biophysik, Physik Department, TU München, Garching, Deutschland

Cell shape, mechanics and motility are mainly determined by crosslinked and bundled actin-networks. As in living cells many different actin binding proteins (ABPs) are used simultaneously, it is necessary to study their mechanical function in well-defined in vitro systems where the type and concentration of the ABP can be controlled. By rheological methods we determine the viscoelastic properties of bundled and crosslinked actin networks. The ABPs filamin and fascin are both known to bundle actin filaments. However, the bundle networks formed exhibit pronounced differences in their viscoelastic properties. We investigate composite networks tuning the concentration of either fascin or filamin in the presence of the other ABP. Interestingly, the concentration dependence of the viscoelastic network response is only slightly modified by the presence of the second ABP. These findings suggest that a combination of these two ABPs does not lead to a phase separation, but to an accessory contribution to the viscoelastic properties of the composite network. Further we find networks with a frequency response resembling that of living cells. These findings underline that in vitro actin networks with only a few combined ABPs might be sufficient to rationalize main aspects of the mechanical properties of cells.

BP 19.6 Wed 18:45 PC 203

Semiflexible Polymer Conformations in Entangled Networks — •Hauke Hinsch and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, LMU München, Germany

Biopolymers are ubiquitous in nature and play a crucial role for cell mechanics and motility. One prominent example is the semiflexible filamentous actin that constitutes the cytoskeleton by forming large networks. In the absence of cross-links the network's polymers are mutually constrained only by entanglements. We report on theoretical work and simulations on various distribution functions, investigate the implications for the network's equilibrium configuration and compare our findings to recent experimental observations. Particularly, we challenge the assumption that for large ensembles in the absence of any other interactions than topology the behavior of free polymers is recovered.

BP 19.7 Wed 19:00 PC 203

Conformations of zipped filaments — •Petra Gutjahr[1], Reinhard Lipowsky[1], and Jan Kierfeld[2] — [1]Max Planck Institute of Colloids and Interfaces, Theory & Bio-Systems, 14424 Potsdam, Germany — [2]Technical University of Dortmund, Theoretical Physics I, 44221 Dortmund, Germany

We study the zipping of two filaments with an attractive interaction and pinned filament ends based on experiments using microscopic pillar arrays. For the cases of weak and strong attraction between filaments, we analyze the influence of the filaments' stiffness and thermal fluctuations on the zipped equilibrium shape. Thereby we propose a scheme, by which the magnitude of the attraction between the filaments can be deduced from experimentally observed conformations. Our results should be applicable to actin filaments bundles induced by various crosslinker proteins and multivalent cations, but also to bundles formed by other types of semiflexible polymers.

BP 19.8 Wed 19:15 PC 203

Semiflexible chains in disordered media — •Abigail Klopper[1], Sebastian Schoebl[2], and Klaus Kroy[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Institut für Theoretische Physik, Universität Leipzig, Leipzig

Cellular function is intimately connected with the mechanical and dynamical properties of an underlying cytoskeletal structure, which can be described as a random network of stiff polymers. One attempt to understand this relationship involves determining how these properties are influenced by the conformational statistics of *single* polymers within the network. This calls for shrewd modeling of the polymers' immediate environment - capturing the spatial confinement caused by cellular crowding within a simplified theoretical framework. In this spirit, the problem may be recast in terms of a wormlike chain embedded within a matrix of quenched random obstacles. Despite the prolific attention paid to the analogous problem in flexible polymer networks in recent years, little is understood about how their stiffer counterparts respond to such an environment. This can be partly attributed to the difficulties encountered when stiffness and inextensibility criteria are imposed simultaneously with quenched disorder constraints. With the view to circumvent these problems, we use a weakly bending

rod formalism and employ replica theory to calculate disorder-averaged equilibrium properties of a stiff biopolymer in a quenched random environment.

BP 20: Regulation and Signaling

Time: Thursday 9:30–12:00 Location: C 243

Invited Talk BP 20.1 Thu 9:30 C 243

Modeling noisy concentration gradients inside single cells — Filipe Tostevin[1], Pieter ten Wolde[2], and •Martin Howard[1,3] — [1]Dept of Mathematics, Imperial College London, SW7 2AZ, UK — [2]AMOLF Institute, Amsterdam, The Netherlands — [3]Dept of Systems Biology, John Innes Centre, Norwich NR4 7UH, UK

Many biological systems require precise positional information to function correctly. Examples include positioning of the site of cell division and determination of cell fate during embryonic development. This positional information is often encoded in concentration gradients. A specific protein is produced only within a small region, and subsequently spreads into the surrounding space. This leads to a spatial concentration gradient, with the highest protein concentration near the source. By switching on a signal only where the local concentration is above a certain threshold, this gradient can provide positional information. However, intrinsic randomness in biochemical reactions will lead to unavoidable fluctuations in the concentration profile, which in turn will lead to fluctuations in the identified position. We therefore investigated how precisely a noisy concentration gradient can specify positional information. We found that time-averaging of concentration measurements potentially allows for great precision to be achieved even with remarkably low protein copy numbers. We have applied our results to a number of examples in cell biology, including positioning of the site of cell division in yeast.

Invited Talk BP 20.2 Thu 10:00 C 243

Non-equilibrium dynamics of gene expression — •Johannes Berg — Institute for Theoretical Physics, Cologne University, Zülpicher Str.77, 50937 Köln

The dynamics of gene expression is characterized by two key elements: (i) The transcription of genes is driven by transcription factor molecules. The number of transcription factors present in a cell changes constantly, keeping the system out of equilibrium. (ii) The transcription of a gene involves a small number of molecules, leading to a noisy dynamics marked by large fluctuations.

In this talk I discuss a simple mapping between models of gene expression and stochastic systems driven out of equilibrium. Using this mapping, results of nonequilibrium statistical mechanics such as the Jarzynski equality and the fluctuation theorem are demonstrated for gene expression dynamics. Applications of this non-equilibrium approach include the determination of mRNA degradation rates and regulatory interactions between genes from experimental gene expression data.

BP 20.3 Thu 10:30 C 243

Links between biochemistry and regulatory network design in a bacterial stress response system — •Georg Fritz[1], Christiane Koller[2], Korinna Burdack[2], Ulrich Gerland[1], and Kirsten Jung[2] — [1]Institute for Theoretical Physics, Universität zu Köln — [2]Department of Microbiology, LMU München

The evolutionary driving forces and constraints that have shaped the design of biomolecular networks are poorly understood in general. Here, we focus on a conditional stress response system, the Cad system of *E. coli*, which is triggered under acidic stress only if lysine is abundant externally. Through lysine import, decarboxylation, and cadaverine export, it effectively expels H^+ from the cytoplasm. A salient feature of the Cad system is that its expression is transient, even when the low-pH and high-lysine conditions for its induction persist. The transient behavior is believed to be caused by a negative feedback via external cadaverine.

We have experimentally recorded the dynamics of the Cad system with a high time resolution, and formulated a quantitative model for its function and regulation. Our analysis suggests that the system design is linked to the biochemical properties of a key system component, the antiporter CadB: Limited specificity of the antiporter causes a futile transport cycle at high external cadaverine levels. Interestingly, the external cadaverine threshold for the negative feedback appears quantitatively consistent with the specificity of the antiporter, suggesting that the regulatory feedback and the biochemistry of the antiporter are evolutionarily linked.

BP 20.4 Thu 10:45 C 243

Fluorescence cross-correlation spectroscopy measurements in vivo reveal the asymmetric incorporation of siRNAs into RISC and the localisation of the complex in human cells — Thomas Ohrt, •Wolfgang Staroske, Jörg Mütze, and Petra Schwille — Biophysics Group, BIOTEC/TU Dresden

Short double stranded RNA molecules have emerged as key regulators of gene expression, controlling developmental programs as well as functioning as a defence mechanism against viruses and transposons. Small RNAs use Argonaute-containing complexes called RNA-Induced Silencing Complex (RISC) to identify cognate RNA transcripts whose expression is to be silenced. By combining laser scanning microscopy, fluorescence correlation and cross-correlation spectroscopy (FCS/FCCS) and biochemical methods, we have exploited the interaction of short interfering RNAs with RISC in vivo. We established a functional and stable EGFP-Ago2 expressing 293 cell line, with expression levels suitable for FCS/FCCS. Using this in vivo system combined with highly sensitive FCS and FCCS it is possible to gain vast information on relative binding, concentration and mobility. Analysis of various microinjected fluorescently labelled siRNAs with FCCS showed the asymmetry dependent incorporation of the antisense strand into RISC over time in human cells. Measurements in various cell compartments showed the localisation of loaded RISC complex in human cells.

BP 20.5 Thu 11:00 C 243

Boolean Model of Fission Yeast Cell Cycle predicts mutations — •Maria Davidich and Stefan Bornholdt — Intitute for Theoretical Physics

A Boolean model [1] of the key regulators of the fission yeast cell cycle was built. The advantage of the model is that it is purely constructed on a wiring diagram of known biochemical reactions; no extra parameters enter the model. However, even though one needs much less information about the system, the model reproduces the right sequence of protein activity states during the cell cycle. This sequence appears to be robustly implemented in the regulatory network, its last state G1 corresponds to the biggest attractor of the system. Surprisingly, this simple model can also describe mutations of the regulatory proteins. We test the model starting from the different initial conditions corresponding to overexpression and underexpression of the proteins. The tests show that other attractors agree with mutations found in experiments.

[1] Davidich M.I., Bornholdt S. Boolean network predicts cell sequence of fission yeast. www.arhiv.org/abs/0704.2200 (Submitted to PLOS ONE)

BP 20.6 Thu 11:15 C 243

On the effect of transcription factor fluctuations at promoter logic gates — •Christian Fleck, Moritz Gerstung, and Jens Timmer — Institute of Physics, Hermann-Herder-Str. 3a, University of Freiburg, Germany

Biological organism constantly respond to changing cellular and environmental signals. These signals are integrated at cis-regulatory modules or promoter logic gates. Hence, the output causally depends on the degree of occupancy of the individual target sides within the cis-regulatory module. Because many TFs are present in low copy numbers per cell, the regulatory processes are inevitably subject to noise. A substantial preliminary for an understanding of how noise alters the output of promoter logic gates is knowledge about how fluctuations in TF abundance affect single operator occupancy. The inherent non-linearity arising from the bimolecular interaction impedes the analytical investigation of this phenomenon substantially. We present a detailed analysis of a TF-operator interaction finding noise correction terms to the macroscopic description. While the correction is always

negative for single binding sites, we discover more diverse effects on the logic gates comprising multiple binding sites.

BP 20.7 Thu 11:30 C 243

Compartment Model for IRE1 Signalling of the Unfolded Protein Response — •Ronny Straube — Department of Systems Biology, Max-Planck-Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg, Germany

In recent years it became apparent that sustained stress in the endoplasmic reticulum (ER) is related to the emergence of several neurodegenerative diseases such as Alzheimer, Parkinson and ALS as well as diabetes and drug resistance of tumor cells. ER stress is caused by the accumulation of unfolded proteins in the secretory pathway. This leads to the activation of an extensive transcriptional response called Unfolded Protein Response (UPR) to restore ER homeostasis. UPR signalling occurs via 3 distinct and temporarily ordered pathways mediated by PERK, ATF6 and IRE1. As a result, proapoptotic and prosurvival signal molecules are activated simultaneously. So far it is unclear how the cell integrates this information to decide in favour of one or the other. However, recent experiments show that sustained signalling via the IRE1 pathway of the UPR promotes cell survival. Here, I propose the first model of the IRE1 signalling pathway which is based on the known molecular details of the interaction network and which shows good agreement with published experimental data.

[1] Lin et. al. (2007), Science **318**, 944-949.

BP 20.8 Thu 11:45 C 243

Mechanisms of sperm chemotaxis — •Benjamin M. Friedrich and Frank Julicher — Max-Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, Dresden

Sperm cells swim towards the egg propelled by a flagellum which beats regularly. In many species sperm show chemotaxis, i.e. they move upwards a gradient of chemoattractant molecules released by the egg. Sperm cells sample the local chemoattractant concentrations with receptors on the surface of their flagellum. A signaling cascade within the flagellum transduces the concentration stimulus and elicits a swimming response by changing the flagellar beat [1,2]. We propose an effective description of this signaling cascade and derive consequences for experiments. In the limit of low chemoattractant concentrations, the concentration stimulus is Poissonian shot noise since the binding of chemoattractant molecules to the receptors is a discrete process. We therefore study also the influence of fluctuations in the concentration stimulus on the chemotaxis mechanism and derive measures for the fidelity of chemotaxis.

[1] B. Kaupp *et. al.*: NCB **5**, 109 (2003)
[2] B.M.F., F.J.: PNAS **109** (2007)

BP 21: Population Dynamics and Evolution

Time: Thursday 12:15–13:15 Location: C 243

BP 21.1 Thu 12:15 C 243

Clonal interference in large populations — •Su-Chan Park and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Köln, Germany

Clonal interference, the competition between lineages arising from different beneficial mutations in an asexually reproducing population, is an important factor determining the tempo and mode of microbial adaptation. The standard theory of this phenomenon neglects the occurrence of multiple mutations as well as the correlation between loss by genetic drift and clonal competition, which is questionable in large populations. Working within the Wright-Fisher model with multiplicative fitness (no epistasis), we determine the rate of adaptation asymptotically for very large population sizes and show that the standard theory fails in this regime. Our study also explains the success of the standard theory in predicting the rate of adaptation for moderately large populations. Furthermore we show that the nature of the substitution process changes qualitatively when multiple mutations are allowed for, since several mutations can be fixed in a single fixation event. As a consequence, the index of dispersion for counts of the fixation process displays a minimum as a function of population size, while the origination process of fixed mutations becomes completely regular for very large populations. We find that the number of mutations fixed in a single event is geometrically distributed as in the neutral case.

Reference: S.-C. Park and J. Krug, PNAS 104, 18135 (2007).

BP 21.2 Thu 12:30 C 243

Stability of food webs with structured populations — •Christian Guill and Barbara Drossel — TU Darmstadt, Institute of Condensed Matter Physics, Hochschulstraße 6, D-64289 Darmstadt

Most existing models of population dynamics in food webs treat species as homogeneous aggregations of identical individuals. They neglect the fact that not all individuals of a species are reproducing, but are juveniles that invest their energy intake into growth in body size. Here, we investigate model food webs with populations that are structured in terms of physiological state (juvenile/adult). Each stage of a species has its own feeding relationships and population dynamics, but the stages are coupled through maturation and reproduction. This leads to time-dependent traits of the species as a whole, such as its mean body size. Since body size is a key factor in determining predation behaviour and also influences metabolic rates, structuring of populations changes the population dynamics and stability of the entire network. Simulation results obtained from networks with structured populations are compared to networks with unstructured populations.

The population dynamics in ecosystems with structured populations are studied in more detail in the example of a real aquatic system consisting of a homogeneous resource (zooplankton), two consumers (salmon species), and a top predator (trout) with structured populations. Simulation results are tested against empirical data of the system.

BP 21.3 Thu 12:45 C 243

Cyclic dominance and biodiversity in well-mixed populations — •Jens Christian Claussen[1] and Arne Traulsen[2] — [1]Institut für Theoretische Physik u. Astrophysik, Christian-Albrecht Universität Kiel — [2]Max-Planck-Institut für Evolutionsbiologie, 24306 Plön

Coevolutionary dynamics is investigated in chemical catalysis, biological evolution, social and economic systems. The dynamics of these systems can be analyzed within the unifying framework of evolutionary game theory. Here, we show that even in well-mixed finite populations, where the dynamics is inherently stochastic, biodiversity is possible with three cyclic dominant strategies. We show how the interplay of evolutionary dynamics, discreteness of the population, and the nature of the interactions influences the coexistence of strategies. We calculate a critical population size above which coexistence is likely.

BP 21.4 Thu 13:00 C 243

Protein Thermodynamics and Population Dynamics — •Miriam Fritsche[1], Andreas Buhr[1], Ugo Bastolla[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany — [2]Centro de Biología Molecular 'Severo Ochoa', Campus UAM, Cantoblanco, 28049 Madrid, Spain

When investigating proteins one has to take into account both the physical constraints on folding stability and the biological constraints on their evolution, being the driving force of nature [1]. Based on previous work [2] we investigate thermodynamical properties of proteins during evolution applying a model which consists of mutations as well as purifying selection. In addition to the explicit consideration of thermodynamic stability, we account for the effect of mutational and translational load in the evolutionary process, therewith sheding light on the impact the spectrum of mutations has on natural selection. Investigating the interplay between protein thermodynamics, population dynamics as well as genomic features we are able to better understand several properties of proteins as well as their evolution, for instance, the existence of a strong mutation bias in the genome of intracellular bacteria.

[1] *Structural Approaches to Sequence Evolution*, U. Bastolla, M. Porto, H.E. Roman and M. Vendruscolo, ed., Springer, Berlin, 2007
[2] U. Bastolla, M. Porto, H.E. Roman and M. Vendruscolo, Phys. Rev. Lett. **89**, 208101 (2002); J. Mol. Evol. **56**, 243 (2003); Proteins **58**, 22 (2005); Mol. Biol. Evol. **22**, 630 (2005); BMC Evol. Biol. **6**, 43 (2006)

BP 22: Cell Mechanics

Time: Thursday 10:30–11:45 Location: PC 203

BP 22.1 Thu 10:30 PC 203

Shear Rheology of a Cell Monolayer — Pablo Fernandez[1], Lutz Heymann[2], •Benjamin Tränkle[3], Albrecht Ott[3,4], Nuri Aksel[2], and Pramod Pullarkat[5] — [1]E22 Biophysik, Technische Universität München, D-85748 Garching — [2]Technische Mechanik und Strömungsmechanik, Universität Bayreuth, D-95440 Bayreuth — [3]Experimentalphysik I, Universität Bayreuth, D-95440 Bayreuth — [4]Biologische Experimentalphysik, Universität des Saarlandes, D-66041 Saarbrücken — [5]on leave from Experimentalphysik I, Universität Bayreuth, D-95440 Bayreuth

We report a systematic investigation of the mechanical properties of fibroblast cells using a novel Cell Monolayer Rheology (CMR) technique. The new technique provides quantitative rheological parameters averaged over $\sim 10^6$ cells, making the experiments highly reproducible. Using this method, we are able to explore a broad range of cell responses not accessible using other present day techniques. Within the explored strain rates (10^{-3}–$1\,s^{-1}$) and strain amplitudes (1%–100%), nonlinear behaviour is only revealed by the effect of a nonzero average stress on the response to small, fast deformations. The response becomes linear at long timescales as well as large amplitudes. This counterintuitive linear behaviour is due to the dynamic nature of the cell cytoskeletal crosslinks and/or filaments, since it can be abolished by making them permanent with a fixation agent. These experiments provide a broad framework for understanding the mechanical responses of the cytoskeleton to different imposed mechanical stimuli.

BP 22.2 Thu 10:45 PC 203

Manipulation of stretch-activated calcium channels with the optical stretcher — •Markus Gyger and J. A. Käs — Universität Leipzig, Institut für Experimentelle Physik I, Linnéstr. 5, 04103 Leipzig

Cellular response to deforming forces can be measured with the optical stretcher. Cells are trapped by two anti-parallel laser beams. By increasing the laser power the momentum transfered to the cell surface causes visible deformations. This can be used to probe the global mechanical behaviour of single cells in suspension. For low stresses and small deformations most of the cells deform viscoelasticly. However, for higher stretching powers the cells start to counteract the deformations. Sometimes this active response to deformation results in a contraction of the cell relative to its initial, undeformed state. This raises interesting questions regarding the mechanisms by which cells register and respond to the applied forces. Under physiological conditions many must react to mechanical stimuli. As a prominent example, hair-cells in the Cochlea of vertebrate ears are known to open transmembrane calcium channels upon mechanical stresses. Calcium is one of the most important secondary messengers and is involved in most of the known mechano-activated cell responses. Since its normal concentration in the cell soma is very low and increases only by influx from outside the cell or release from intracellular calcium stores upon stimulus, the influx can be made visible by appropriate fluorescent dyes. The aim of this 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 22.3 Thu 11:00 PC 203

Dynamic states of rolling adhesion: dependance on rates for formation and rupture of molecular bonds — •Christian B. Korn and Ulrich S. Schwarz — University of Heidelberg, Im Neuenheimer Feld 267, D-69120 Heidelberg, Germany

Motivated by rolling adhesion of white blood cells in the vasculature, we study how cells move in linear shear flow above a wall to which they can adhere via specific receptor-ligand bonds. We perform computer simulations based on a Langevin equation accounting for hydrodynamic interactions, thermal fluctuations and adhesive interactions. In contrast to earlier approaches, we resolve both receptor and ligand positions. We identify five different dynamic states of motion in regard to the translational and angular velocities of the cell. We express these states in a state diagram for the parameter subspace spanned by the dynamic rates for bond formation and rupture. In particular, we show that if on- and off-rates are sufficiently balanced the cell's translational and angular velocities become sychronized. This corresponds to rolling in a macroscopic sense while otherwise the cell is slipping.

In order to analyze the generic interplay between bond formation and rupture, we also define and analytically solve a simple model system based on a one-step master equation. The analytical results show qualitative agreement with the mean velocity data obtained from the computer simulations.

BP 22.4 Thu 11:15 PC 203

Stress relaxation, stiffening and fluidization of adherent cells — •Philip Kollmannsberger and Ben Fabry — Physics Department, University Erlangen-Nuremberg, Henkestr. 91, 91052 Erlangen

The linear rheology of adherent cells is characterized by a wide distribution of relaxation times, as seen by a creep or stress relaxation response that follows a weak power law over several time decades. However, stress relaxation of living cells in the non-linear range where stress stiffening occurs has been poorly characterized and are not well understood. We used a magnetic tweezer setup with real-time force control to apply forces of more than 20 nN to beads bound to the cytoskeleton of adherent cells. Deformations in response to stepwise increasing and repeated force application were analyzed using a nonlinear superposition model that allowed us to dissect stress relaxation processes from stiffening responses. Results show that the creep modulus becomes nonlinear and decreases with increasing force. In addition, stresses relaxed in most beads according to a power-law in time with a slope between 0.2 and 0.3 independent of the stress magnitude. Force-induced fluidization and yielding leads to an increase in the power-law exponent. This was indicative either of a disruption of the beads when the force was further increased, or of a substantial plastic deformation after the force was removed. We interpret our results in terms of a model where dynamic stability and turnover of molecular interactions carrying the mechanical stress are determined by an energy landscape with a wide distribution of energy well depths and associated trap stiffnesses.

BP 22.5 Thu 11:30 PC 203

The use of scanning probe techniques and laser micromanipulation to isolate and mechanostimulate highly potent adult mesenchymal stem cells — •Karla Müller[1], Matthias Zscharnack[2], Jörg Galle[3], and Josef Käs[1] — [1]Inst. for Soft Matter Physics, University of Leipzig — [2]Applied Stem Cell Biology, Center for Biotechnology and Biomedicine, University of Leipzig — [3]Interdiciplinary Centre for Bioinfomatics, University of Leipzig

Degenerative joint diseases due to rheumatism, joint dysplasia or traumata are particularly widespread in countries with high life expectancies. Today hyaline cartilage and bone defects resulting from joint destruction can be treated by appropriate transplantations from (and thereby destroying) intact joint areas. An alternative approach is the use of adult mesenchymal stem cells. These cells have the potential to differentiate into various cell types, such as osteoblast-like cells and chondrocyte-like cells. The aim of MS CartPro is to develop a closed, aseptic bioreactor for the production of autologous grafts for cartilage regeneration. We establish the sorting of most potent cells out of a heterogeneous cell sample by exploring the phase space of viscoelastic properties and relating these to the individual cells ability to differentiate into the desired tissue type. In order to non-invasively probe the mechanical properties of suspended cells, the Optical Stretcher is a highly adequate tool. Mechanostimulation is achieved by indenting adherent stem cells with a modified AFM tip in order to push them towards a chondrocyte like differentiation.

BP 23: Electrical Stimulation and Recording

Time: Thursday 12:00–13:15 Location: PC 203

BP 23.1 Thu 12:00 PC 203

Study of neural cells on organic semiconductor ultra thin films — •Eva Bystrenova[1], Ilaria Tonazzini[1], Pablo Stoliar[1], Pierpaolo Greco[1], Marta Jelitai[2], Adina Lazar[1], Martin Huth[3], Soumya Dutta[1], Chiara Dionigi[1], Marcello Cacace[1], Bert Nickel[3], Emilia Madarasz[2], Claudia Martini[4], and Fabio Biscarini[1] — [1]ISMN-CNR, Bologna, Italy — [2]IEM- HAS, Budapest, Hungary — [3]LMU, Munich, Germany — [4]Dept. PNPB, Univ. of Pisa, Italy

Many technological advances are currently being developed for nanofabrication, offering the ability to create and control patterns of soft materials. We report the deposition of cells on organic semiconductor ultra-thin films. This is a first step towards the development of active bio/non bio systems for electrical transduction. Thin films of pentacene, whose thickness was systematically varied, were grown by high vacuum sublimation. We report adhesion, growth, and differentiation of human astroglial cells and mouse neural stem cells on an organic semiconductor. Viability of astroglial cells in time was measured as a function of the roughness and the characteristic morphology of ultra thin organic film, as well as the features of the patterned molecules. Optical fluorescence microscope coupled to atomic force microscope was used to monitor the presence, density and shape of deposited cells. Neural stem cells remain viable, differentiate by retinoic acid and form dense neuronal networks. We have shown the possibility to integrate living neural cells on organic semiconductor thin films. Project EU-NMP-STRP 032652 BIODOT.

BP 23.2 Thu 12:15 PC 203

Very high-k oxide dielectric on silicon chip for capacitive stimulation of nerve cells — •Biljana Mesic and Herbert Schroeder — IEM im Institut für Festkörperforschung und CNI, Forschungszentrum Jülich GmbH, D-52425 Jülich

Thin insulating films of the perovskite-type mixed-oxides such as (Ba,Sr)TiO3 or SrTiO3 have very large dielectric constants of k>200. Compared to the materials presently used for capacitive stimulation of nerve cells directly on silicon chips such as TiO2 or HfO2 with about k=40, such enlarged capacitance would allow increased stimulation. We have fabricated an electrode stack directly on a conducting, highly doped silicon wafer. Due to the conductive diffusion barrier layer included in the stack it is stable up to 600°C, which then allows high temperature deposition of perovskite-type mixed-oxides with very high dielectric constants up to k=450.

In this contribution we report the fabrication of the thin film electrode stack on the silicon chip which then was used as bottom electrode for a capacitor with thin film oxide dielectric (BST) and platinum top electrodes. Detailed electrical characterization (capacitance, leakage current) is also presented proving the desired properties.

BP 23.3 Thu 12:30 PC 203

Neuronal cells on GaN-based materials — •H. Witte[1], M. Charpentier[1], M. Mueller[1], T. Voigt[2], M. Deliano[3], B. Garke[1], P. Veit[1], T. Hempel[1], A. Diez[1], A. Reiher[1], F. Ohl[3], A. Dadgar[1], J. Christen[1], and A. Krost[1] — [1]Inst. of Experimental Physics, Otto-von-Guericke-University Magdeburg, Magdeburg — [2]Inst. of Physiology, Otto-von-Guericke-University Magdeburg, Magdeburg — [3]Leibniz Institute of Neurobiology, Magdeburg

Group-III-nitride-based devices can be used for recording electrical activities of cell signals using the main advantage of high chemical and physiological stability. However, for the application of these materials in neural tissue their biocompatibility should be proofed. We have investigated the interactions between group-III-semiconductors and (1) dissociated neuron networks of embryonic rat cerebral cortex, and (2) neurons within the primary auditory cortex of Mongolian gerbils (rodents). The neuron networks were cultured within more than two days on the surfaces of GaN, AlGaN, AlN and GaO/GaN layers and were analyzed using optical and electron microscopy. In addition, pieces of nitrides were implanted into the cortex of living gerbils and remained there for several months. The reactions of the ambient neuron tissue were investigated by histological methods. Furthermore, the impact of the neuron cell cultures on the substrate surfaces were analyzed using atomic force microscopy and X-ray photoelectron spectroscopy. All investigations showed the stability and the non-toxic behavior of the pure GaN layers whereas the Al-containing layers were somewhat affected.

BP 23.4 Thu 12:45 PC 203

Realisierung von GaN FET-Arrays zur ortsaufgelösten Messung von elektrochemischen Potentialen in flüssigen Medien — •Mathias Müller[1], Jürgen Bläsing[1], Thomas Hempel[1], Michael Charpentier[1], Oliver Schulz[2], Antje Reiher[2], Hartmut Witte[1], Armin Dadgar[1,2], Jürgen Christen[1] und Alois Krost[1,2] — [1]Otto-von-Guericke-Universität, Magdeburg — [2]AZZURRO Semiconductors AG, Universitätsplatz 2, 39106 Magdeburg

GaN, AlGaN und AlN, als chemisch weitgehend inerte Halbleiter, sind hervorragend geeignet zur Analyse systemspezifischer Parameter in chemisch reaktiven Lösungen. Da für viele chemische Reaktionen der pH-Wert von großer Bedeutung ist, wird dieser mit Hilfe von GaN/AlGaN/GaN FET-Arrays ortsaufgelöst bestimmt. Bei diesen Bauelementen wirkt das elektrochemische Potential der Elektrolytlösung als Gate. Um die mittels MOVPE auf Saphir-Substraten abgeschiedenen FETs prozessieren zu können, muss ein Lithographiemasken-Layout für die FET-Arrays entwickelt werden. Die Sensorgrößen und -abstände werden dabei so gewählt, dass in verschiedenen Lösungen Änderungen des chemischen Potentials analysiert werden können. Die Güte der GaN/AlGaN/GaN-Struktur wird dabei durch Röntgendiffraktometrie, Hall-Effekt-Messungen und C-V-Messungen an den zu prozessierenden Wafern bestimmt. Die Abhängigkeit des Source-Drain-Stromes vom pH-Wert wird am Beispiel einer Titrierung mit 100 mMol NaCl / 10 mMol Hepes Lösung demonstriert. Dabei wird der pH-Wert mit verdünnter NaOH oder HCl eingestellt.

BP 23.5 Thu 13:00 PC 203

Einfluss des Substratmaterials auf die dielektrischen Übertragungs-eigenschaften planarer Multielektrodenanordnungen in Zellnetzwerke — •M. Charpentier, M. Müller, H. Witte, A. Dadgar und A. Krost — Institute of Experimental Physics, University of Magdeburg, 39016 Magdeburg

Planare Mehr-Elektrodenanordnungen sind weit verbreitet für Anwendungen zum Anregen und Auslesen von neuronalen Netzwerken. Hierfür werden vorrangig Metallelektroden oder auf Silizium-Bauelementen basierende Strukturen verwendet. Als alternative Materialien werden aber auch Gruppe-III-Nitride angewendet, da sie chemisch und biologisch sehr resistent sind. Aus diesem Grunde haben wir den Einfluss von GaN, AlGaN und AlN als Substrat von planaren Elektrodenstrukuren auf die dielektrischen Übertragungseigenschaften elektrischer Signale von den Elektroden in die Zellkulturlösungen untersucht. Neben den Einzelschichten wurden auch High Electron Mobility Transistor (HEMT) -Strukturen genutzt und mit verschiedenen Elektrolytlösungen mit variierenden pH-Werten und Leitfähigkeiten benetzt und dielektrisch charakterisiert. Dies geschah durch frequenzabhängige Widerstands- und Kapazitätsmessungen im Frequenzbereich 20Hz....1MHz in einer Dreielektrodenanordnung. An Elektrolyt / HEMT-Strukturen wurden auch Hall-Effektmessungen durchgeführt, um den Einfluss des Elektrolyten auf die Ladungsträgerkonzentration im 2D-EG zu analysieren. Mit diesen Untersuchungen ist es möglich, den Einfluss des Substrates in entsprechenden Ersatzschaltbildern genauer zu spezifizieren.

BP 24: Actin Dynamics

Time: Thursday 14:00–16:45 Location: C 243

Invited Talk BP 24.1 Thu 14:00 C 243

A biochemical reconstitution approach of the coordinated actin assembly dynamics in motile and morphogenetic processes. — •Marie-France Carlier, Louis Renault, Guillaume Romet-Lemonne, Emmanuele Helfer, Beata Bugyi, Kim Ho Diep Le, Dominique Didry, and Stéphane Romero — CNRS, Gif-sur-Yvette, France

In living cells, the actin cytoskeleton is composed of polar actin filaments that are assembled at a steady state in well organized arrays, and co-exist with a pool of monomeric actin. Filaments turnover via a treadmilling mechanism, in which the pool of polymerizable monomeric ATP-actin, generated by pointed end depolymerization of all filaments in these arrays, drives the growth of filament barbed ends. Filament barbed end growth is also controlled by machineries that link signalling to the actin cytoskeleton. We are interested in understanding the physical chemical principles underlying the coordinated turnover of actin filaments in these different meshworks and their synergetic action in motility and porphogenetic processes. For this we propose a systemic biology approach. I will show a few examples as follows. In vitro reconstitution assays of actin-based propulsion of N-WASP-functionalized beads or liposomes illustrate the role of the interplay between membrane and cytoskeleton dynamics in directional movement ; reconstitution of the rapid processive assembly of filaments profilin-actin by immobilized formins mimicks filopodia extension ; reconstitution of the synergy between Spire and formin suggests a possible functional basis of the genetic interplay between these two proteins in embryogenesis.

BP 24.2 Thu 14:30 C 243

Protrusion force generation of fish keratocytes — •Claudia Brunner, Michael Gögler, Allen Ehrlicher, Bernd Kohlstrunk, and Josef Käs — University of Leipzig

Cell motilitiy is a fundamental process associated with many phenomena in nature, such as immune response, wound healing, and metastasis.On the molecular level, actin polymerization and molecular motors, are involved in cell motility but the mechanism as a whole is not very well understood. Rapidly migrating cells, such as keratocytes, move forward through active protrusion at the leading edge, and retraction/deadhesion of the cells rear, indicating two force generating centers.

Our SFM-based technique uses the vertical and lateral deflection of a modified cantilever and allows direct measurements of the forces exerted by the cell. We present direct measurements of the forward forces generated at the leading edge of the lamellipodium, the cell body and retrograde forces within the lamellipodium. Through selective manipulation of molecular components by addition of different drugs, such as Jasplakinolide, Cytochalasin D, and ML-7 the measured forces and velocity changes can be compared. This leads to new insights concerning the importance of different force generating processes and reveals actin polymerization as the dominant force generating process at the leading edge. On the other hand myosin does not seem to be responsible for the retrograde flow.

BP 24.3 Thu 14:45 C 243

Actin polymerization and ATP hydrolysis kinetics — •Xin Li[1], Jan Kierfeld[1,2], and Reinhard Lipowsky[1] — [1]MPI of Colloids and Interfaces, Science Park Golm, 14424 Potsdam — [2]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik I, 44221 Dortmund

Actin polymerization plays an important role in many aspects of cell dynamics. This active process involves the hydrolysis of ATP molecules, which takes place within an ATP-rich cap and can be spatially separated from the assembly process. In this study, we theoretically compare different mechanism for the coupling between ATP hydrolysis and actin polymerization and describe their effects on experimentally observable quantities, such as cap length, total hydrolysis rate, and actin filament growth rate.

BP 24.4 Thu 15:00 C 243

Actin flow and cellular traction at focal adhesions: measurements and theoretical interpretation — •Benedikt Sabass[1], Margaret Gardel[2], Clare Waterman[3], and Ulrich Schwarz[1] — [1]University of Heidelberg, BQ 0013, Im Neuenheimer Feld 267, D-69120 Heidelberg, Germany — [2]University of Chicago, IL, USA — [3]NIH, Bethesda, MD, USA

The dynamic nature of cell-substrate contacts (focal adhesions) is an essential ingredient of the communication between cells and their environment. In particular the intracellular motion of actin flow and its connection to external cellular traction seems to be crucial for cellular decision making at focal adhesions. We have developed a novel assay to simultaneously measure retrograde actin flow and cellular traction force with high spatial resolution. The resulting data demonstrates a biphasic relationship between actin speed and traction. Moreover, we find that maximum traction is always exerted at a speed level which is independent of biochemical perturbations. This suggests the existence of a robust sensory mechanism relating internal flow dynamics to traction in the environment. We also discuss physical models for bond dynamics which are able to explain the experimentally found data.

15 min. break

BP 24.5 Thu 15:30 C 243

Actin dynamics in SCAR-deficient cells — Hellen Ishikawa-Ankerhold[1], Till Bretschneider[1], Günther Gerisch[1], Annette Müller-Taubenberger[1,2], Robert Insall[3], Eberhard Bodenschatz[4], and •Carsten Beta[5,4] — [1]MPI für Biochemie, Martinsried, Germany — [2]Institut für Zellbiologie, LMU München, Germany — [3]School of Biosciences, University of Birmingham, UK — [4]MPI fuer Dynamik und Selbstorg., Goettingen, Germany — [5]Institut fuer Physik, Universitaet Potsdam, Germany

The dynamical properties of the actin cytoskeleton provide the basis for motility, phagocytosis, and division of eukaryotic cells. Directed polymerization of actin in the cell cortex has been identified as the underlying source of force generation. A key player in the formation of a dense cortical actin network is the seven-subunit Arp2/3 complex that initiates the nucleation of branches on existing filaments. Its activity is controlled by SCAR/WAVE proteins of the WASp (Wiscott-Aldrich Syndrome protein) family that are downstream effectors of receptor-mediated signalling pathways. Here we analyze the temporal patterns of actin polymerization in the cortex of mutant cells lacking members of the pentameric SCAR complex. The results highlight the actin machinery as a self-organizing system that can be described by the concepts of non-equilibrium dynamics. We furthermore report evidence that the cortical dynamics is linked to the chemosensory pathway, so that receptor signals are transmitted to the actin system, even if SCAR is missing.

BP 24.6 Thu 15:45 C 243

A microscopic description of actin-based propulsion of beads — •azam gholami[1], martin falcke[1], and erwin frey[2] — [1]Hahn-Meitner-Institute, Dept. Theoretical Physics, GlienickerStr. 100, 14109 Berlin, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics and Center of NanoScience, Ludwig-Maximilians-Universität, Theresienstr. 37, 80333 München, Germany

Beads propelled by actin polymerization have been widely used as a model system for Arp2/3 dependent actin-based movement. VCA-grafted beads were shown to exhibit the same characteristic motion as the pathogen Listeria monocytogenes. All existing microscopic models, such as the elastic Brownian ratchet model do not explicitly consider geometry, such as the size of object or the curvature. Here, we generalize our simple model of actin-based motility to include the curvature of the obstacle. We find that small and large beads move approximately at the same speed which is different from the tethered ratchet model which predicts faster movement with larger beads.

BP 24.7 Thu 16:00 C 243

Measurement of Force by Actin Gel Polymerization: A Combined AFM and Epifluorescence Study — •Stephan Schmidt[1], Pia Zissman[1], Walter Zimmermann[1], Emmanuèle Helfer[2], Marie-France Carlier[2], and Andreas Fery[1] — [1]Universität Bayreuth, Germany — [2]CNRS-LEBS, Gif-sur-Yvette, France

The ability to generate forces and move actively is one of the key features of micro-organisms and nature has found various pathways to accomplish it. In processes associated with active movement of eukaryotic cells and some bacteria such as Listeria monocytogenes force generation is driven by actin filament growth against the membrane. The

biochemistry of the involved processes are well understood, whereas the molecular scale mechanism of force generation is still matter of debate. We use a simplified in vitro assay composed of purified proteins and artificial colloids. Force measurements on actin networks are performed using colloidal probe AFM techniques, were the growing actin network is clamped between an AFM spring and a solid substrate. Using fluorescence microscopy we observe the gel extension in direct conjunction with the AFM measurement. Results suggest that force stalling is due to buckling and (induced) symmetry breaking at the stressed site of the gel. By changing the composition of the medium we vary the actin density and use different probes to control the size of the gel. In these experiments, the amount of force generated can be well explained by the size and density of the polymerizing network. Further we show experiments and theory concerning confinement effects on symmetry breaking of actin gels.

BP 24.8 Thu 16:15 C 243

Physical principles of self-organized cell locomotion — •Konstantin Doubrovinski — Universität des Saarlandes, Geb E26, Postfach 151150, 66041 Saarbrücken

Experiments on crawling cell fragments of fish keratocytes indicate that cell locomotion can emerge from self-organization of the cytoskeleton. The underlying physical mechaism, however, is still poorly understood. Recent experiments on human neutrophils, which are the most abundant white blood cells, indicate that intracellular spiral waves of the protein HEM, which regulates actin polymerization are essential for driving membrane portrusions at the leading edge [1]. We propose a physical description of spiral waves in human neutrophils, based on experimental findings. A key element of our description is the treatment of interactions between the cytoskeleton and the membrane through a phase-field. In addition to persistent uni-directional locomotion, we find that the system can self-organize into polymerization waves lateral to the membrane. Such waves have been observed in spreading cells [2] and indicate a common mechanism of cell locomotion and spreading.

[1] Weiner et. al. (2007) PLoS Biol 5 e221
[2] Doebereiner et. al. (2006) Phys. Rev. Lett. 97 038102

BP 24.9 Thu 16:30 C 243

Modeling and Mimicking Lamellipodial Actin Network Growth — •Florian Huber, Björn Stuhrmann, and Josef Käs — Institute for Soft Matter Physics, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Most cells are able to perform directed migration, which is of enormous relevance for many different biological systems and indispensable for multicellular organisms. Typically the cell migrates by formation of lamellipodial structures, i.e. a thin active actin network. Its formation and appearance is regulated by various actin related proteins.

The key molecular players involved in these processes have been identified and have already been used to generate *in vitro* actin network growth. The required next step towards reproducing cellular conditions is to confine the polymerizing actin gel in sub-micron sized structures. These structures are obtained with a combination of several microfabrication techniques that also allow selective functionalization with the polymerization inducing peptide VCA. We use fluorescence microscopy to visualize the emerging actin network. Speckle microscopy will be applied to further analyze its properties.

For the first time we operate with a restricted protein pool that allows to mimic the self-sustaining character of the lamellipodial machinery. Moreover, we directly link experiment to Monte-Carlo simulation and mathematical modeling. All three approaches allow controlled variation of various biochemical and physical parameters in order to better understand the complex interplay between the essential cytoskeletal proteins.

BP 25: Protein Structure and Folding

Time: Thursday 14:30–17:00 Location: PC 203

BP 25.1 Thu 14:30 PC 203

Transition states in protein folding — •Thomas Weikl — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Abteilung Theorie und Bio-Systeme, Wissenschaftspark Golm, 14424 Potsdam

Conformational transitions of proteins are often apparent two-state processes. Examples are the folding and unfolding of small single-domain proteins, or the opening and closing of ion channels. The dynamics of two-state processes is thought to be governed by a transition-state barrier between the two states. Transition states are short-lived and cannot be observed directly in experiments. However, a mutational analysis of the two-state dynamics can provide indirect access. In a mutational analysis, experimentalists measure the effect of point mutations on the folding and unfolding rates of small proteins, or the opening and closing rates of ion channels. I will present models that help to reconstruct folding transition states from mutational data. The models are based on identifying cooperative substructural elements of proteins, and on calculating mutation-induced free-energy changes for these elements.

References:

[1] C. Merlo, K. A. Dill, and T. R. Weikl, PNAS 102, 10171 (2005).
[2] T. R. Weikl and K. A. Dill, J. Mol. Biol. 365, 1578 (2007).
[3] T. R. Weikl, Biophys. J., in press (2008).

BP 25.2 Thu 14:45 PC 203

Algorithm for selection of fast folding proteins — •Dmitry Gridnev and Martin Garcia — Kassel University, Heinrich-Plett-Str. 40, Germany

We discuss the following problem: from a large number of given amino acid chains select potentially good folders. In the framework of the lattice model of proteins we propose an algorithm, which uses the Monte Carlo dynamics and tests the rate of convergence of an amino acid chain in the configuration space. To test this algorithm we have hidden one known good folder among one thousand of other chains with a random amino acid decomposition. Our results show that the designed good folding sequence comes on top in the list of folders from good to bad. We also discuss how this method could be generalized to more sophisticated atomistic models.

BP 25.3 Thu 15:00 PC 203

Relation of Evolutionary Dynamics to Molecular Mechanics — •Kay Hamacher — Bioinformatics & Theo. Biology Group, Dept. of Biology, Technische Universität Darmstadt, Schnittspahnstr. 10, 64287 Darmstadt, Germany

We investigate the connection between sequence evolution under selective pressure induced by drugs and the functional and molecular-stability characteristics of a protein.

To this end we analyze sequence data of the human immunodeficiency virus (HIV) type 1 protease for more than 45,000 patients. We then formulate a chemo-physical-model for the stability and the functional modes of the protease and correlate the findings on the sequence evolutionary dynamics to extensive *in-silico*-mutagensis studies performed with this chemo-physical-model. First we derive a physical explanation for the particular important mutation V82F-I84V.

In a second step we discuss interactions in the β-sheet dimerization interface to be most important for maintaining function and stability of the protease. These interactions are at the same time evolutionary conserved - implications of and comparisons to experimental and other theoretical results are finally discussed.

BP 25.4 Thu 15:15 PC 203

Thermodynamics and kinetics of a protein-like heteropolymer model with two-state folding characteristics — Anna Kallias, •Michael Bachmann, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, D-04009 Leipzig

We present results of Monte Carlo computer simulations of a coarse-grained hydrophobic-polar Gō-like heteropolymer model and discuss thermodynamic properties and kinetics of an exemplified heteropolymer, exhibiting two-state folding behavior [1]. We find that thermodynamic and kinetic properties as, for example, the folding temperature within this model, are quantitatively consistent. It turns out that general, characteristic folding features of realistic proteins with a single free-energy barrier can also be observed in this simplified model, where the folding transition is primarily driven by the hydrophobic force. As further recent results [2], our study shows that characteristic features

of protein folding are intrinsic properties of heteropolymers and thus even observable on mesoscopic scales.

[1] A. Kallias, M. Bachmann, and W. Janke, J. Chem. Phys., in print (2007).

[2] S. Schnabel, M. Bachmann, and W. Janke, Phys. Rev. Lett. **98**, 048103 (2007).

BP 25.5 Thu 15:30 PC 203

Insights from atomistic computer simulations of halophilic proteins — •Joachim Dzubiella — Physics Department, Technical University Munich, Germany

Halophilic (salt-loving) proteins, typically found in Archaea, can maintain their native structure and function in aqueous environment only at relatively high salt concentrations (>1-2M). As they are highly negatively charged at physiological conditions the competition between hydrophobic and hydrophilic solvation is strongly amplified and tuned by salt type and concentration. By performing atomistic molecular dynamics (MD) computer simulations the influence of salt on effective interactions between amino acids, protein secondary structures, and the stability of small coiled-coil proteins is investigated. Possible salt-induced specific and non-specific (de)stabilization mechanisms are identified and critically discussed.

BP 25.6 Thu 15:45 PC 203

Molecular machines involving electron tunneling — •Igor Goychuk — Institut für Physik, Universität Augsburg, Germany

ATP-driven molecular machinery of living cells involves various molecular motors operating far from the thermodynamic equilibrium. They are generally believed to be essentially classical nanoengines. Nitrogenase molecular machines present, however, a clear counter-example because of the long-range electron tunneling involved in the overall reaction of nitrogen fixation (ammonia production) which these enzymes perform: the energy derived from ATP hydrolysis is used to pump electrons into the nitrogenase reaction center. The theory of quantum dissipative dynamics driven by non-equilibrium fluctuations [1] presents a general theoretical framework for such and similar electron tunneling pumps. I will discuss a tentative mechanism [2,3] based on the stochastically driven spin-boson model [4] and general principles of the free energy transduction in biology [5].

[1] I. Goychuk, P. Hänggi, Adv. Phys. **54**, 525 (2005), and references therein.

[2] I. V. Kurnikov, A. K. Charnley, D. N. Beratan, J. Phys. Chem. B, **105**, 5359 (2001).

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[5]T.L. Hill, Free Energy Transduction in Biology (Academic Press, New York, 1977).

BP 25.7 Thu 16:00 PC 203

Protein structure prediction using structure profiles — •Katrin Wolff[1], Andrea Cavalli[2], Harri Hopeauroho[2], Michele Vendruscolo[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Department of Chemistry, University of Cambridge, UK

Protein structure predictors using knowledge-based energy functions and homology modelling have faced huge progress over the last few years whilst still allowing for further improvement. Here, we investigate the possibility to improve an existing predictor by incorporating information from structure profiles. A specific class of such profiles can be used to reconstruct the protein structure's contact matrix [1], from which the three-dimensional structure can be efficiently recovered [2]. Such profiles can be predicted to good accuracy from sequence (see e.g. [3]). It therefore seems promising to include profile information into existing predictors. Using the program collection 'almost' [4] we perform a series of prediction steps consisting of Monte Carlo-minimization with fragment insertion, filtering by the structure profile's cost function and subsequent refinement of predicted structures. We compare conventionally predicted structures to those including the structure profile as an additional input for several known protein structures and show that RMSDs to the target structure significantly decrease.

[1] M. Porto *et al.*, Phys. Rev. Lett. **92**, 218101 (2004).

[2] M. Vendruscolo *et al.*, Fold. & Des. **2**, 295 (1997).

[3] A. R. Kinjo *et al.*, BMC Bioinformatics **7**, 401 (2006).

[4] A. Cavalli *et al.*, Proc. Nat. Acad. Sci. **104**, 9615 (2007)

BP 25.8 Thu 16:15 PC 203

Global Dynamics of Yeast Alcohol Dehydrogenase — •Biehl Ralf[1], Hoffmann Bernd[2], Fallus Peter[3], Monkenbusch Michael[1], Merkel Rudolf[2], and Richter Dieter[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany — [2]Institut für Bio- und Nanosysteme, Forschungszentrum Jülich, Germany — [3]Institut Laue-Langevin, Grenoble, France

The dynamics of proteins is a keystone to the understanding of their function as nanomachines or while metabolizing toxic by-products. To understand these processes we need information on length scales comparable to the size of the protein, which determine their functionality. Neutron spin echo spectroscopy is a versatile tool to determine the dynamics of macromolecules on these nanometer length and a nanosecond timescale. We will present NSE results from the protein Yeast Alcohol Dehydrogenase, which is a compact tetramer build up from 2 dimeric subunits involved in the production of ethanol. It binds the cofactor NAD in a cleft before catalysing the ethanol production. At low concentration around 1% the protein dynamics is observable with only small influence of protein-protein interactions at lowest q. The main characteristics of the protein dynamics can be described as the translational diffusion at low q and additional rotational diffusion at higher q, compatible with a rigid body model. We find additional dynamics at the onset of rotational diffusion, which is modelled in a first approach by a contribution due to elastic normal modes. The influence of the bound cofactor leads to a shift of the elastic contribution to higher q attributed to stronger coupling between the main domains.

BP 25.9 Thu 16:30 PC 203

Accurate sequence alignment statistics for different protein models — •Stefan Wolfsheimer[1], Inke Herms[2], Sven Rahmann[3], and Alexander K Hartmann[1] — [1]Institut für Physik, Universität Oldenburg, Germany — [2]AG Genominformatik/COMET, Technische Fakultät,Universität Bielefeld, Germany — [3]Fachbereich Informatik, TU Dortmund, Germany

Searching for homologous sequences or identifying proteins are well studied fields in bioinformatics. For these purposes a large sequence database is searched with a query by sequence alignment algorithms. The Smith-Waterman algorithm is a famous representative of those. A meaningful interpretation of the score is given by a p-value, which states the probability of the score within a selected null model.

Exact results are only known for gapless alignment of infinitely long uncorrelated protein models, where the amino acids are independent and identically distributed (i.i.d.). For this case a Gumbel distribution is expected. It turned out that real proteins do not fulfill these restrictions: first they are finite and secondly the i.i.d. assumption might not be the best description. Therefore we study more complex systems which incorporate information from secondary structure annotation to obtain a more plausible null model.

By generalized ensemble Monte Carlo simulations we obtain the score distributions down to very small probabilities ($p \sim 10^{-100}$). We find strong deviations from the expected form in the rare-event tail. Our results indicate that p-values are overestimated in the high scoring regime, when assuming a Gumbel extrapolation.

BP 25.10 Thu 16:45 PC 203

MONTECARLO SIMULATIONS OF PROTEIN FOLDING UNDER CONFINEMENT — •Pedro Armando Ojeda May[1], Aurora Londono[2], Nan-Yow Chen[3], and Martin Garcia Rimsky[1] — [1]Kassel Universitaet, Heinrich-Plett-St- 40 34132 Kassel — [2]Department of Molecular Biology, IPICYT Mexico — [3]Academia Sinica, Taiwan

We present a theoretical investigation of the folding of small proteins assisted by chaperones. We describe the proteins in the framework of an effective potential model which contains the Ramachandran angles as degrees of freedom. The cage of chaperonins is modeled by an external confining potential which is also able to take into account hydrophobic and hydrophilic effects inside the cavity. Using the Wang-Landau algorithm [Phys. Rev. Lett. **86**, 2050 (2001)] we determine the density of states $g(E)$ and analyze in detail the thermodynamical properties of the confined proteins for different sizes of the cage. We show how the confinement through the chaperon dramatically reduces the phase space available for the protein leading to a much faster folding process. Slightly hydrophobic cages seem to make the native structure more stable. However, not any confining potential helps folding. If the inner walls of the cage are strongly hydrophobic, a denaturation process is induced, in which the proteins partially unfold and stick to

the walls.

BP 26: Posters II

Time: Thursday 17:00–19:30 Location: Poster A

BP 26.1 Thu 17:00 Poster A

Fast $\mathcal{O}(N^2)$ Hydrodynamics for Brownian Dynamics Simulations — •Tihamér Geyer and Uwe Winter — Zentrum für Bioinformatik, Universität des Saarlandes, Saarbrücken, D–66041 Saarbrücken

In Brownian Dynamics (BD) simulations, the solvent molecules are replaced by a continuous solvent, thus greatly reducing the complexity and the required numerical effort. The polarizability of the solvent molecules is thereby taken into account by a shielded Coulomb interactions while the mechanical displacement of the solvent leads to hydrodynamic interactions (HI). Due to the many-body nature of this (effective) interaction, which introduces a correlation into the random motion of the particles, it is more complicated to evaluate. Effectively, HI is calculated from a factorization of the $6N \times 6N$ diffusion matrix, for which the runtime scales as $\mathcal{O}(N^3)$. This makes it prohibitive to include HI into BD simulations with more than a hundred particles.

Here we report on an approximation to the hydrodynamic interaction, which, at weak coupling, preserves the statistical moments of the correlated random motion of the particles. Due to this approximation, the hydrodynamic corrections to the particle displacements can be evaluated with a runtime $\propto \mathcal{O}(N^2)$, i.e., it scales as the evaluation of the direct interactions. With this form it is now possible to include HI into simulations with virtually arbitrarily many particles.

Here we present first test runs that show that the errors introduced through the approximation are negligible compared to the benefit of including the hydrodynamic corrections to the continuum solvent model.

BP 26.2 Thu 17:00 Poster A

Effect of high pressure on the global and internal dynamics of multimeric proteins studied by quasielastic neutron scattering experiment. — •Marie-Sousai Appavou[1], Sebastian Busch[2], Wolfgang Doster[3], Ana Gaspar[2], and Tobias Unruh[2] — [1]Forschungszentrum Jülich GmbH, IFF-JCNS, Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany — [3]Technishe Universität München, Physik Department E 13, Garching, Germany

Pressure is a physical parameter, which in contrast to temperature, allows to separate volume changes from entropic effects. Moreover, pressure is increasingly utilized in the sterilization and bio-conservation processes in food and pharmaceutical industries. In the range up to 2000 bar, essentially association-dissociation phenomena of biomolecular assemblies are observed. The unfolding of monomeric proteins typically requires pressures exceeding 3 kbar. Pressure can also be used to investigate the effect of density changes on molecular motions. Quasi-elastic neutron scattering allows exploring structural fluctuations of proteins on the pico-second time scale. In this contribution we present a series of neutron scattering spectra of hemoglobin and beta-casein as a function of pressure. For this project we have built a new scattering cell with high transmission, which can sustain pressures up to 2000 bar. Dynamic changes as a result of water reorganisation and subunit dissociation will be discussed.

BP 26.3 Thu 17:00 Poster A

Effective Connectivity profile: A Structural Representation that Evidences the Relationship between Protein Structures and Sequences — Ugo Bastolla[1], Angel R. Ortiz[1], Markus Porto[2], and •Florian Teichert[2] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 6-8, 64289 Darmstadt, Germany — [2]Centro de Biología Molecular "Severo Ochoa", (CSIC-UAM), Cantoblanco, 28049 Madrid, Spain

We recently defined the vectorial Effective Connectivity profile (EC) to describe protein structures [1] which is highly correlated with the average hydrophobicity profile (HP) of simulated proteins with stable native structure. We showed analytically that the optimally stable HP belongs to a family of profiles that we call the Generalized Effective Connectivity family (GEC), of which the EC is a distinctive member, as well as the previously defined revised PE profile [2]. This mathematical relationship unveils the close relationship between different vectorial representations derived from structural and from sequence data, as we could demonstrate. Finally, we show that structurally similar proteins have similar EC profiles, a property that we exploit to perform protein structure alignments [3].

[1] U. Bastolla, A.R. Ortíz, M. Porto, and F. Teichert, (submitted).
[2] F. Teichert and M. Porto, Eur. Phys. J. B **54**, 131-136 (2006).
[3] F. Teichert, U. Bastolla, and M. Porto, BMC Bioinformatics **8**, 425 (2007).

BP 26.4 Thu 17:00 Poster A

SABERTOOTH: Protein Structural Alignment Based on a Vectorial Structure Representation — •Florian Teichert[1], Ugo Bastolla[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 6-8, 64289 Darmstadt, Germany — [2]Centro de Biología Molecular "Severo Ochoa", (CSIC-UAM), Cantoblanco, 28049 Madrid, Spain

The task of computing highly accurate structural alignments of proteins in very short computation time is still challenging. We tackle this issue that arises mostly from the complexity of protein structures by representing a protein fold's topology in the form of a vectorial profile [1,2], consisting of only one real number per amino acid. Doing so, the alignment of spatial structures is carried out by maximizing the overlap of profile vectors. This simplification results in favourable scaling of computation time with chain length in comparison with other algorithms while we achieve an accuracy that is comparable to established alignment tools, like Dali, as we have shown [3]. The algorithm discussed is implemented in the 'SABERTOOTH' alignment server, freely accessible at `http://www.fkp.tu-darmstadt.de/sabertooth/`.

[1] F. Teichert and M. Porto, Eur. Phys. J. B **54**, 131-136 (2006).
[2] U. Bastolla, A.R. Ortíz, M. Porto, and F. Teichert, (submitted).
[3] F. Teichert, U. Bastolla, and M. Porto, BMC Bioinformatics **8**, 425 (2007).

BP 26.5 Thu 17:00 Poster A

Kinetic clustering analysis of protein (un)folding trajectories from molecular dynamics simulation — •Lothar Reich and Thomas R. Weikl — Max-Planck-Institute of Colloids and Surfaces, Wissenschaftspark Golm, 14424

Small fast-folding proteins reach their folded state within microseconds. In the past years, the folding dynamics of these proteins has become accessible by molecular dynamics (MD) simulations. Central questions are: Which partially folded or metastable states dominate the folding/unfolding process, and can we describe the folding/unfolding process on a network of such states? We have performed extensive MD simulations of the Pin WW Domain, a fast-folding three-stranded beta-sheet protein, and have analyzed the folding/unfolding trajectories with a novel kinetic clustering method, the Perron-Cluster-Cluster analysis (PCCA). Our analysis reveals a complex network of metastable states.

BP 26.6 Thu 17:00 Poster A

Stretching of a DNA/HU-protein complex 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 interact with the DNA in a non-specific way [1]. Its major function is the binding, compaction and stabilization of DNA. We applied steered molecular dynamic (SMD) simulations to DNA which is bound to a HU protein. 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].

[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 26.7 Thu 17:00 Poster A

Restrained Protein Folding Dynamics in the Tube Model — •Katrin Wolff[1], Michele Vendruscolo[2], and Markus Porto[1]

— [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Department of Chemistry, University of Cambridge, UK

The study of protein folding dynamics through all-atom molecular dynamics requires significant computational efforts, and coarse-grained models are therefore of great interest. Here, we use the tube model [1], which has been shown to be computationally very effective in reproducing the folding behaviour of proteins [1,2,3]. In order to drive the folding dynamics towards a specific protein structure, we augment the energy function with a term based on a structural profile. For single-domain proteins, this structural profile has been shown to contain sufficient information to reconstruct the contact map of the target structure [4]. When directly applied to folding, the use of the structural profile is conceptually very different from the use of the contact map, since the latter would result in a Gō-type model. By contrast, the structural profile entries contain global information about the protein structure rendering this approach similar to the actual protein folding process [5]. We show that by adopting this strategy we are able to fold several small to medium-size single-domain proteins.

[1] T.X. Hoang *et al.*, Proc. Natl. Acad. Sci. USA **101**, 7960 (2004).
[2] T.X. Hoang *et al.*, Proc. Natl. Acad. Sci. USA **103**, 6883 (2006).
[3] S. Auer *et al.*, Phys. Rev. Lett. **99**, 178104 (2007).
[4] M. Porto *et al.*, Phys. Rev. Lett. **92**, 218101 (2004).
[5] K. Wolff, M. Vendruscolo, and M. Porto, submitted.

BP 26.8 Thu 17:00 Poster A

Proteins under extreme conditions - new SAXS setup at beamline BL9 of DELTA synchrotron — •Christina Krywka[1], Christian Sternemann[1], Roland Winter[2], and Metin Tolan[1] — [1]Fachbereich Physik, Universität Dortmund, D-44221 Dortmund, Germany — [2]Fachbereich Physikalische Chemie, Universität Dortmund, D-44221 Dortmund, Germany

The biological activity and the chemical properties of proteins depend on the structure of the solvent and its thermodynamic parameters. Understanding the effects of cosolvents on the structure and dynamics of proteins is crucial for a deeper insight into protein stability, folding, aggregation and fibrillation processes. The latter play an important role in many conformational diseases, such as Alzheimer, Creutzfeldt-Jakob, and Parkinson. Recently, we could show that these fibrillation processes are strongly influenced by the type and concentration of cosolvents. In order to determine the effects of different types of cosolvents on the native and unfolded states of the model protein Staphylococcal Nuclease (SNase) we have performed Small-Angle-X-ray-Scattering (SAXS) measurements at temperature and pressure conditions where unfolding of the protein sets in. The experimental equipment which had to be developed in the course of the ongoing project comprises of a high-pressure, temperature controlled sample cell with the ability to perform SAXS-measurements at pressures up to 7 kbar in a wide temperature range (-15°C to 80°C). This contribution will provide an outline of recent high-pressure data of SNase and the experimental setup installed at the multi-purpose beamline BL9.

BP 26.9 Thu 17:00 Poster A

(Structure-) Mechanical properties of nanocoposite silk and wood at macro and molecular scales. — •Igor Krasnov[1], Imke Diddens[1], Tomasz Pazera[1], Sergio S. Funari[2], Richard Davies[3], Manfred Burghammer[3], and Martin Müller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel — [2]Hasylab at Dasy, Hamburg — [3]ESRF, Grenoble, France

Using an in situ combination of tensile tests and X*ray fiber diffraction, we have directly determined the mechanical roperties of both the crystalline and the disordered phase of the biological nanocomposite silk and wood.

The measurements at single fibers and bundels was done in controlled enviromental conditions such as temperature and humidity. We have adapted a model from linear viscoelastic theory, which fully accounts for the semicrystalline orphology of studying materials. The viscoelastic parameters (modulus, viscosity, relaxation times) were determined at a wide range of time scales.

The observed interplay of morphology, mechanical and enviromental properties will have strong impact on the design of novel high*performance nanocomposite fibers.

BP 26.10 Thu 17:00 Poster A

Mechanical properties of Wood investigated using X-Ray Scattering under defined humidity conditions — •Tomasz Pazera[1], Igor Krasnov[1], Imke Diddens[1], Florian Kunze[1], Henning Vogt[1], Richard Davies[3], Manfred Burghammer[3], Sergio S. Funari[2], and Martin Müller[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]HASYLAB at DESY, Hamburg — [3]ESRF, Grenoble, France

Wood is a composite material that mainly consists of stiff cellulose crystals surrounded by a softer, water adsorbing matrix. The mechanical properties of pine earlywood have been studied in combined X-ray diffraction and stretching experiments at defined humidity conditions. We observed explicit variations in both the crystal strain and the stress-strain curves of wood. The most radical discrepancy in the behaviour of the whole wood-fibre was estimated to happen between 85%-100% relative humidity. In this range, the matrix shows strong macerating effects. By stretching in direction of the fibre axis we received information about changes in the correlation of crystal strain and force transfer inside the fibre at different humidities. Furthermore, an investigation of single fibres shows explicit changes in the orientation of the microfibrils in the cell wall.

BP 26.11 Thu 17:00 Poster A

Nanotomography of Biomaterials — •Stephanie Röper[1], Christian Zeitz[2], Christian Dietz[1], Nadine Drechsel[1], Anke Bernstein[3], Nicolaus Rehse[1], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [2]Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken — [3]Experimentelle Orthopädie, Martin-Luther-Universität Halle-Wittenberg, D-06097 Halle/Saale

Biomaterials such as bone and teeth are nanocomposites of proteins and minerals. At the molecular length scale these materials have a stiff inorganic component (hydroxylapatite) that reinforces the soft organic matrix (type I collagen) through a recurring structural motif. To gather information of the nanometer scaled structure of these materials we use nanotomography. For this scanning probe microscopy (SPM) based method the specimen is ablated layer-by-layer by wet chemical etching and imaged with tapping mode SPM after each etching step. In our experiments we focus on cortical human bone (embedded and native) and human teeth. The stepwise etching is done in-situ in the SPM with an automated setup. We will present our latest volume images of human bone and teeth and discuss new concepts for adjusting the imaging parameters to maintain a good imaging quality.

BP 26.12 Thu 17:00 Poster A

The influence of pH and temperature on the self-assembly of amelogenin and its relevance for the biomineralization of enamel — •C. Gilow[1], B. Aichmayer[1], F.B. Wiedemann-Bidlack[2], H.C. Margolis[2], and P. Fratzl[1] — [1]Max Planck Institute of Colloids and Interfaces, D-14424 Potsdam, Germany — [2]The Forsyth Institute, Boston, MA 02115-3782, USA

In the early stages of dental enamel formation, amelogenin is the most abundant matrix protein. The self-assembly of amelogenin to so-called "nanospheres" is believed to control the growth and alignment of hydroxyapatite crystals in the developing enamel tissue. Previous studies [1] on the formation of these "nanospheres" and their subsequent temperature-induced aggregation showed that the interaction between the "nanospheres" is controlled by the hydrophilic C-terminus of the protein. Further studies by Wiedemann-Bidlack et al. [2] revealed that the pH-value is the dominant parameter which regulates the higher-order assembly of amelogenins. In the current study measurements with small-angle X-ray and neutron scattering techniques are used to elucidate the structure of these protein agglomerates, which - in spite of their commonly used name were found to strongly deviate from a spherical shape. Through a systematic study of the effects of temperature and pH as well as a more detailed characterisation of the shape of the "nanospheres" we hope to get a clearer understanding of the processes involved in the mineralization of dental enamel.

1.Aichmayer, B., et al., J Struct Biol, 2005. 151: 239.
2.Wiedemann-Bidlack, F.B., et al., J Struct Biol, 2007. 160: 57.

BP 26.13 Thu 17:00 Poster A

2-Photon laser scanning microscopy of cartilage materials — •Thorsten Bergmann[1], Jörg Martini[1], Maik Tiemann[1], Michael Dickob[2], Ronald Schade[3], Klaus Liefeith[2], Katja Tönsing[1], and Dario Anselmetti[1] — [1]Bielefeld University, Exp. BioPhysics & Appl. NanoSc., Bielefeld, Germany — [2]Orthopedic Surgery, Bielefeld, Germany — [3]IBA e.V., Department of Biomaterials, Heilbad Heiligenstadt, Germany

2-photon laser scanning microscopy (2PLSM) is a powerful tool for label-free investigation of living cells and strongly scattering tissue

samples. In our experiments, strongly scattering native hyaline cartilage has been imaged with this technique using multifocal 2PLSM and analyzed in descanned and non-descanned detection mode. Intensity, wavelength and fluorescence lifetime sensitive detection methods were used for imaging the autofluorescence of the extracellular matrix (ECM) as well as the chondrocytes, the only cells within this tissue. Spectral and lifetime separation of chondrocytes from the ECM allow to quantify the chondrocyte density. The intensity and the structural differences of the detected fluorescence signal from the ECM can be used for differentiation of arthritic and non-arthritic cartilage. Additionally, results of an investigation of collagen scaffolding materials and a comparison concerning chondrocyte density will be discussed.

[1] J. Martini, K. Tönsing, M. Dickob, D. Anselmetti: Proc. of SPIE, 5860: 16-21, 2005 [2] J. Martini, K. Tönsing, M. Dickob, R. Schade, K. Liefeith, D. Anselmetti: Proc. of SPIE, 6089: 274-282, 2006 [3] J. Martini, K. Tönsing, D. Anselmetti: BIOspektrum 5, 489-492, 2006

BP 26.14 Thu 17:00 Poster A

Magnetic Relaxation Dispersions of Biomolecules: Effects of Field-Cycling — •Talea Köchling, Konstantin Ivanov, Sergey Korchak, Alexandra Yurkovskaya, and Hans-Martin Vieth — Institute für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

The dynamics of biomolecules is reflected in the spin-lattice relaxation times T1 of individual nuclei. From the change of T1 at variation of the external magnetic field intramolecular mobility can be determined. Combining a field-cycling unit, which shuttles the NMR probe along the bore axis of the spectrometer cyromagnet, with high resolution NMR spectroscopy we are able to measure T1 of individual nuclei between 1 uT and 7 T. Our experiments show that such relaxation dispersion is strongly affected by scalar couplings among the spins. Spins having substantially different T1 at high field relax at low field with a common T1 due to strong coupling. Furthermore peaks or dips are seen at fields corresponding to crossings of spin levels. An adequate theoretical approach to modelling the dispersion curve and extracting motional parameters is presented and experiments on amino acids and peptides (for example, tyrosine and enkephalin) are discussed. It shows that for proper interpretation of relaxation dispersion curves scalar couplings must be taken into account as long as $1/J<T1$.

BP 26.15 Thu 17:00 Poster A

Biological NMR Spectroscopy: Hyperpolarization at Variable Field — •Sergey Korchak, Konstantin Ivanov, Talea Köchling, Alexandra Yurkovskaya, and Hans-Martin Vieth — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

For optimization of nuclear spin hyperpolarization and its transfer to target spins of choice field-cycling schemes have been devised that make use of scalar spin-spin interaction J in the strong coupling regime. A field-cycling unit is described shuttling the NMR probe along the bore axis of the spectrometer cryomagnet and allowing field variation between 1 uT and 7 T combined with high resolution detection. By incrementing spin evolution times an oscillatory exchange of polarization between spins is observable allowing efficient manipulation of polarization flow. We studied coherent transfer of chemically induced dynamic nuclear polarization (CIDNP) in the amino acids histidine, tyrosine and tryptophan and observed well-pronounced quantum beats in their transfer kinetics indicating the coherent nature of the process. In the field dependence of the CIDNP transfer efficiency features such as peaks and dips were found corresponding to anti-crossings of the nuclear spin levels in the molecule. In experiments performed at very low field (about 1 uT) where hetero-nuclei become strongly coupled coherent CIDNP transfer between protons and fluorine atoms was found. An adequate theoretical approach to the phenomena studied was developed. This work was supported by the EU (Bio-DNP grant # 011721 and IFF # 22008) and INTAS (grant # 05-1000008-807).

BP 26.16 Thu 17:00 Poster A

LED illumination for video-enhanced DIC imaging of single — •Volker Bormuth[1], Jonathon Howared[1], and Erik Schäffer[2] — [1]Max Planck Institute for Molecular Cell Biology and Genetics, Pfotenhauerstr.108, 01307 Dresde — [2]Biotechnology Center (BIOTEC), Tatzberg 47-51, 01307 Dresden

In many applications high-resolution video-enhanced differential interference contrast microscopy is used to visualize and track the ends of single microtubules. We show that single ultrabright light emitting diodes from Luxeon can be used to replace conventional light sources for these kinds of applications without loss of function. We measured the signal-to-noise ratio of microtubules imaged with three different light emitting diode colours (blue, red, green). The blue light emitting diode performed best, and the signal-to-noise ratios were high enough to automatically track the ends of dynamic microtubules. Light emitting diodes as light sources for video-enhanced differential interference contrast microscopy are high performing, low-cost and easy to align alternatives to existing illumination solutions.

BP 26.17 Thu 17:00 Poster A

Coherent anti-Stokes Raman scattering (CARS) microscopy - a means to visualize molecular distribution in complex, biological samples — •susana chatzipapadopoulos[1], denis akimov[2], michael schmitt[1,2], and jürgen popp[1,2] — [1]Institute of Photonic Technology, Jena, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University of Jena, Germany

Coherent anti-Stokes Raman scattering (CARS) microscopy is a non linear Raman mapping technique which provides vibrational contrast with high chemical selectivity and high 3D sectioning capability. CARS is applied to complex, biological samples in order to visualize the molecular distribution of various types of molecules with high efficiency, high chemical selectivity and low acquisition times without the need of staining. Unfortunately the CARS signal is not background free and also is derived from the bulk media. In order to develop techniques to yield pure molecular contrast we analyze different, non-linear and linear contrast mechanisms contributing to the CARS image.

BP 26.18 Thu 17:00 Poster A

Mechanically actuated silicon microgrippers for micromanipulation of biological matter — •Marius M. Bliderean[1], Jochen Sterr[2], Stephan Kleindiek[2], Matthias G. Langer[3,4], Francois Grauvogel[3], Monika Fleischer[1], and Dieter P. Kern[1] — [1]University of Tübingen, Institute of Applied Physics, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Kleindiek Nanotechnik GmbH, Aspenhaustrasse 25, 72770 Reutlingen, Germany — [3]Department of Applied Physiology, University of Ulm, 89081 Ulm, Germany — [4]Carl Zeiss NTS GmbH, 73447 Oberkochen, Germany

Controlled gripping during the manipulation of objects is widely desired in the fields of microbiology and microassembly. Therefore it is important, especially when targeting biological structures to measure or calculate the forces exerted by the end segment of the manipulator. This way one would know exactly when the object under investigation is grabbed and what pressures are applied to it. Moreover, for handling objects only micrometers in size, microgrippers or tweezers with fine end-segments are required. On the other hand the manipulator has to be attached to a motor or actuator, which implies that the gripper has to be millimeters in size at its other end. The mechanical assembly of the gripper and the actuator proves to be a crucial step in realizing the system. This work presents solutions to the two challenges mentioned above: a method for determining the gripping forces combining experimental with simulation results, and a procedure for the secure construction of our micromanipulator. Finally results from tests of the system on micrometer-sized objects will be shown.

BP 26.19 Thu 17:00 Poster A

Carbon Coated Nanomagnets for Biomedical Applications — •A.U.B. Wolter[1], Y. Krupskaya[1], C. Mahn[1], S. Hampel[1], D. Haase[1], A. Leonhardt[1], A. Vyalikh[1], A. Werner[2], A. Taylor[2], K. Krämer[2], B. Büchner[1], and R. Klingeler[1] — [1]Leibniz Institute for Solid State Research, IFW Dresden, 01069 Dresden, Germany — [2]Universitätsklinikum Carl Gustav Carus, 01307 Dresden, Germany

There is a rapidly increasing interest in applying carbon nanotubes (CNT) in biomedicine since they can be filled with tailored material, thereby acting as chemically and mechanically stable nanocontainers. Furthermore, the carbon shells enhance the possibilities for exohedral functionalization, this way targeting e.g. pathological tissue. We report on a systematic approach to exploit the potential of filled CNT to act as magnetic nano-heaters, temperature sensors and contrast agents which allow a diagnostic and therapeutic usage on a cellular level. Here, we present a detailed field and frequency dependent study of different concentrations of Fe-filled CNT suspensions, which imply their potential for magnetic nano-heaters in a hyperthermia cancer treatment. Indeed, there is a substantial temperature increase of Fe-CNT under applied AC magnetic fields. Furthermore, filled CNT can also be used for diagnostic purposes such as contrast agents in MRI or for the simultaneous detection of the resulting temperature increase, since the nanocontainers can be filled with (additional) appropriate sensor

materials. An example is their filling with copper or silver halides, which exhibit a strongly temperature dependent NMR signal so that nanoscaled contactless temperature sensors are realised.

BP 26.20 Thu 17:00 Poster A

A robust surface plasmon resonance biosensor with high resolution — •Sebastian Horstmeier, Andy Sischka, Christoph Pelargus, Katja Tönsing, and Dario Anselmetti — Experimentelle Biophysik und Angewandte Nanowissenschaft, Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld

We present a simple, robust and easy to use surface plasmon resonance (SPR) biosensor with high resolution which is based on a previous study [1] and can be used in biophysical applications as well as for educational purposes, e.g. practical courses. SPR-based biosensors are able to investigate biochemical reactions according to their kinetics without labeling the molecules. Using the Kretschmann-Raether-configuration the SPR-angular shifts are detected by a method based on a quadrant photo diode like in atomic force microscopy (AFM). The goldfilm is divided into two areas, one for reference measurement, the other for analysing the specific binding-reaction. SPR-angular changes due to the bulk solution as well as errors caused by thermal drift, mechanical stress or fluctuations of the laser are eliminated by the reference measurement which is made parallel under the same conditions. Using this method changes of the refractive index in the order 10^{-8} refractive index units (RIU) can be measured. The experimental setup and first results will be presented and discussed.

[1] H.Q. Zhang, S. Boussaad and N.J. Tao: *High-performance differential surface plasmon resonance sensor using quadrant cell photodetector*, Review of Scientific Instruments, **74**(1):150-153, 2002

BP 26.21 Thu 17:00 Poster A

Magnetic Properties of Iron Nanowires Encapsulated in Carbon Nanotubes — •K. Lipert[1], M. Lutz[1], T. Mühl[1], K. Krämer[2], A. Taylor[2], R. Klingeler[1], and B. Büchner[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, PF 270116, D-01171 Dresden, Germany — [2]Universitätsklinikum der Technischen Universität Dresden, Fetscherstraße 74, D-01307 Dresden, Germany

Introducing nanomagnets into carbon shells provides a promising route to synthesize novel magnetic nanoparticles with well defined geometrical dimensions. Carbon shells provide wear resistance and oxidation protection, can stabilize novel magnetic molecules and enhance possibilities for exohedral functionalisation. Here, we report on a systematic approach to study magnetic nanoparticles encapsulated in carbon nanotubes and nanospheres which are exploited for an application in biomedicine, i.e. as contrast agents or for hyperthermia cancer treatment. We present thorough magnetic and structural studies on ensembles and on individual particles. The ensemble studies are done both inside and outside biological systems. XRD patterns and TEM pictures are shown along with hysteresis loops measured at carbon nanotubes inside cancer cells as well as grown on silicon oxide substrates. Magnetic studies of individual Fe filled CNTs performed by means of the MFM technique and the micro hall magnetometry setup based on a GaAs nanoscaled Hall-cross are presented which provide an insight into the magnetisation reversal.

BP 26.22 Thu 17:00 Poster A

Two-focus fluorescence correlation spectroscopy with an EM-CCD detector — •Markus Burkhardt, Jonas Ries, and Petra Schwille — Biophysics/ BIOTEC/ TU Dresden, Tatzberg 47-51, 01307 Dresden, Germany

Fluorescence Correlation Spectroscopy (FCS) extracts thermodynamic and kinetic parameters from time dependent fluorescence intensity fluctuations of labeled biomolecules in solution. In a standard FCS setup, the fluorescence signal is collected from one specific focus position and detected by a single photon sensitive point detector. Two-focus FCS is based on the information from two spatially fixed laser foci. It enhances the precision of diffusion coefficient determination by evaluating the spatial cross-correlation.

Spatially resolved detection, employing an electron multiplying CCD (EMCCD) camera, is a versatile method perfectly suited for two-focus FCS measurements. The distances between the two laterally shifted focal volumes can be changed easily and they can be determined accurately by imaging a microscopic ruling.

We demonstrate two-focus FCS measurements for different fluorescent molecules and under various measurement conditions.

BP 26.23 Thu 17:00 Poster A

Searching the proper Model for F_1-ATPase rotation — •Florian Werz[1], Alexander Kovalev[1], Nawid Zarrabi[1], Carsten Tietz[1], Michael Börsch[1], Dirk Bald[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Germany — [2]Department of Structural Biology, Vrije Universiteit Amsterdam, Netherlands

The F-type ATP-Synthase is a composed rotary motor enzyme in the plasmamembrane of prokaryotes and in the inner membrane of mitochondria of eukaryotes, respectively, producing the universal fuel ATP, which is used to sustain nearly every chemical reaction in cells. The F_1-part of the enzyme can work in reverse hydrolyzing ATP and rotating backwards showing 120° steps resulting from the threefold symmetry of its $\alpha_3\beta_3$-stator-complex. We recorded trajectories up to half an hour with high time resolution (down to $\Delta = 1$ms) of Polystyrol beads attached to the rotating γ-subunit of single F_1-ATPase using wide field microscopy. We recorded the same molecule for different concentrations of ATP and ADP and therefore different rotational speeds. Analyzing data by hidden Markov models (HMM) we found to reproduce dwell time histograms a model with three or more consecutive states per visible state was required. Introduction of an additional state corresponding to the ADP-inhibited state, which stops rotation of F_1-ATPase for relative long times (up to minutes), significantly improved the fit.

BP 26.24 Thu 17:00 Poster A

Interferometric detection of nanosize diamond particles — •Thomas Wolf, Steffen Steinert, Carsten Tietz, Fedor Jelezko, and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

In recent years nanodiamonds have become available with well defined size distributions. It is possible to functionalize these diamonds with many different chemical groups to achieve biocompatibility and use them as markers. Aim of this work is to show the sensitivity of detecting scattering of these diamonds. We use a confocal setup combined with an interferometric detection scheme. The backscattered light of the sample passes the pinhole and is then recombined with the reference beam on our detector, thus yielding an interference pattern. As detector we use a splitted Si-diode to measure the difference signal. In this way it is possible to detect shifts in this interference pattern due to the light scattering of the diamonds. Using such a setup allows the detection of 50nm polystyrene or 10nm gold beads. The high refractive index of diamond should render it possible to detect diamonds down to a size of 10nm. Detecting this size would mean a step towards using nanodiamonds as non-toxic, non-bleaching biological markers.

BP 26.25 Thu 17:00 Poster A

Dynamic Force Spectroscopy studies of native and synthetic point mutated transcription regulators — •Andre Körnig[1], Katrin Wollschläger[2], Norbert Sewald[2], Dario Anselmetti[1], and Robert Ros[1] — [1]Experimental Biophysics and Applied Nanoscience, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld — [2]Bioorganic Chemistry, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld

For many aspects of cellular regulation the specific interaction between proteins and DNA is fundamental. Especially the recognition of specific DNA target sequences by transcription regulators is a central issue for the regulation of gene expression. We are using atomic force microscope (AFM) based force spectroscopy to investigate the molecular mechanism of the interaction of the transcription regulator PhoB with DNA target sequences on a single molecule level. In order to investigate the contribution of single amino acids to the specificity and strength of the binding as well as the role of the protein environment we compare the wild type protein with point mutants and peptides representing the PhoB recognition helix. This allows a quantitative analysis of the dissociation rates of those complexes and gives insights into the energy landscape of the respective interaction.

BP 26.26 Thu 17:00 Poster A

Quantitative Optical Tweezers for Single Molecule Manipulations in 3D — •Andy Sischka, Christoph Kleimann, Katja Tönsing, and Dario Anselmetti — Experimentelle Biophysik & Angewandte Nanowissenschaft, Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielelfeld

We introduce a novel way of measuring minute forces and manipulate single molecules like DNA by means of a quantitative optical tweezers system that is operated in reflection mode using a single laser beam

[1].

Our optical setup is based on a compact, stable optical tweezers configuration (2D) that is compatible with an inverted optical microscope (Zeiss Axiovert) [2] and was modified in order to allow quantitative analysis and molecular manipulation in three dimensions (3D) with remarkably high precision.

The optical setup was tested by manipulating individual λ-DNA molecules in the vicinity of a nanopore similar to a previous study [3], and allowed quantitative single molecule experiments with minimal optical interference, and insights into the threading dynamics of DNA into a nanopore.

[1] A. Sischka et al., Rev. Sci. Instrum., submitted, 2008.
[2] A. Sischka et al., Rev. Sci. Instrum. 74, 4827, 2003.
[3] U.F. Keyser et al. Nature Phys 2, 473, 2006.

BP 26.27 Thu 17:00 Poster A

Single-molecule Spectroscopy on Phytochromes — •Jana B Nieder, Marc Brecht, and Robert Bittl — Fachbereich Physik, Freie Universität Berlin, Arnimalle 14, 14195 Berlin, Germany

Phytochromes are red light sensitive photoreceptors controlling flowering, shade avoidance and germination in plants. Their cofactor biliverdin is a linear tetrapyrroles whos conformation is strongly affected by the protein environment. The tight binding by the protein surrounding is the basis for the metastable PR and PFR conformational states. The switching between these isomeric states is reversibly triggered by Red and Far Red light.

Physical properties of the interaction between the pigment and its protein surrounding are accessible by single-molecule spectroscopy at low temperatures . Under low temperature conditions major protein rearrangements are inhibited and the phytochromes are trapped in the dark stable state (here PR). The fluorescence emission of single Agp1 molecules (phytochrome from Agrobacterium tumefaciens) shows marked time dependence. The pigment-protein interaction causes intensity and spectral changes. This spectral fine-tuning is observed by comparison of signals from different molecules and within time-dependent spectra of individual Agp1 molecules. For some of the analysed Agp1 molecules narrow lines in the vibronic energy range could be resolved. The spectral fine-tuning affects all vibrational lines simultaneously. For these molecules the vibrational energies can directly be extracted. In this work detection of vibrational information of single chromophores in their natural protein environment is achieved.

BP 26.28 Thu 17:00 Poster A

Cantilever Based Apertureless Scanning Near-Field Optical Microscopy in Aqueous Solution — •Jan Paskarbeit, Heinrich Frey, Christoph Pelargus, Robert Ros, and Dario Anselmetti — Experimental Biophysics & Applied Nanosciences, Department of Physics, Bielefeld University, Germany

Scanning near-field optical microscopy strives for the highest optical resolution, far beyond the classical diffraction limit of Abbé, and simultaneously provides topographical information. In conventional fluorescence SNOM a metallised glass fibre with an aperture of about 50nm is used to illuminate the sample locally. The main drawbacks are, dependent on the size of the aperture, either reduced light throuput or low optical resolution. We presented already a cantilever based setup, in which the tip of an aluminium or silver coated full body glass tip is used as illumination in air and which could be operated at an optical resolution of 15nm on individual fluorescent dye molecules [1]. Especially for applications in life sciences the operation in aqueous solution is essential. In addition to our recent numerical simulations, we present results of gold, silver and aluminium coated glass tips for SNOM operations in liquids with respect of SNOM performance and stability.

[1] Frey, H. G., C. Bolwien, A. Brandenburg, R. Ros und D. Anselmetti: Optimized apertureless optical near-field probes with 15 nm optical resolution. Nanotechnology, 17(13):3105*3110, 2006.

BP 26.29 Thu 17:00 Poster A

Scanning FCS applied to precise measurement of diffusion coefficients — •Susan Derenko, Zdeněk Petrášek, and Petra Schwille — Biophysics Group, Biotechnologisches Zentrum, TU Dresden, Germany

Although fluorescence correlation spectroscopy (FCS) is a useful technique to obtain diffusion coefficients of fluorescent molecules in solution, the precision of the measurement is limited due to difficulties in the determination of the fixed volume size in standard FCS. In order to avoid the reference to the inaccurate volume size, the beam is scanned in a circle with either two galvanometer scanners or a 2-axis piezo scanner. The diffusion coefficent is then related to the scan radius R and the scanning freqency using the spatial cross-correlated signal. The radius needs to be calibrated carefully and is therefore the most important value for the calculation of the diffusion coefficient D.

To test the applicability of the new approach, several dyes were tested under two-photon excitation, and the important parameters, mainly radius and frequency, were optimized. The method is being extended to one-photon excitation, where triplet-effects of the fluorescent molecules have to be considered. Further, operation under non-ideal conditions and in biological samples will be investigated.

BP 26.30 Thu 17:00 Poster A

Single molecule microscopy using total internal reflection — •Andreas Veenendaal, Jan Peter Siebrasse, Constanze Husche, and Ulrich Kubitscheck — Institute of Physical and Theoretical Chemistry, Bonn, Germany

In single molecule fluorescence microscopy one often wants to reduce the fluorescence background emitted by fluorophores not located in the plane of interest. With total internal reflection fluorescence (TIRF) microscopy this is achieved by reflecting the light at the coverslip/probe interface (coverslip (glass) n = 1.51; sample (e.g. cell) n = 1.33), and thus generating an evanescent wave illuminating the sample. The intensity of the evanescent wave decays exponentially with a penetration depth of roughly half the wavelength of the incident light. We realised objective type TIRF using an NA 1.45 objective from Zeiss. Using this technique we characterized several red fluorescent dyes attached to the surface by a PEG-biotin-streptavidin system at the single molecule level. As a first biological application we studied the transport dynamics of single nuclear pore complexes.

BP 26.31 Thu 17:00 Poster A

Coated particles as enhanced probes for optical tweezers — •Anita Jannasch[1], Volker Bormuth[1], Jonathon Howard[1], and Erik Schäffer[2] — [1]MPI of Molecular Cell Biology and Genetics Dresden — [2]BIOTEC Dresden

In an optical trap, micron-sized dielectric particles in aqueous solutions can be held by a tightly focused laser beam. The optical force on the particle is composed of an attractive gradient force in the direction of highest light intensity, and a scattering force in the light propagation direction, that pushes the particle away from the focus and thereby weakens the trap. To optimize the trapping potential, we reduce the scattering force by using coated microspheres. The shell of the particle is designed such that it acts as an anti-reflection coating. We characterized such particles and found in comparison with the same-sized uniform microspheres a more than two-fold strengthening of the trap. By improving the trapping potential higher overall forces can be achieved with the same laser power, or vice versa the same force can be reached by using less laser power. A higher maximal force increases the range of possible experiments, and a reduced laser intensity leads to less photo-toxic interactions relevant for biological applications, like in vivo cell measurements.

BP 26.32 Thu 17:00 Poster A

Live imaging of signalling complexes using pulsed dual-colour microscopy — •Steffen Steinert[1], Felix Neugart[1], Andrea Zappe[1], Lutz Graeve[2], Carsten Tietz[1], and Jörg Wrachtrup[1] — [1]University Stuttgart — [2]University Hohenheim

Communication between cells is mediated via messenger molecules which bind to a receptor that eventually induces oligomerisation with other molecules and transduce a certain signal. The CNTF receptor is a GPI-anchored protein involved in many signalling pathways which control apoptosis, differentiation and other key cellular functions. In order to gain information about the characteristics of the CNTF receptor at the membrane as well as its internal trafficking, colocalisation analysis with other distinct markers is required. For that purpose we set up a widefield and confocal microscope with pulsed dual-colour excitation which enables us to track two different proteins without crosstalk between the fluorophores. The high sensitivity and adjustable temporal resolution in ms-range of the widefield system facilitates a rapid image acquisition even on single-molecule level. Due to the simultaneous detection of the emission of both fluorophores, FRET signals are detected automatically. FCCS is used to study potential interactions at almost native protein concentrations. It was shown that gp130, an important glycoprotein which is known to associate with CNTF-receptor upon stimulation, and CNTF receptor have comparable diffusion constants in the range of 10-9cm*/s. However, FCCS

revealed that both proteins are not pre-associated in the membrane, but both become part of the signalling complex after stimulation.

BP 26.33 Thu 17:00 Poster A

1D diffusion model for inter-site communication by Type III restriction enzymes — •Subramanian Ramanathan[1], Kara van Aelst[2], Mark D. Szczelkun[2], and Ralf Seidel[1] — [1]Biotechnology Center, Dresden University of Technology, Germany — [2]Department of Biochemistry, University of Bristol, UK

Type III restriction enzymes use ATP hydrolysis to communicate between distant target sites on DNA, which subsequently triggers DNA cleavage. Due to amino acid sequence similarities these enzymes belong to the superfamily 2 of helicases. They are therefore generally believed to be molecular motors that directionally translocate DNA in order to communicate between their target sites. However, the low ATPase activity of these enzymes does not support DNA translocation and alternative models involving passive diffusive looping have been suggested. In order to gain insight into the communication mechanism of type III restriction enzymes we used magnetic tweezers to investigate DNA cleavage of multiple single molecules in parallel. This allowed us to measure the cleavage kinetics while keeping the DNA stretched. We observed rapid DNA cleavage even at the highest stretching forces, where DNA looping is completely abolished. Furthermore, the cleavage rates did not change over a large range of forces. These results provide direct evidence for a communication mechanism between the target sites in 1D, i.e. enzyme movement along the DNA contour, rather than in 3D by diffusive DNA looping. Therefore, given the low ATP consumption, we suggest diffusion rather than active translocation as being the mechanism by which the enzymes move along DNA.

BP 26.34 Thu 17:00 Poster A

Single Molecule FRET studies of RNA Polymerese II — •Joanna Andrecka[1], Robert Lewis[1], Florian Brueckner[2], Patrick Cramer[2], and Jens Michaelis[1] — [1]Department of Chemistry and Biochemistry, Ludwig-Maximilians-Universität München, Butenandtstr.11, 81377 Munich, Germany — [2]Gene Center Munich and Department of Chemistry and Biochemistry, Feodor-Lynen-Strasse 25, Ludwig-Maximilians-Universität München, 81377 Munich, Germany

Single-pair Fluorescence Resonance Energy Transfer (FRET) was used to track RNA exiting from RNA Polymerase (Pol II) in elongation complexes [1]. Measuring the distance between the RNA 5'-end and three known locations within the elongation complex allowed us to determine its position by means of triangulation. RNA leaves the polymerase active center cleft via the previously proposed exit tunnel, and then disengages from the enzyme surface. When the RNA reaches lengths of 26 and 29 nucleotides, its 5'-end associates with Pol II at the base of the dock domain. Since the initiation factor TFIIB binds to the dock domain and exit tunnel, exiting RNA may contribute to TFIIB displacement during the initiation to elongation transition and may prevent TFIIB re-association during elongation.

[1] J. Andrecka, R. Lewis, F. Brueckner, E. Lehmann, P. Cramer, J. Michaelis: Single-molecule tracking of mRNA exiting from RNA polymerase II, PNAS (accepted)

BP 26.35 Thu 17:00 Poster A

A Bayesian Approach to 3D Position Determination on the Nanometer Scale by Single-Pair FRET Experiments — •Adam Muschielok[1], Joanna Andrecka[1], Patrick Cramer[1,2], and Jens Michaelis[1] — [1]Department Chemie und Biochemie, Ludwig-Maximilians-Universität München — [2]Gene Center, Ludwig-Maximilians-Universität München

It is often desired to infer the relative position of a domain of a protein/nucleic acid complex that can't be localized by crystallographic means due to its high flexibility. Measurements of distances between two fluorescent dyes based on Fluorescence Resonant Energy Transfer (FRET) can yield this information if one dye molecule (target) is attached to the domain of interest and distance measurements to at least three other dye molecules (anchors) sitting in different but well known positions are carried out. Since the domain of interest is highly flexible, single-molecule measurements are necessary in order to understand the underlying dynamics. We present a new, Bayesian approach to analyze such experiments that is capable of inferring the target dye position and its uncertainty. Based on our measurements, we calculate the probability density distribution of the target dye position and display confidence volumes in the context of crystallographic structure. In contrast to ordinary trilateration this method is able to manage an arbitrarily large number of measurements and accounts for uncertainties in the anchor dye positions, the corresponding Förster radii and the FRET efficiency measurements itself. We apply this method to study yeast RNA polymerase II elongation complexes.

BP 26.36 Thu 17:00 Poster A

Untersuchung supramolekularer Kapseln mittels Dynamischer Einzelmolekül-Kraftspektroskopie — •Tobias Schröder[1], Björn Schnatwinkel[2], Dario Anselmetti[1] und Jochen Mattay[2] — [1]Experimentelle Biophysik, Fakultät für Physik, Universität Bielefeld, Bielefeld — [2]Organische Chemie 1, Fakultät für Chemie, Universität Bielefeld, Bielefeld

Eckel et al. zeigten erstmalig, dass die Einzelmolekül-Kraftspektroskopie zur Charakterisierung der Bindung in (photoschaltbaren) supramolekularen Wirt-Gast-Systemen genutzt werden kann.[1,2] Basierend auf diesen Experimenten werden erste Resultate der Kraftspektroskopie an supramolekularen Kapseln präsentiert und diskutiert. Durch Immobilisierung der Kapselbausteine am Cantilever und einem geeigneten Substrat können supramolekulare Kapseln mittels Dynamischer Einzelmolekül-Kraftspektroskopie untersucht werden.

[1] R. Eckel, R. Ros, B. Decker, J. Mattay, D. Anselmetti, Angew. Chem. 2005, 117, 489*492; Angew. Chem. Int. Ed. 2005, 44, 484*488. [2] C. Schäfer, R. Eckel, R. Ros, J. Mattay, D. Anselmetti, J. Am. Chem. Soc. 2007, 129, 1488*1489.

BP 26.37 Thu 17:00 Poster A

Computational studies of the visual pigment rhodopsin — •Minoru Sugihara[1,2], Peter Entel[1], and Volker Buss[2] — [1]Theoretical Low-Temperature Physics, University of Duisburg-Essen — [2]Theoretical Chemistry, University of Duisburg-Essen

Rhodopsin, the visual pigment in the vertebrate eye, is one of the prototypical G-protein-coupled receptors (GPCRs), which are responsible for signal transduction in mammalian cells. Like all membrane proteins, GPCRs are difficult to crystalize and no high-resolution structure of any GPCRs was known until 2000. There are now five structures of the rhodopsin dark state deposited with the Protein Data Bank and the resolution was extended to 2.2 angstrom [1], however it is still insufficient to unequivocally define the functionally important parts like the chromophore. In this work we address the chromophore geometries in rhodopsin and the first photo-intermediate, bathorhodopsin, by applying quantum mechanical / molecular mechanical (QM/MM) methodolgy based on the X-ray crystal structures [1,2,3]. Based on the calculated chromophore geometries, the spectral tuning mechanisms of the chromophore is discussed [2,4].

[1] Okada, T.; Sugihara, M.; Bondar, A.-N.; Elstner, M.; Entel, P.; Buss, V. J. Mol. Biol. 2004, 342, 571. [2] Schreiber, M.; Sugihara, M.; Okada, T.; Buss, V. Angew. Chem. 2006, 45, 4274. [3] Sugihara, M.; Hufen, J.; Buss, V. Biochemistry 2006, 45, 801. [4] Sekharan, S.; Sugihara, M.; Buss, V. Angew. Chem. Int. Ed. 2007, 46, 269.

BP 26.38 Thu 17:00 Poster A

Emergent vascular network inhomogeneities and resulting blood flow patterns in a growing tumor — •Michael Welter and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

We present and analyze a theoretical model for tumors growing in a host tissue that is vascularized with an arterio-venous blood vessel network. The tumor grows by coopting a massive vascular plexus which is progressively created by angiogenic sprouting. In the center, drastic vessel regression is apparent, accompanied by necrosis in unperfused regions. Few vessels survive, threading the tumor, cuffed by viable tumor cells (TCs). Via Monte-Carlo simulation, we analyze our hybrid cellular-automaton model where this behavior is realized by stochastical processes like sprouting, vessel removal, TC proliferation or TC death. Further we show current simulation results of the time-dependent distribution of drug injected into the blood stream.

BP 26.39 Thu 17:00 Poster A

Formation of Compartment Boundaries in Growing Tissues — •Jonas Ranft[1], Katharina Landsberg[2], Thomas Bittig[1], Reza Farhadi Far[1], Amani Said[2], Christian Dahmann[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstraße 108, 01307 Dresden, Germany

During the development of living organisms, tissues grow due to cell division. As the tissues grow, sharp boundaries between different cell populations within the tissue can emerge. The position of such compartment boundaries plays an important role in the patterning of the tissue. However, the mechanisms of the formation of these boundaries remain still unclear. We developed a stochastic model to describe epithelial tissue growth. The dynamics is described by balancing potential forces with friction forces that account for tissue viscosity. The potential forces describe adhesive forces as well as elastic forces. Our simulations show that a reduced attraction between cells of different types (which corresponds to a reduced cell-cell adhesion) can lead to the dynamic formation of a straight boundary during the growth process. This is a possible explanation of the presence of a straight interface between two cell populations with similar bulk mechanical properties.

BP 26.40 Thu 17:00 Poster A

Effect of fluctuations for the formation of spatial patterns of gene expression — •Thorsten Erdmann and Pieter Rein ten Wolde — FOM Institute for Atomic and Molecular Physics (AMOLF), Kruislaan 407, 1098 SJ Amsterdam, The Netherlands

During development of a drosophila embryo, the segmented structure of the adult body is determined by a sequentially refined pattern of gene expression domains along the anterior-posterior axis. The first zygotic genes to be expressed are the gap-genes. These are activated by the morphogen molecule bicoid and interact with each other by mutual repression or activation. The anterior-to-posterior gradient of morphogen concentration induces a stripe-pattern of domains in which one gene is predominantly expressed and the relative concentration of the corresponding protein is high. This pattern is very precise and robust against variations, e.g., in embryo length or morphogen concentration. Moreover, the domain boundaries are rather sharp although the small number of molecules makes fluctuations of protein concentration important and although small fluctuations in morphogen concentration close to the activation threshold strongly alter the expression level of a gene. We use a stochastic model for gene expression, protein diffusion and decay to investigate how domains of gene expression are positioned in space and how fluctuations affect the sharpness of their boundaries. Besides looking at a single target gene activated by the morphogen gradient we also investigate how a single morphogen gradient can control expression patterns of several, interacting genes.

BP 26.41 Thu 17:00 Poster A

A physical model for Bicoid controlled enhancers in *Drosophila* — •Wolfram Möbius[1,2] and Ulrich Gerland[2] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), LMU München — [2]Institute for Theoretical Physics, Universität zu Köln

Transcription activity of genes in eukaryotes is regulated by regions called cis-regulatory modules (CRM), in some cases located several thousands of base pairs up- or downstream of the gene of interest. While function of these CRMs, also called enhancers, has been qualitatively understood in terms of activating and repressing proteins binding to the DNA, a quantitative mapping from DNA sequence to transcription activity is still missing. In early Drosophila development, the protein Bicoid forms a concentration gradient along the embryo axis and controls various target genes which are expressed in different regions. We use this experimentally known mapping of Bicoid concentration to gene activation in vivo as well as Bicoid binding data to study correlations between Bicoid assembly at CRMs and transcription activity of the target genes.

BP 26.42 Thu 17:00 Poster A

Signal integration and stochastic decision making phosphorelay signal transduction — •Ilka Bischofs[1,2], Josh Hug[1], Aiwen Liu[1], David Lee[1], Denise Wolf[2], and Adam Arkin[1,2] — [1]University of Berkeley, USA — [2]Lawrence Berkeley Lab, Berkeley, USA

Phosphorelays are common architectures for integrating multiple signals in prokaryotic signal transduction. In B. *subtilis* a phosphorelay controls stress response induction in response to adverse environmental conditions. We investigate mechanisms of signal integration and stochastic decision making by time lapse microscopy of fluorescent reporter strains to quantify the dynamics of population heterogeneity. Through theoretical modelling we furthermore demonstrate that the complex feedback architecture found in the spo-relay confers robust signal amplification and robust integration of starvation and quorum signals.

BP 26.43 Thu 17:00 Poster A

On schemes of sequential transcription logic — •Georg Fritz[1,2] and Ulrich Gerland[1] — [1]Institute for Theoretical Physics, Universität zu Köln — [2]Department of Physics, LMU München

Many regulatory processes in molecular biology do not merely transform a set of simultaneous input conditions into an output signal, but instead yield a response that depends also on signals received in the past. For instance, such "sequential"regulatory logic is well documented in the development of multicellular organisms, where individual cells condition their phenotypic response not only on the present input signals, but also on the history of signals at the specific location in the tissue. In digital logic circuits, sequential logic elements are typically implemented by arrays of NAND-gates connected by feedback loops and comprise latches, flip-flops, and registers. Here, we explore the design characteristics of sequential regulatory logic in biology, starting with bacterial systems, where the basic molecular mechanisms for regulation are well understood. We previously showed that a specific "data-latch"may be readily implemented by cells through the use of protein heterodimerization [1]. We now use an unbiased *in silico* evolution approach to study the more general design principles of sequential transcription logic based on existing protein-protein interactions and simple transcriptional regulation.

[1] G. Fritz, N. Buchler, T. Hwa, and U. Gerland, Systems and Synthetic Biology **1**, 89-98 (2007)

BP 26.44 Thu 17:00 Poster A

Metabolic Synchronization of Yeast Cells — •Christian Warnke, Marcus J. B. Hauser, and Thomas Mair — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung Biophysik, Magdeburg, Germany

Yeast cells exhibit synchronization of their glycolytic activity when exposed to sugar. This behaviour is manifested as the appearance of oscillations in all intermediates of the glycolytiy pathway. The synchronization process is mediated via the extracellular exchange of the signalling molecule acetaldehyde, an intermediate of the glycolytic pathway. We have investigated the synchronization of yeast cells at varying extracellular acetaldehyde concentrations and at different metabolic states of the cells. We found a pronounced difference in the synchronization behaviour in response to acetaldehyde for the yeast strains Saccharomyces cerevisiae and Saccharomyces carlsbergensis. Our data indicate that these different behaviours can be explained by the different fermentative capacity of the two strains.

BP 26.45 Thu 17:00 Poster A

Simulation of protein kinase C alpha (PKCα) membrane translocation processes — •Martin Peglow and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

PKCα is a versatile key for decoding the cellular calcium toolkit. During their measurements of PKCα membrane translocations, which are activated through intracellular Ca^{2+} release, Reither and Lipp [1] found two populations of so called Local Translocation Events (LTEs). One population whose life times correspond to the duration of the underlaying Ca^{2+}-signals and a second population the so called long lasting LTEs ($T > 4s$). The source or appearance of the long lasting LTEs can't be explained for sure. Theoretical assumptions for possible mechanisms shall be verified by our simulations. An efficient Monte Carlo algorithm for simulations of reaction-diffusion kinetics in single cells, the "Next Subvolume Method" [2], is presented here.

[1] Dr. Gregor Reither, EMBL Heidelberg and Prof. Peter Lipp, Institut für Molekulare Zellbiologie Universität des Saarlandes, JCB, 174, 521, (2006)
[2] J. Elf, A. Doncic, M. Ehrenberg, Proceeding of SPIE, 5110, (2003)

BP 26.46 Thu 17:00 Poster A

Designing Biomolecule-Nanoparticle Interfaces for the Regulation of Cell Fate — •Lisa Maus[1], Roberto Fiammengo[1], Oliver Dick[2], Malte Wittmann[2], Hilmar Bading[2], and Joachim P. Spatz[1] — [1]Max-Planck-Institute for Metals Research, Dept. of New Materials & Biosystems & University of Heidelberg, Dept. of Biophysical Chemistry, Heisenbergstr. 3, D - 70569 Stuttgart — [2]University of Heidelberg, Interdisciplinary Center for Neurosciences, Dept. of Neurobiology, Im Neuenheimer Feld 364, D - 69120 Heidelberg

We are aiming at designing stable nanoparticles functionalized with biomolecules to study cell death pathways in primary hippocampal neurons. Due to their unique properties metal nanoparticles show great promise as drug delivery systems and intracellular contrast agents. Especially gold nanoparticles have been studied intensely, due to their high biocompatibility and well known thiol chemistry. The synthesized particles are passivated with PEG thiol derivatives to prevent aggregation in high ionic strength solutions. They are further functionalized with a peptide that is known to specifically block NMDA receptors (N-methyl-D-aspartate) crucial for calcium influx in postsynaptic neurons. Elevated intracellular calcium levels triggered by calcium entry through synaptic NMDA receptors promote cell survival. In contrast, calcium entry through extrasynaptic NMDA receptors seems to initiate cell death cascades. This concept of differential signalling by synaptic and extrasynaptic NMDA receptors is important for the understanding of neuronal diseases such as stroke in which brain damage may be caused by activation of extrasynaptic NMDA receptors.

BP 26.47 Thu 17:00 Poster A

Glycolytic oscillations in a layer of interacting cells — •Jana Schütze and Jana Wolf — AG Theoretische Biophysik, Humboldt-Universität zu Berlin

Synchronisation of glycolytic oscillations in populations of yeast cells has been intensively analysed experimentally as well as theoretically. There is evidence that the individual cells communicate by exchanging products of glycolysis as acetaldehyde, for which the plasma membrane is permeable. Whereas previous models considered well stirred cell suspensions we here analyse the dynamics in a layer of cells. We aim to understand the conditions for wave initiation as observed in experiments where glucose was added to starved cells in a limited region of a cell layer.

For the generation of oscillations in the individual cells a two-component model containing an autocatalytic step is used. Cells are embedded in an extracellular medium in which the added glucose and the extracellular product can diffuse. Intercellular coupling takes place via the exchange of the end product. For single cells and a small number of interacting cells, the oscillations can be studied by using bifurcation analysis. In two-dimensional spatial arrangements of cells where glucose injection is continuously confined to a limited number of cells, waves of glycolytic oscillations can be observed. The strength of the product coupling as well as the stationary glucose distribution effect the existence and the range of waves, the propagation velocity and the period of the oscillations.

BP 26.48 Thu 17:00 Poster A

Formation of Domains in Bacterial Flagella — •Reinhard Vogel and Holger Stark — Institute for Theoretical Physics, TU Berlin, Germany

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 characterised by their pitch, radius and helicity (polymorphism). Finally the flagellum assumes its original form and returns into the bundle.

In general, the helical shape of the bacterial flagellum can assume 11 different configurations depending e.g. on mechanical loading, temperature and chemical composition of the solution. In recent optical tweezer experiments, Darnton and Berg [1] pulled at the flagellum and induced transformations between different helical configurations but they also observed the simultaneous occurrence of two configurations separated by a transition region. We investigate this domain formation based on the helical Kirchoff-rod model and the Calladine model [2] for the bacterial flagellum and present first results of our theoretical study.

[1] N.C.Darnton H.C. Berg, Biophys. J. 92, 2230-2236 (2007)
[2] C.R. Calladine,Nature (London) 255, 121 (1997)

BP 26.49 Thu 17:00 Poster A

Which Network Connectivities generate a given Dynamics? II: Network Reconstruction — •Frank van Bussel[1,2], Lishma Anand[1,2], Raoul-Martin Memmesheimer[1,2], and Marc Timme[1,2] — [1]Network Dynamics Group, MPI f. Dynamics & Self-Organization — [2]Bernstein Center for Computational Neuroscience, Göttingen

We present two alternative perspectives towards understanding relations between structure and dynamics in neural networks. In the first contribution, we present a design method [1], that enables us to find all networks as well as the structurally optimal network that generate a given neural spiking dynamics.

In this second part, we present a method to reconstruct the connectivity of a given network from its response dynamics to external driving signals. For a given driving signal, measuring how the collective state changes, reveals information about how the units are interconnected [2]. Sufficiently many repetitions for different driving conditions yield the entire network connectivity from measuring the response dynamics only [3]. We discuss possible applications to dimensionally reduced time series from coupled high-dimensional systems.

[1] R.-M. Memmesheimer and M. Timme,
Phys. Rev. Lett. 97:188101 (2006); Physica D 224:182 (2006).
[2] M. Timme, Europhys. Lett. 76:367 (2006).
[3] M. Timme, Phys. Rev. Lett. 98:224101 (2007).

BP 26.50 Thu 17:00 Poster A

Which Network Connectivities generate a given Dynamics? I: Optimal Network Design — •Raoul-Martin Memmesheimer[1,2], Lishma Anand[1,2], Frank van Bussel[1,2], and Marc Timme[1,2] — [1]Network Dynamics Group, MPI f. Dynamics & Self-Organization — [2]Bernstein Center for Computational Neuroscience, Göttingen

We present alternative perspectives towards understanding relations between structure and dynamics in neural networks.

First, can we design a network, e.g. by modifying the features of units or interactions, such that it exhibits a desired dynamics? Here we positively answer this question analytically for a class of networks of spiking neural oscillators [1, 2], by finding the set of all networks that exhibit a given arbitrary periodic spike pattern as an invariant dynamics. We illustrate the applicability of the method by designing networks that exhibit a predefined dynamics and simultaneously minimize the networks' wiring costs, i.e. are structurally optimal.

In a second contribution "Network Reconstruction" we present a method to infer the connectivity of a given network from its response dynamics to external driving signals [3,4].

[1] R.-M. Memmesheimer and M. Timme,
Phys. Rev. Lett. 97:188101 (2006).
[2] R.-M. Memmesheimer and M. Timme, Physica D 224:182 (2006).
[3] M. Timme, Europhys. Lett. 76:367 (2006).
[4] M. Timme, Phys. Rev. Lett. 98:224101 (2007).

BP 26.51 Thu 17:00 Poster A

Spectral measures of different integrate-and-fire neurons and how stimulus-induced synchrony varies among them — •Rafael Vilela and Benjamin Lindner — Max Planck Institute for the Physics of Complex Systems - Dresden

Integrate-and-fire (IF) neurons have found wide-spread applications in computational neuroscience, in particular, in stochastic versions of these models. Here we present results on the white-noise driven perfect, leaky, and quadratic integrate-and-fire models and focus on the spectral statistics (power spectra, cross spectra, and coherence functions) in different dynamical regimes (noise-induced and deterministic firing regimes with low or moderate noise). We make the models comparable by tuning parameters such that the mean value and the coefficient of variation of the interspike interval agree for all of them. We find that under these conditions, the power spectrum under white-noise stimulation is very similar while the response characteristics (characterized by the cross spectrum between a fraction of the input noise and the output spike train) differs in part drastically. We also investigate how two neurons of the same kind (e.g. two leaky integrate-and-fire neurons) synchronize if they share a common noisy input. We show that depending on the dynamical regime either two quadratic IF models or two LIFs are best synchronized. Our results suggest that for network simulations when choosing among simple integrate-and-fire models, the details of the model have a strong effect on synchronization behavior and regularity of the output.

BP 26.52 Thu 17:00 Poster A

Poisson-Nernst-Planck description of nonequilibrium membrane potentials — •David Hofmann and Joachim Dzubiella — Physics Department, TU-Munich

The time-dependent Nernst-Planck and Poisson equations are solved numerically for a model cell membrane between aqueous reservoirs containing several ionic species. The steady state situation is analyzed and compared to the Goldman-Hodgkin-Katz equation, the analytical description of a cell membrane resting potential. Furthermore the full non-equilibrium situation is analyzed in order to describe the dynamic evolution of an action potential. The results are compared to

the Hodgkin-Huxley model and available experimental data.

BP 26.53 Thu 17:00 Poster A

A Paradigm for Phenotype Decision: Non-linear Dynamics Coupled to Low Number Stochastic Effects — •Jan-Timm Kuhr[1,3], Madeleine Leisner[2,3], Joachim Rädler[3], Berenike Maier[2,3], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, Germany — [2]Institut für Allgemeine Zoologie und Genetik, Westfälische Wilhelms Universität, Germany — [3]Department für Physik, Ludwig-Maximilians-Universität München, Germany

Many organisms show a variety of phenotypes, even in populations consisting of genetically identical individuals. An example is the bacterium *B. subtilis*: Upon overpopulation a fraction cells switches to the "competent" phenotype, developing the trait of taking up genetic material from the surrounding medium and integrating it into their own genome, thereby speeding up evolution of the species. The bulk population, reproducing asexual, holds up a status quo while competent cells increase genetic variability by switching to quasi-sexual reproduction.

Here we present a scheme describing this extraordinary process by non-linear dynamics coupled to low-number stochastic effects of the involved molecular components. A two-component system is derived, explaining different phenotypes by bifurcation analysis and switching by intrinsic fluctuations intensified by auto-feedback. All parameters where chosen in accordance with previous experiments. The model quantitatively reproduces our experimental findings and explains the fractional onset of competence development on the single cell level.

BP 26.54 Thu 17:00 Poster A

influence of mass–dependent metabolic rates on food web stability — •Boris Kartascheff and Barbara Drossel — TU Darmstadt, Institute of Condensed Matter Physics, Hochschulstr. 6, D-64289 Darmstadt

Most basic approaches to modeling food web dynamics lead to a negative relation between the complexity and the stability of networks, if complexity is measured in terms of connectance or species number. This is in contrast to empirical data, which suggest that complex food webs are at least as likely to persist in time as simpler predator–prey systems.

In this study, we investigate the effect of allometric scaling, i.e. of metabolic rates that decrease as an inverse power of the body mass (which in turn depends on the trophic level), on food web stability. We randomly initiate networks and evaluate how many species survive until population dynamics reaches a stationary state. We investigate the effect of allometric scaling on the stability of networks with different structure (random, layered, niche models) and with different population dynamics (without and with adaptive foraging).

In this way, we are able to reveal the generic mechanisms that allow certain food web models to show remarkably increased stability when allometric scaling is included. Besides computer simulations, we also apply analytical methods to obtain answers to the question whether the existence of different sized species in ecosystems is crucial to their stability.

BP 26.55 Thu 17:00 Poster A

Dynamics of RNA evolution on realistic fitness landscapes — •Klaus Blindert — University of Cologne, Germany

The folding and function of RNA molecules strongly constrains the evolution of their sequences, by producing complex epistatic interactions between individual sequence positions. For instance, the deleterious effect of a mutation can often be compensated by a different mutation, which either directly or indirectly restores the folded basepairing pattern. To analyye the evolutionary dynamics of such compensatory effects, we use realistic models for RNA folding and fitness functions derived from existing structural alignments. We study the relative importance of direct (that is restoring a Watson-Crick base pair) and indirect compensation (e.g. lowering the free energy of the motif at an unrelated site) using simple RNA structural motifs such as hairpins. Our evolutionary model is based on the well-established Wright-Fisher model. To explore a wide range of parameters in our simulations, we apply a new technique, which approximates the evolutionary dynamics of multiple alleles under mutation, genetic drift and weak selection.

BP 27: Membrane Morphology and Adhesion

Time: Friday 10:15–12:45 Location: C 243

Invited Talk BP 27.1 Fri 10:15 C 243

Secretion of protein-coated vesicles — •Pierre Sens — CNRS, PhysicoChimie Théorique - ESPCI, Paris

Cellular trafficking generally involves spherical or tubular membrane vesicles, the formation of which often rely on the aggregation of membrane proteins (COPI, COPII, Clathrin and Caveolae). I will review some of the theoretical models that have been developed to describe this phenomenon, with particular emphasis on systems driven out of equilibrium by the expenditure of energy through the activity of GTPases proteins. I will show how vesicle secretion and traffic can be very efficiently regulated by the alteration of the GTP hydrolysis cycle, which is known to be affected, for instance, by the presence of cargo.

BP 27.2 Fri 10:45 C 243

Fluctuations of red blood cell membranes — •Thorsten Auth[1,2], Nir S. Gov[1], and Samuel A. Safran[1] — [1]Weizmann Institute of Science, Rehovot 76100, Israel — [2]Forschungszentrum Jülich, IFF, 52425 Jülich, Germany

We model the red blood cell membrane by a lipid bilayer that is coupled to a polymerized membrane. Using experimental fluctuation spectra, this model allows us to determine the elastic constants and to quantify the active, ATP-driven fluctuations. The extensive experimental studies on and the easy availability of red blood cells make them especially attractive for setting up and testing theoretical models to quantitatively explain the experimental results. However, using a simple fluid-polymerized membrane model, several basic aspects regarding the mechanical properties of the cell membrane are not completely understood. On the one hand, static deformation experiments indicate that the cell is very stiff with a high shear modulus of the order of $10^{-3} - 10^{-2}\,\mathrm{k_B T\,nm^{-2}}$. On the other hand, the relatively large fluctuation amplitudes, observed in light scattering/video microscopy spectra at wavevectors, $q \approx 0.010\,\mathrm{nm^{-1}}$, indicate that the shear modulus is small. Furthermore, experiments that measure the fluctuation amplitude as a function of the position on the cell are — within the continuum theory — compatible only with a vanishing shear modulus. We have performed simulations of inhomogeneous membranes and find that localized fluctuations, due to irregularities of the cytoskeleton, are capable to explain both riddles.

BP 27.3 Fri 11:00 C 243

Adhesion dynamics of fluctuating membranes — •Ellen Reister-Gottfried and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

We study a system consisting of a fluctuating membrane close to a flat substrate that may adhere to the substrate via receptor-ligand bonds that we model as springs with a certain stiffness. We keep the position of the ligands on the substrate fixed and assume such a high abundance of receptors in the membrane that lateral diffusion has no influence on the adhesion process. While the energy of the membrane and the bonds combined with an appropriate Onsager coefficient determine the equation of motion for the membrane, the binding and unbinding of receptor-ligand pairs is expressed with Kramers rates, that depend on the local distance between membrane and substrate. Applying stochastic simulations we study the adhesion process of an initially unbound membrane as a function of binding energy, spring stiffness, and bending rigidity of the membrane. We analyse two limiting cases: the average distance between the membrane and substrate is *i)* either fixed or *ii)* variable allowing center of mass movement of the membrane. For *i)* we find that membrane fluctuations together with the height dependent reaction rates increase the number of bonds compared to a flat membrane. Furthermore, strong spatial correlations between the bonds are observed. In situation *ii)* equilibrium calculations for a flat membrane reveal a bimodal binding probability for certain

binding energies. Our simulations show that membrane fluctuations break this bimodality. Additionally, spatial correlations are reduced compared to *i)*.

BP 27.4 Fri 11:15 C 243

Large scale organization in crowded membranes — •Stefan Semrau[1], Timon Idema[2], Cornelis Storm[2], and Thomas Schmidt[1] — [1]Physics of Life Processes, Leiden University, The Netherlands — [2]Lorentz Institute for Theoretical Physics, Leiden University, The Netherlands

Over the past years, the classical fluid mosaic model - in which membrane proteins have ample space to explore the entire membrane - has undergone some serious revision. In actuality, the membrane environment is highly crowded and heterogeneous. Crowding has profound implications for the dynamical behavior of the proteins, and is therefore a determining factor for the mechanisms of cell signaling. Only very recently the importance of membrane mediated interactions in such processes was recognized. Here we use two-phase GUVs (giant unilamellar vesicles) with multiple budded, liquid ordered domains to model this class of interactions. Such budded domains repel as our recent analytical model of completely phase separated GUVs (Semrau, Idema et al.) suggests. Here we measure the strength of the repulsion by analysis of domain diffusion and find that it gives rise to a preferred domain size. Furthermore, we observe that the interaction strength has peaks at distinct domain sizes. These sizes correspond to the addition of a domain to a shell of domains surrounding a central, pinned domain. This implies that in a crowded system governed by membrane mediated interactions clustering of proteins of similar size or interaction strength is promoted.

15 min. break

BP 27.5 Fri 11:45 C 243

Coarse-grained simulation studies of peptide-induced pore formation in lipid membranes — Gregoria Illya[1,2] and •Markus Deserno[2,3] — [1]Institut für Anorganische und Physikalische Chemie, TU Darmstadt, Petersenstraße 20, 64287 Darmstadt — [2]MPI für Polymerforschung, Ackermannweg 10, 55128 Mainz — [3]Department of Physics, Carnegie Mellon University, 5000 Forbes Ave, Pittsburgh PA 15213, USA

We investigate generic aspects of the impact of antimicrobial peptides on lipid membranes using a solvent-free coarse-grained simulation technique. Lipids are modeled as strings of four beads, peptides as bead-composed cylinders with hydrophilic caps and a transmembrane hydrophobic region with possibly small hydrophilic strips. As a function of hydrophobic peptide-lipid attraction the preferred state of the peptide changes from desorbed to adsorbed to inserted, and peptides can mutually catalyze their own insertion. In the presence of hydrophilic strips along the transmembrane region peptides aggregate to form pores in the bilayer, whose size and morphology depends on the generic interaction parameters. For instance, whether pores appear as "toroidal" or "barrel stave" is triggered by the strength of an additional hydrophobic peptide-peptide cohesion beyond the hydrophilicity-driven pore formation.

BP 27.6 Fri 12:00 C 243

Phase Separation in Membranes on Corrugated Substrates — •Bartosz Rozycki, Thomas R. Weikl, and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany

We study separation of two liquid phases in lipid membranes that strongly adhere to a corrugated solid substrate. Both mean field theory and Monte Carlo simulations show that the spatial distribution of the two liquid phases are governed by membrane curvature. [1] For small curvature amplitudes, the membrane undergoes complete separation of the two liquid phases. For larger membrane curvature amplitudes, the two phases form patterns which follow the membrane curvature contour lines. These theoretical results are in agreement with recent experiments [2,3] and explain a possible control mechanism of domain arrangement in biological membranes.

[1] Bartosz Rozycki, Thomas R. Weikl, Reinhard Lipowsky (in preparation). [2] Tae-Young Yoon et. al, Nature Matherials 5, 281 (2006). [3] Raghuveer Parthasarathy, Cheng-han Yu, and Jay T. Groves, Langmuir 22, 5095 (2006).

BP 27.7 Fri 12:15 C 243

Curvature induced interaction between a membrane protein and a fluctuating model membrane: the influence on membrane dynamics and protein diffusion — •Stefan Leitenberger, Ellen Reister-Gottfried, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

In our work the influence of an interaction between a curved protein and a fluctuating membrane whose energy is given by the Helfrich Hamiltonian on the dynamics of the system is analyzed. We derive coupled equations of motion for the membrane dynamics and the lateral protein diffusion. In a first step, the influence of the protein on the membrane dynamics is neglected. Within this approximation we calculate the curvature-coupled diffusion coefficient, which is enhanced compared to free diffusion. This increase is caused by the additional force acting on the protein. To probe our results and overcome other approximations of the calculations, we set up simulations that also neglect the changed membrane dynamics. Comparing the results we find qualitative agreement, however, the diffusion coefficients achieved in the simulations are smaller since the particle tries to follow energetically favorable positions. Correlations between protein position and local membrane shape are not accounted for correctly in the analytical calculations. In a second step, the influence of the curvature-coupling on the membrane dynamics is taken into account. Using an extension of our simulation scheme we study the changed height correlations of the membrane and the effect on the lateral protein diffusion as a function of the protein's spontaneous curvature and bending rigidity.

BP 27.8 Fri 12:30 C 243

Contact lines for fluid surface adhesion — •Martin Michael Müller[1,2], Markus Deserno[1,3] und Jemal Guven[4] — [1]Max Planck Institute for Polymer Research, D-55128 Mainz, Germany — [2]Laboratoire de Physique Statistique, ENS, F-75231 Paris Cedex 05, France — [3]Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15213, USA — [4]Instituto de Ciencias Nucleares, UNAM, Apdo. Postal 70-543, 04510 México D.F., Mexico

When a fluid membrane or a similar surface adheres to a substrate, the location of the contact line adjusts in order to minimize the overall energy. This implies boundary conditions which depend on the characteristic surface deformation energies. In this talk a general geometrical framework is presented within which these conditions can be derived in a completely systematic way [1,2]. Both adhesion to a rigid substrate as well as adhesion between two fluid surfaces will be treated and illustrated for several important Hamiltonians involving both curvature and curvature gradients.

[1] M. Deserno, M. M. Müller, and J. Guven, Phys. Rev. E **76**, 011605 (2007). [2] M. M. Müller, Phd thesis, available at http://www.geomnat.com/veroeff_en.php

BP 28: Molecular Recognition

Time: Friday 10:45–12:45 Location: PC 203

BP 28.1 Fri 10:45 PC 203

Influence of Sequence Correlations on Molecular Recognition — •Hans Behringer and Friederike Schmid — Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld

Equilibrium aspects of molecular recognition are investigated using coarse-grained models for the recognition process of two rigid biomolecules. To this end, a two-stage approach is adopted. First, the structure of the target molecule is fixed and learned by a probe molecule resulting in an ensemble of probe sequences. In a second step the recognition ability of the designed probe ensemble with respect to the chosen target sequence is tested by comparing the free energy of association with the previously fixed target structure and a different competing structure. Particular attention is paid to the influence of correlations in the hydrophobicity distributions on the recognition sites of the molecules on the recognition ability of the probe molecules.

Behringer, H., A. Degenhard, F. Schmid 2007, Coarse-Grained Lat-

tice Model for Investigating the Role of Cooperativity in Molecular Recognition, *Phys. Rev. E* **76**, 031914.

BP 28.2 Fri 11:00 PC 203

Structure based prediction of protein-DNA recognition — Sahand Jamal Rahi[1], •Peter Virnau[2], Mehran Kardar[1], and Leonid A. Mirny[1,3] — [1]Massachusetts Institute of Technology — [2]Johannes Gutenberg-Universität Mainz — [3]Harvard-MIT Division of Health Sciences and Technology

Binding of proteins to specific DNA sites is central for several vital biological processes, such as regulation of genes, replication of DNA and repair of DNA damage. The challenge can be formulated as follows: Given the structure of a protein-DNA binding complex, predict sites in the genome which the protein recognizes, i.e., to which it binds with significant affinity. In this talk, we will discuss the predictive quality of atomistic force-fields in conjunction with molecular mechanics calculations and compare results with predictions from bioinformatics for the PurR protein-DNA complex. We will also compare binding energies derived from simulations with experimental binding energies for several amino acid and DNA point mutations.

BP 28.3 Fri 11:15 PC 203

The impact of defects on the binding affinity of surface bound oligonucleotide-duplexes — Thomas Naiser[1], Oliver Ehler[1], •Jona Kayser[1], Timo Mai[1], Wolfgang Michel[1], and Albrecht Ott[1,2] — [1]Experimentalphysik I, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]Biologische Experimentalphysik, Universität des Saarlandes, D-66041 Saarbrücken, Germany

It is not fully understood how point defects and loop insertion affect the stability of DNA duplexes. This is for example of interest in the context of genotyping microarrays which base on the reduced binding affinity of non-perfect match duplexes. In order to study the complex problem of surface based hybridization in more detail, we performed array based hybridization experiments in simple and well controlled situations without competitive binding. The microarrays are produced in our lab using Light Directed Polymerization (LDP) of phosphoramedites on a dendrimer substrate. This technique provides a high flexibility in array design. We report a strong positional dependence of the influence of single base bulges and single base mismatches with increasing importance towards the middle of the strand. To explain the observed behavior we propose a molecular zipper. Direct comparison between binding affinities of DNA/DNA and RNA/DNA duplexes shows that for RNA/DNA purine-purine mismatches are most destabilizing whereas for DNA/DNA the affected base pair is the relevant parameter. We attribute these differences to the different structures of the duplexes (A vs. B form).

BP 28.4 Fri 11:30 PC 203

Physical-Chemistry Analysis of Microarray Data — •K. Myriam Kroll[1], Gerard Barkema[2,3], and Enrico Carlon[1] — [1]Institute for Theoretical Physics, KU Leuven, Celestijnenlaan 200D, B-3000 Leuven, Belgium — [2]Institute for Theoretical Physics, Universiteit Utrecht, Leuvenlaan 4, 3584 CE, Utrecht, The Netherlands — [3]Institute-Lorentz for Theoretical Physics, University of Leiden, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands

DNA microarrays are comparably novel devices which allow to monitor the gene expression level of thousands of genes simultaneouly on a genome-wide scale. The underlying principle of these DNA chips is the hybridization process between surface-bound DNA sequences (probes) and the so-called target sequences (DNA or RNA) which are floating in solution. From the amount of hybridized targets, information about the presence of certain genes in solution can be extracted and conclusions concerning the gene expression level can be drawn. However, due to non-specific binding the measured signal contains a noisy background component which makes the data analysis and interpretation rather difficult. In this talk, we focus on the theoretical analysis of the publicly available data of microarray experiments performed on Affymetrix GeneChips. By combining well-established models from physical chemistry (Nearest Neighbor Model) and statistical mechanics, we construct a functional to predict the background intensity on every single spot on the chip. We then compare the results to other background subtraction schemes and show that our approach performs better on a global scale.

BP 28.5 Fri 11:45 PC 203

Switchable DNA layers - a versatile instrument for protein detection on a chip — •Wolfgang Kaiser[1], Erika Pringsheim[1], Jelena Knezevic[1], Kenji Arinaga[2], Shozo Fujita[2], Naoki Yokoyama[2], Ulrich Rant[1], and Gerhard Abstreiter[1] — [1]Walter Schottky Institut, Technische Universität München, Deutschland — [2]Fujitsu Laboratories Ltd., Atsugi, Japan

We present a new technique to detect label free protein targets by switchable DNA-layers. The concept is to "switch" surface bound DNA molecules by applying external AC fields. By varying the electrical field the DNA molecule changes its orientation from lying to upright and back, which is monitored in real-time by observing the fluorescence of a dye-label on the distal end of the DNA. Distance dependent energy transfer from the dye to the metal surface governs the fluorescence emission.

For the detection of proteins, the DNA is additionally functionalized with a chemical label which acts as a specific binding site for proteins. When proteins bind to this label, we observe a distinct shift in the switching behavior. At high switching frequencies DNA-protein-complexes can be discriminated from uncomplexed DNA due to their different hydrodynamic mobility. We present sensing experiments of streptavidin and antibiotin, and discuss the influence of the proteins' weight and hydrodynamic diameter (measured by dynamic light scattering) to the switching dynamics.

Switchable DNA layers make the determination of the hydrodynamic mobility / weight of proteins in a chip-compatible format possible.

BP 28.6 Fri 12:00 PC 203

Beyond modular structure in protein-interaction networks — Stefan Pinkert[1], •Jörg Reichardt[2], and Jörg Schultz[1] — [1]Dept. of Bioinformatics, University of Würzburg — [2]Institute f. Theoretical Physics, University of Würzburg

The availability of large-scale databases on protein-protein interaction (PPI) has lead to a surge of research for structure in this data and biological information following from it. The paradigm of these approaches is that the inner workings of the cell are organized into relatively independent modules. Researchers have hence been trying to discover biological information in PPI networks by looking for densely connected groups of proteins, so-called modules or clusters, which are only sparsely connected to the rest of the network. In this contribution, we show that this search for cohesive clusters in PPI networks falls short of the rich structure present in these data and can only represent a small portion of the biological information present in these networks. We introduce an analysis method which is able to overcome these limitations and apply it to the Human Protein Reference Database (HPRD). We provide an insight into the large scale organization of the human protein interaction network and discuss possible biases in the network coming from the combination of yeast-2-hybrid, in vitro and in vivo experiments.

BP 28.7 Fri 12:15 PC 203

separation of specific sequence oligonucleotides from a yeast genome using single primer abrupt termination PCR (SPAT-PCR) — •harish bokkasam — Department of Biological Experimental Physics, University of Saarbrücken, Saarbrücken, Germany

As a step towards gene expression analysis with short DNA fragments (20-50 bp), we develop a novel technique for fishing out a sequence specific oligonucleotide from a yeast genome. This method is based on SPAT-PCR, using a single primer and a temperature jump resulting in abrupt termination of the PCR cycle and interruption of the elongation of the primer on the RNA template. We design a complementary primer to select the specific sequence oligonucleotide (SSON). The intermediate product, consisting of the required SSON, excess primer and RNA template, is visualized and subsequently separated using gel-electrophoresis. The obtained SSON then serves as template for PCR amplification. The accuracy of this method can further be tested by using the obtained SSON as a target in array-based hybridisation experiments.

BP 28.8 Fri 12:30 PC 203

Stochastic dynamics of protein assembly — •Jakob Schluttig and Ulrich Schwarz — University of Heidelberg, Bioquant, BQ 0013 BIOMS Schwarz, INF 267, D-69120, Heidelberg, Germany

The growing interest in structure and dynamics of protein assemblies requires the development of computer time-efficient modelling methods. In our approach, we combine efficient methods from stochastic dynamics with molecular information derived from all-atom simulations. In order to bridge these two fields, we use the concept of an encounter complex, which denotes an intermediate state of mutual entanglement

separating the spatially completely separated reaction partners and the bound state. The stochastic transport process preceeding the formation of the encounter complex is described with a Langevin equation. The effect of anisotropic proteins and anisotropic intermediates is studied using non-diagonal mobility matrices. Long-ranged (electrostatic) interactions can be taken into account using appropriate drift terms. We apply our methods to several cases of biological interest, including bi-molecular reactions like barnase-bastar and large assemblies like viral capsids.