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Fachverband Biologische Physik (BP)

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Overview of Invited Talks and Sessions

(lecture rooms H 1028 and H 1058; Poster A)

Plenary, Keynote and Prize Talks related to BP

PV I	Mon	8:30– 9:15	H 0105	**Survival in the face of the unknown: some lessons from bacteria** — •Stanislas Leibler
PV III	Mon	14:00–14:45	ER 270	**Soft Matter and Life Sciences: Research with Neutrons** — •Dieter Richter
PV XIX	Thu	13:15–14:00	H 0105	**Mechanics and Growth of Tissues** — •Jean-Francois Joanny
PV XX	Thu	14:00–14:45	H 0105	**How superficial is adhesion? Common fundamentals of gecko, bacteria, protein and thin film adhesion** — •Karin Jacobs
PV XXII	Thu	14:00–14:45	EW 201	**3D imaging of lung tissue during total liquid ventilation** — •Christian Schnabel, Sven Meissner, Maria Gaertner, Edmund Koch
PV XXIV	Fri	8:30– 9:15	H 0105	**Role of van der Waals Interactions in Physics, Chemistry, and Biology** — •Matthias Scheffler

Invited Talks

BP 1.1	Mon	9:30–10:00	H 1058	**Friction and Hydration Repulsion Between Hydrogen-Bonding Surfaces** — •Roland Netz
BP 2.1	Mon	9:30–10:00	H 1028	**Membrane tension regulates motility by controlling lamellipodium organization** — •Julie Plastino
BP 1.7	Mon	11:30–12:00	H 1058	**Cryo electron microscopy of biological materials** — •Wolfgang Baumeister
BP 6.1	Mon	15:00–15:30	H 1028	**Intercellular Interactions and the Mystery of Growth Control** — •Boris Shraiman
BP 10.1	Tue	9:30–10:00	H 1058	**Surface topology effect on cell interaction at the nanoscale** — •Giuseppe Battaglia
BP 13.1	Wed	9:30–10:00	H 1058	**Chemo-mechanics of a ring-shaped helicase during unwinding** — •Michael Schlierf, Ganggang Wang, Xiaojiang Chen, Taekjip Ha
BP 14.1	Wed	9:30–10:00	H 1028	**Membrane transformations in vesicles enclosing aqueous two-phase polymer solutions** — •Rumiana Dimova
BP 15.1	Wed	15:00–15:30	H 1058	**Electron Paramagnetic Resonance in Protein Science** — •Malte Drescher
BP 16.1	Wed	15:00–15:30	H 1028	**Molecular Crowding Creates Traffic Jams of Kinesin Motors On Microtubules** — •Cecile Leduc, Kathrin Padberg-Gehle, Vladimír Varga, Dirk Helbing, Stefan Diez, Jonathon Howard
BP 16.2	Wed	15:30–16:00	H 1028	**Collective properties of molecular motors** — •Jean-François Joanny
BP 23.1	Thu	15:00–15:30	H 1028	**Actin network architecture determines myosin motor activity** — •Laurent Blanchoin
BP 31.1	Fri	9:30–10:00	H 1058	**High-speed imaging of organogenesis in entire zebrafish with SPIM** — •Jan Huisken

Invited Talks of the Joint Symposium 100 Years of X-ray Diffraction

Organizers Leonore Wiehl, Gerhard Grübel and Joachim Rädler. For more details see SYXD.

SYXD 1.1	Mon	15:00–15:30	H 0105	**Disputed discovery: The beginnings of X-ray diffraction in crystals** — •Michael Eckert
SYXD 1.2	Mon	15:30–16:00	H 0105	**Why are quasicrystals quasiperiodic?** — •Walter Steurer
SYXD 1.3	Mon	16:00–16:30	H 0105	**Coherent Diffraction Imaging with Free-Eletron Lasers** — •Massimo Altarelli
SYXD 1.4	Mon	16:30–17:00	H 0105	**X-ray free-electron lasers - emerging opportunities for structural biology** — •Ilme Schlichting
SYXD 1.5	Mon	17:00–17:30	H 0105	**Structure analysis by x-ray diffraction and x-ray imaging: beyond crystals, beyond averages, and beyond modeling** — •Tim Salditt

Invited Talks of the Joint Symposium Control of Network Dynamics

Organizers Eckehard Schöll and Stefan Bornholdt. For more details see SYND.

SYND 1.1	Thu	9:30–10:00	H 0105	**Controlling Complex Networks with Compensatory Perturbations** — •Adilson E. Motter
SYND 1.2	Thu	10:00–10:30	H 0105	**Toward control, prediction, and optimization of biological and engineering complex networks** — •Kazuyuki Aihara
SYND 1.3	Thu	10:30–11:00	H 0105	**Design of robust functional networks as complex combinatorial optimization problem** — •Alexander S. Mikhailov
SYND 1.4	Thu	11:00–11:30	H 0105	**Braess Paradox, (In-)Stability and Optimal Design: Nonlinear Dynamics of Modern Power Grids** — •Marc Timme, Dirk Witthaut, Martin Rohden, Andreas Sorge
SYND 1.5	Thu	11:30–12:00	H 0105	**Delay-Coupled Laser Networks: Complex Behavior, Synchronization and Applications** — •Ingo Fischer

Invited Talks of the Joint Symposium Origin of Life

Organizers Karin Jacobs, Karsten Kruse, Albrecht Ott and Ulrich Gerland. For more details see SYOL.

SYOL 1.1	Fri	9:30–10:00	H 0105	**From sequence to function: Random polymerization and modular evolution of RNA** — •Susanna C. Manrubia
SYOL 1.2	Fri	10:00–10:30	H 0105	**Spontaneous autocatalysis and periodic switching in a prebiotic broth** — •Eva Wollrab, Sabrina Scherer, Karsten Kruse, Albrecht Ott
SYOL 1.3	Fri	10:30–11:00	H 0105	**Thermal solutions for molecular evolution** — •Dieter Braun
SYOL 1.4	Fri	11:00–11:30	H 0105	**Systems chemistry: Self-replication and chiral symmetry breaking** — •Guenter von Kiedrowski

Invited Talks of the Joint Focus Session Systems Biology of Bacteria (with jDPG)

AGjDPG 4.1	Tue	9:30–10:00	E 020	**Stochastic gene regulation strategies in bacteria** — •Ulrich Gerland
AGjDPG 4.2	Tue	10:00–10:30	E 020	**The evolutionary advantage of being round** — •Oskar Hallatschek
AGjDPG 4.3	Tue	10:30–11:00	E 020	**Optimal control strategies in living cells** — •Markus Kollmann
AGjDPG 4.4	Tue	11:00–11:30	E 020	**Bacterial communication systems** — •Ilka Bischofs

Invited Talks of the Joint Focus Session Statistics of Cellular Motion (with DY)

Organizers Carsten Beta, Peter Dieterich, Rainer Klages and Lutz Schimansky-Geier.

BP 11.1	Tue	9:30–10:00	H 1028	**Data-driven modeling of cell trajectories: a do-it-yourself kit** — •Henrik Flyvbjerg
BP 11.2	Tue	10:00–10:30	H 1028	**The statistics of eukaryotic chemotaxis** — •Eberhard Bodenschatz
BP 11.3	Tue	10:30–11:00	H 1028	**Dynamics of directed cell migration** — •Albrecht Schwab, Otto Lindemann, Peter Dieterich

BP 11.4	Tue	11:00–11:30	H 1028	**Medley swimming of sleeping sickness parasites** — •Vasily Zaburdaev, Sravanti Uppaluri, Thomas Pfohl, Markus Engstler, Rudolf Friedrich, Holger Stark

Invited Talks of the Joint Focus Session Nonlinear Dynamics of the Heart (with DY)

Organizer Ulrich Parlitz.

DY 14.1	Wed	9:30–10:00	MA 001	**Modelling Excitation Contraction Coupling** — •Martin Falcke
DY 14.2	Wed	10:00–10:30	MA 001	**Modeling of electrical and mechanical function of the heart** — •Alexander Panfilov
DY 14.3	Wed	10:30–11:00	MA 001	**Mechanisms for calcium alternans** — •Blas Echebarria, Enric Alvarez-Lacalle, Carlos Lugo, Angelina Peñaranda, Inma R. Cantalapiedra
DY 14.4	Wed	11:00–11:30	MA 001	**Synchronization as a mechanism of chaos control; Applications to cardiac arrhythmias.** — •Flavio H. Fenton, Stefan Luther, Philip Bittihn, Daniel Hornung, Eberhard Bodenschatz, Robert F. Gilmour Jr
DY 14.5	Wed	11:30–12:00	MA 001	**Cardiac dynamics from a nonlinear system's perspective - from basic science to applications** — •Stefan Luther

Invited Talks of the Joint Focus Session Stress Relaxation in Polymers - From single molecules to biological cells (with CPP)

Organizers Robert Magerle and Klaus Kroy.

CPP 32.1	Thu	9:30–10:00	C 243	**Stress relaxation and chain dynanics in entangled polymer melts** — •Ralf Everaers
CPP 32.5	Thu	10:45–11:15	C 243	**Slow stress relaxation in recoiling polymers** — •Ulrich F. Keyser
CPP 32.9	Thu	12:00–12:30	C 243	**Cytoskeletal stress in collective cell migration** — •Xavier Trepat

Sessions

BP 1.1–1.11	Mon	9:30–13:00	H 1058	**Proteins I**
BP 2.1–2.12	Mon	9:30–13:00	H 1028	**Physics of Cells I**
BP 3.1–3.14	Mon	9:30–13:15	MA 001	**Statistical Physics of Biological Systems I (with DY)**
BP 4.1–4.5	Mon	15:00–17:30	H 0105	**Symposium SYXD: 100 years of X-ray diffraction: from the Laue experiment to new frontiers (with KR, CPP, DF, MA, MM, GP)**
BP 5.1–5.10	Mon	15:00–17:30	H 1058	**Statistical Physics of Biological Systems II (with DY)**
BP 6.1–6.9	Mon	15:00–17:30	H 1028	**Physics of Cells II**
BP 7.1–7.42	Mon	17:30–19:30	Poster A	**Posters: Proteins**
BP 8.1–8.16	Mon	17:30–19:30	Poster A	**Posters: Biopolymers and Biomaterials (with CPP)**
BP 9.1–9.8	Tue	9:30–12:30	E 020	**Focus: Systems Biology of Bacteria (with jDPG)**
BP 10.1–10.12	Tue	9:30–13:00	H 1058	**Biopolymers and Biomaterials (with CPP)**
BP 11.1–11.11	Tue	9:30–13:30	H 1028	**Focus: Statistics of Cellular Motion (with DY)**
BP 12.1–12.5	Wed	9:30–12:00	MA 001	**Focus: Nonlinear Dynamics of the Heart (with DY)**
BP 13.1–13.12	Wed	9:30–13:00	H 1058	**DNA/RNA and Related Enzymes**
BP 14.1–14.12	Wed	9:30–13:00	H 1028	**Membranes and Vesicles**
BP 15.1–15.9	Wed	15:00–17:30	H 1058	**Proteins II**
BP 16.1–16.8	Wed	15:00–17:30	H 1028	**Molecular Motors**
BP 17.1–17.42	Wed	17:30–19:30	Poster A	**Posters: Physics of Cells**
BP 18.1–18.39	Wed	17:30–19:30	Poster A	**Posters: Statistical Physics in Biological Systems**
BP 19.1–19.5	Thu	9:30–12:00	H 0105	**Symposium SYND: Control of Network Dynamics (with DY and SOE)**
BP 20.1–20.12	Thu	9:30–13:00	H 1058	**Regulation**
BP 21.1–21.9	Thu	9:30–12:30	C 243	**Focus: Stress Relaxation in Polymers - From single molecules to biological cells (with CPP)**
BP 22.1–22.10	Thu	15:00–17:30	H 1058	**Statistical Physics of Biological Systems III (with DY)**
BP 23.1–23.7	Thu	15:00–17:00	H 1028	**Cytoskeletal Filaments**

BP 24.1–24.13	Thu	17:30–19:30	Poster A	**Posters: DNA/RNA and Related Enzymes**
BP 25.1–25.7	Thu	17:30–19:30	Poster A	**Posters: Molecular Motors**
BP 26.1–26.24	Thu	17:30–19:30	Poster A	**Posters: Membranes and Vesicles**
BP 27.1–27.16	Thu	17:30–19:30	Poster A	**Posters: Cytoskeletal Filaments**
BP 28.1–28.11	Thu	17:30–19:30	Poster A	**Posters: Imaging**
BP 29.1–29.10	Thu	17:30–19:30	Poster A	**Posters: Regulation**
BP 30.1–30.4	Fri	9:30–11:30	H 0105	**Symposium SYOL: Origin of Life (with CPP and DY)**
BP 31.1–31.7	Fri	9:30–11:30	H 1058	**Imaging**
BP 32.1–32.13	Fri	9:30–13:00	H 1028	**Physics of Cells III**

Annual General Meeting of the Biological Physics Division

Wednesday 19:00–20:00 H 1028

- Bericht der drei Sprecher
- Manöverkritik und Planung Frühjahrstagung Regensburg 2013
- Verschiedenes

BP 1: Proteins I

Time: Monday 9:30–13:00 Location: H 1058

Topical Talk BP 1.1 Mon 9:30 H 1058

Friction and Hydration Repulsion Between Hydrogen-Bonding Surfaces — •Roland Netz — FU Berlin

The dynamics and statics of polar surfaces are governed by the hydrogen-bonding network and the interfacial water layer properties. Insight can be gained from all-atomistic simulations with explicit water that reach the experimentally relevant length and time scales. Two connected lines of work will be discussed: 1) On surfaces, the friction coefficient of bound peptides is very low on hydrophobic substrates, which is traced back to the presence of a depletion layer between substrate and water that forms a lubrication layer. Conversely, friction forces on hydrophilic substrates are large. A general friction law is presented and describes the dynamics of hydrogen-bonded matter in the viscous limit. 2) The so-called hydration repulsion between polar surfaces in water is studied using a novel simulation technique that allows to efficiently determine the interaction pressure at constant water chemical potential. The hydration repulsion is shown to be caused by a mixture of water polarization effects and the desorption of interfacial water.

BP 1.2 Mon 10:00 H 1058

Temperature-induced denaturation of protein layers at solid-liquid interfaces - an x-ray reflectivity study — •Irena Kiesel[1], Michael Paulus[1], Julia Nase[1], Sebastian Tiemeyer[1], Christian Sternemann[1], Anne K. Hüsecken[2], Steffen Bieder[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany — [2]Naturwissenschaftlich Technische Fakultät, Fachbereich Physik, Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen, Germany

Protein adsorption at solid-liquid interfaces is crucial for many applications such as in food industry and medical devices. As proteins loose their functionality during denaturation, the state of the adsorbed proteins influence the growth of biofilms (e.g. bacteria) and the acceptance of implants in human body (e.g. growth of cells). Our aim is to understand the denaturation process of proteins at the solid-liquid interface. Until now, most denaturation processes were analysed in protein solutions, which serves as a protein reservoir. We investigate the protein denaturation process in two different environments by heating adsorbed protein layers up to 90° C and analyse them at each temperature step by x-ray reflectivity measurements. Therefor we use the 27 keV x-ray reflectivity set-up at BL9 at the synchrotron light source DELTA, Dortmund. The denaturation process is investigated by analyzing the (layer) electron density profile and with this, information on structural changes in the protein film induced by temperature are obtained.

BP 1.3 Mon 10:15 H 1058

The influence of van der Waals forces on protein adsorption kinetics — •Almuth Hoffmann, Hendrik Hähl, and Karin Jacob — Saarland University, D-66123 Saarbrücken, Germany

In contact with an aqueous solution of proteins, any surface is instantly covered by a thin layer of proteins. It is of great interest for many biological and biomedical applications to understand and control this adsorption process that depends on a multitude of parameters. Concentrating on the influence of the substrate on the adsorption, the surface chemistry has been in focus of many studies. Protein adsorption is mainly influenced by short-range forces arising from the surface chemistry and Coulomb interaction. Yet, it could be shown that proteins also interact with the bulk substrate via van der Waals forces [1,2]. In the present study we show that the adsorption kinetics (as observed by ellipsometry) is affected by the subsurface composition of the substrate. The results are corroborated by simulations, which predict an influence of the van der Waals forces on surface processes (e.g. reorientations, spreading, *) that take place immediately after the initial adsorption. The variation of these surface processes can be investigated by fitting the experimental data with the appropriate model. The rate constants of the surface processes then give insight into the influence of the van der Waals forces.

[1] A. Quinn et al., EPL 81 (2008) 56003.
[2] Y. Schmitt, H. Hähl et al., Biomicrofluidics 4 (2010) 032201.

BP 1.4 Mon 10:30 H 1058

Sequence Independent DNA-to-DNA Binding at a Gold Surface Mediated by a Dimeric Protein — •Tihomir Solomun[1], Alexander Kovalev[1], Robert Wild[2], Harald Seitz[2], and Heinz Sturm[1,3] — [1]Federal Institute for Materials Research and Testing, Unter den Eichen 87, D-12205 Berlin, Germany — [2]Fraunhofer Institut für Biomedizinische Technik, Am Mühlenberg 13, D-14476 Potsdam-Golm, Germany — [3]Technical University Berlin, Pascalstrasse 8-9, D-10587 Berlin, Germany

Confocal fluorescence, surface plasmon resonance (SPR) and atomic force microscopy (AFM) methods were used to study the interaction of a dimeric gene-5-protein (g5p) with an adlayer of single-stranded DNA (ssDNA) oligonucleotides tethered to a gold surface. The data show that a highly stable g5p-ssDNA surface complex is readily formed. The extent of the complexion indicates involvement of cooperative protein-protein interactions. In the case where oligonucleotides are also present in the solution, sequence independent binding takes place between the non-complementary oligonucleotides in the solution and those immobilized on the surface. This binding is rendered possible by dimeric nature of the g5p protein.

BP 1.5 Mon 10:45 H 1058

A novel computer simulation method for simulating the multiscale transduction dynamics of signal proteins — •Emanuel Peter, Bernhard Dick, and Stephan Baeurle — Universität Regensburg, Universitätsstr. 31, 93053 Regensburg

Signal proteins are able to adapt their response to a change in the environment, governing in this way a broad variety of important cellular processes in living systems. While conventional molecular-dynamics (MD) techniques can be used to explore the early signaling pathway of these macromolecules at atomistic resolution [1], their high computational costs limit their usefulness for the elucidation of the multiscale transduction dynamics of most signaling processes, occurring on experimental timescales. To cope with the problem, we introduce in this presentation a novel multiscale-modeling method, based on a combination of the kinetic Monte-Carlo- (KMC) and MD-technique, and demonstrate its suitability for investigating the signaling behavior of the photoswitch light-oxygen-voltage-2-Jα domain from Avena Sativa (AsLOV2-Jα) and an AsLOV2-Jα-regulated photoactivable Rac1-GTPase (PA-Rac1). These applications demonstrate that our approach reliably reproduces the signaling pathways of complex signal proteins, ranging from nanoseconds up to seconds at affordable computational costs [2].

[1] E. Peter, B. Dick, S. A. Baeurle, *Nat.Commun.* (2010), **1**, 122; *Prot. Struct. Funct. Bioinf.* (2011); **doi: 10.1002/prot.23213. [2]** E. Peter, B. Dick, S. A. Baeurle, *submitted* (2011).

BP 1.6 Mon 11:00 H 1058

Characterization of Free Energy Landscape of Villin Headpiece with Principal Components Analysis by Parts (pPCA) — •Abhinav Jain and Gerhard Stock — Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, 79104 Freiburg.

The free-energy landscape of flexible small peptides and nucleic acids can be quite complex, showing numerous metastable conformational states. On the other hand, various computational studies of proteins have given a comparatively simple picture of their energy landscape which is surprising at higher energies where the protein can reversibly fold and unfold. A method to analyze molecular dynamics (MD) simulations of protein folding is proposed, which is based on a principal component analysis (PCA) of the protein's backbone dihedral angles.[1] Adopting extensive MD simulations of the villin headpiece by Pande and co-workers [2], it is shown that "PCA by parts" allows us to characterize the free-energy landscape of the protein with unprecedented detail.

[1] Jain; Hegger; Stock. J. Phys. Chem. Lett. 2010, 1, 2769 - 2773
[2] Ensign; Kasson; Pande. J. Mol. Biol. 2007, 374, 806 - 816.

15 min break

Topical Talk BP 1.7 Mon 11:30 H 1058

Cryo electron microscopy of biological materials — •Wolfgang Baumeister — Max-Planck-Institute of Biochemistry, Martinsried, Germany

Today, essentially all electron microscopy of biological materials aiming for molecular resolution is cryo electron microscopy. Samples are examined in a frozen-hydrated state to avoid artifacts resulting from dehydration or from chemical fixation and staining. Three different imaging modalities are used: Electron crystallography, which can provide atomic resolution structures but requires that the molecules under study form well-ordered two-dimensional crystals. Single particle analysis which is the method of choice for large multi subunit protein complexes; in conjunction with other methods (hybrid methods) it can provide structures with pseudo-atomic resolution. Electron tomography allows to study large (non-repetitive) structures, such as organelles or cells, and to analyze molecular structures in situ, i.e. in their unperturbed functional environments.

In cryo electron tomography the main challenges are sample preparation and the molecular interpretation of tomograms with a poor signal-to-noise ratio. Denoising, automated segmentation, pattern recognition, and subtomogram averaging are the key strategies in tomogram interpretation. Focused ion beam technology is an emerging tool in the micromachining of frozen-hydrated samples. In conjunction with correlative fluorescence microscopy allowing the navigation of complex samples, thin lamellae suitable for tomography can be produced in a targeted manner.

BP 1.8 Mon 12:00 H 1058

Exploring protein self-diffusion in crowded solutions — •Felix Roosen-Runge[1], Marcus Hennig[1,2], Fajun Zhang[1], Robert M.J. Jacobs[3], Helmut Schober[2], Tilo Seydel[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen — [2]ILL, Grenoble, France — [3]CRL, University of Oxford

We report a study on the self-diffusion of a globular protein, bovine serum albumin (BSA), under crowding conditions [1]. Using quasi-elastic neutron backscattering, we access the so far unexplored short-time regime of protein diffusion at nanosecond time and nanometer length scales. After separation of internal motions and rotational diffusion, the translational self-diffusion coefficients are obtained for a volume fraction range from 5% to 40%. At a biologically relevant volume fraction, the self-diffusion is slowed down by a factor of 5 compared to the dilute limit already within nanoseconds. Despite high volume fractions, no anomalous diffusion was observed at the experimental scales. Modeling the non-spherical, soft proteins with an effective hard sphere, our data agree well with predictions from colloid theory for short-time self-diffusion. This finding implies that hydrodynamic interactions are an essential part of an understanding of protein dynamics in macromolecular crowding. Comparisons are made to complementary DLS experiments [2]. The successful modeling is promising for studies on internal dynamics of proteins diffusing freely in aqueous solutions [3].

[1] F. Roosen-Runge et al., PNAS 2011, 108:11815
[2] M. Heinen et al., Soft Matter, DOI:10.1039/c1sm06242e
[3] M. Hennig et al., Soft Matter, DOI:10.1039/c1sm06609a

BP 1.9 Mon 12:15 H 1058

Solution structures and domain motions of human guanylate binding protein 1 — •Andreas Stadler[1], Adrian Syguda[2], Ralf Biehl[1], Christian Herrmann[2], and Dieter Richter[1] — [1]Forschungszentrum Jülich, ICS-1 & JCNS-1 — [2]Ruhr-Universität Bochum

Human guanylate binding protein 1 belongs to the superfamily of large GTPases. The expression of the protein in cells is strongly induced by interferons and other cytokines and it plays an important role in immune response and tumor growth. The crystal structure shows three domains: a globular head which is responsible for catalytic activity, an α-helical middle domain and a long rigid α-helical H12/H13-domain along the whole protein. The protein hydrolyses GTP to GDP and to GMP. Different conformations of the protein can be trapped during the GTP hydrolysis in solution. In the course of GTP hydrolysis, concerted large scale motions between the LG and the H12/H13 domains occur, which affect the enzymatic reaction rate.

We determined the solution structures of the protein in the different conformations during GTP hydrolysis using small angle X-ray scattering. Additionally, we measured the amplitudes and relaxation rates of the domain motions in the nm length- and 100 ns time-scale using neutron spin echo spectroscopy combined with small angle neutron scattering. The obtained results are important for a detailed understanding of the biological function of the protein on a molecular level, as we gain direct insight into the correlation of the domain motions and the enzymatic reaction.

BP 1.10 Mon 12:30 H 1058

Single-molecule fluorescence spectroscopy of the structure and dynamics of the spliceosomal complex — •Mira Prior[1], Thomas Orth[2], Peter Odenwälder[2], Ingo Gregor[1], Reinhard Lührmann[2], and Jörg Enderlein[1] — [1]Third Institute of Physics, Göttingen — [2]Max Planck Institute for Biophysical Chemistry, Göttingen

The spliceosome is the cellular machinery responsible for removing non-coding introns from precursor mRNA. During its catalytic action the spliceosome undergoes compositional and conformational changes. We are investigating the conditions for recruitment and release of particular proteins during the splicing steps. We determine how the changes occur (stepwise or in a correlated manner) and the roles of certain spliceosomal RNA helicases in the restructuring of the complex. The spectroscopic methods we use for investigating the spliceosomal complex are Dual-Focus Fluorescence Correlation Spectroscopy (2fFCS) and Dual-Color-Fluorescence Cross-Correlation Spectroscopy (2-color-FCCS). These methods allow for studying structural and dynamical properties of proteins and small nuclear ribonucleoproteins (snRNPs). 2-color-FCCS in combination with 2fFCS enables the observation of protein-protein interactions and the determination of dissociation constants for protein-protein and protein-mRNA bindings which could not be resolved with standard biochemical methods. In our experiments we focus on the B to Bact transition followed by LSm ring proteins, the thermally-stable splicing factor Cwc25 and on the proteins of the snRNP U2 complex.

BP 1.11 Mon 12:45 H 1058

Stabilization of peptide helices with respect to length and vibrational free energy — •Mariana Rossi, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin

We here address the helix-forming alanine-based Ac-Ala$_n$-LysH$^+$ polypeptide series in the gas phase, for which experiments [1] have indicated helical onset at n=8. We quantify helix stabilization wrt. peptide length and temperature [harmonic approximation for vibrational free energies (FE)], which are effects that can be dissected and accurately benchmarked in the gas phase. After an initial force-field screening, we fully relax thousands of conformers using density-functional theory with the van der Waals (vdW) corrected [2] PBE exchange-correlation potential. α-Helices are the lowest energy structures at $n \approx 7-8$ on the potential energy surface, but only barely. Interestingly, helices are systematically stabilized over globular conformers by inclusion of vibrational FE at 300K. The vibrational entropy is the leading stabilizing term at 300K, but also zero-point-energies favor helical structures by a significant amount. For $n \geq 8$, the α-helix should be the only accessible conformer in the FE surface at 300K, in agreement with experiment [1] and with our own quantitative comparison [3] of calculated *ab initio* anharmonic IR spectra to experimental IR multiphoton dissociation (IRMPD) data for Ac-Ala$_n$-LysH$^+$, n=5, 10, 15. [1] Tkatchenko and Scheffler, PRL 102, 073055 (2009); [2] Kohtani and Jarrold, JACS 108, 8454 (2004); [3] Rossi *et al.*, JPCL 1, 3465 (2010).

BP 2: Physics of Cells I

Time: Monday 9:30–13:00 Location: H 1028

Invited Talk BP 2.1 Mon 9:30 H 1028

Membrane tension regulates motility by controlling lamellipodium organization — •Julie Plastino — Institut Curie, Paris, France

Many cell movements proceed via a crawling mechanism, where assembly of the cytoskeleton pushes out the leading edge membrane. In this scenario, membrane tension has been seen as an impediment to cytoskeleton polymerization and cell motility. Here we exploit a simple model of cell motility, the Caenorhabditis elegans sperm cell, and we

apply osmotic and biochemical treatments that relax or tense the cell membrane, in order to test how membrane tension affects cytoskeleton dynamics and cell movement. Surprisingly, we find that membrane tension reduction is correlated with a decrease in cell displacement speed, whereas an increase in membrane tension enhances motility. We propose and show evidence for the idea that membrane tension optimizes motility by streamlining polymerization in the direction of movement, thus adding a layer of complexity to our current understanding of how membrane tension enters into the motility equation.

BP 2.2 Mon 10:00 H 1028

Mixing dynamics of the actin cytoskeleton in motile cells — •Matthias Gerhardt, Michael Walz, and Carsten Beta — Institut für Physik und Astronomie, Karl-Liebknecht-Strasse 24/25, 14476 Potsdam-Golm, Germany

We investigate the dynamics of the actin cytoskeleton during and immediately after electrofusion of cells of the social amoeba Dictyostelium discoideum. Two cell lines are used, one expressing a green (GFP) the other one a red fluorescent protein (mRFP) linked to a Lim-domain protein that serves as a marker for filamentous actin. Using a custom designed fusion chamber mounted on a confocal microscope, we are able to study the mixing dynamics of the actin cytoskeleton during cell fusion. The fusion process typically proceeds via three stages: I.) The early state is characterized by an initial pore, which connects the cells. F-actin fragments with a green label invade the cell expressing the red label and vica versa. II.) In the intermediate state, the cells are connected by a junction of hour-glass shape. The actin cytoskeleton starts mixing, resulting in a yellow overlay of the two labels. III.) The final state is characterized by a completely mixed actin cytoskeleton in a fused cell. The timescale of mixing and remodeling of the cytoskeleton is surprisingly short, indicating that the active, self-organized processes in the actin cytoskeleton quickly integrate constituents of both cells into one overall cortex of the fused cell.

BP 2.3 Mon 10:15 H 1028

Contractile forces facilitate the enhanced glycosylphosphatidylinositol-anchored receptor CD24-dependent invasiveness of cancer cells — •Claudia Tanja Mierke — University of Leipzig, Institute for Experimental Physics I, Soft Matter Physics Division

The malignancy of tumors depends on the capability of cancer cells to metastasize. The process of metastasis involves cell invasion through the extracellular matrix (ECM). Cell invasion is a fundamental biomechanical process, which usually requires adhesion to the ECM through mainly beta1 heterodimeric integrin receptors. The localization of beta1 integrins to lipid rafts depends on the glycosylphosphatidylinositol-anchored receptor CD24. The expression of CD24 is up-regulated in several tumor types and consistently associated with increased metastasis in patients. Here, the invasion of A125 lung cancer cells with different CD24 expression levels was studied in 3D-ECMs. The hypothesis was that CD24 expression increases the invasion of cancer cells through increased contractile forces. To analyze this, A125 cells (CD24negative) were stably transfected with CD24 and sorted for high and low CD24 expression. The invasiveness of CD24high and CD24low transfectants were determined in 3D-ECMs. The percentage of invasive cells and their invasion depth were increased in CD24high compared to CD24low cells. Fourier-transform-traction-microscopy revealed that CD24high cells generated 5-fold higher contractile forces compared to CD24low cells. Finally, these results suggest that CD24 enhances cell invasion through increased contractile forces.

BP 2.4 Mon 10:30 H 1028

Cell shape and behaviour for accurate chemotaxis — •Luke Tweedy[1,2], Börn Meier[3,4], Jürgen Stephan[3,4], Doris Heinrich[3,4], and Robert Endres[1,2] — [1]Division of Molecular Biosciences, Imperial College, London, United Kingdom — [2]Centre for Integrative Systems Biology and Bioinformatics, London, United Kingdom — [3]Ludwig-Maximilians-University, Munich, Germany — [4]Center for NanoScience, Munich, Germany

The behaviour of an organism often reflects a strategy for coping with its environment. Such behaviour in higher organisms can often be reduced to a few stereotyped modes of movement due to physiological limitations, but finding such modes in amoeboid cells is more difficult as they lack these constraints. Here, we investigate the connection of stereotypical cell shape and movement in the amoeba Dictyostelium discoideum with its ability to accurately chemotax. We show that the incredible variety in amoeboid shape can be reduced to a few principal modes, which capture the majority of variability in the population. The cell*s preference for modes depends on the chemical environment. We further construct a parameter-free model using the principle of maximum caliber, which accurately predicts long-term cell behaviour. Stereotypy in cells may thus inform our understanding of cell physiology, evolution, and strategy, and may even be used to screen cell health.

BP 2.5 Mon 10:45 H 1028

Cytoplasmic streaming in giant algae cells: the role of wall slip — •Katrin Wolff, Davide Marenduzzo, and Mike Cates — SUPA, School of Physics & Astronomy, University of Edinburgh, UK

We present lattice Boltzmann simulations of a microscopic model for cytoplasmic streaming in algal cells such as those of Chara corallina. The fluid motion is driven by myosin motors carrying vesicles or other organelles and moving along actin filaments which are attached to the outer part of the cytoplasm. We address how the high speeds observed in experiments can be achieved by assuming a layer of lower viscosity at the outer wall of the simulated compartment. To this end we introduce a finite slip boundary condition at the wall close to which the motors move. The motivation behind the low-viscosity layer is the assumption that those cell contents populating the cytoplasm do not reach up to the cell wall resulting in a more dilute solution close to the wall. We find that this simplified view, which does not rely on any coupling between motors, cytoplasm and vacuole other than that provided by viscous Stokes flow, accounts very well for the observed magnitude of streaming velocities [1].

[1] K. Wolff, D. Marenduzzo, M. Cates, Cytoplasmic streaming in giant algae cells: the role of wall slip (submitted)

BP 2.6 Mon 11:00 H 1028

Mechanics in Neuronal Development — •Kristian Franze[1,2], Hanno Svoboda[1], Andreas F. Christ[2], Luciano da F. Costa[3], Christine E. Holt[1], and Jochen Guck[2] — [1]Department of Physiology, Development and Neuroscience — [2]Department of Physics, University of Cambridge, UK — [3]Instituto de Fisica de Sao Carlos, University of Sao Paulo, Brazil

During the development of the nervous system, neurons migrate and grow over great distances. During these processes, they are exposed to a multitude of signals influencing their speed and direction. Currently, our understanding of neuronal development is, in large part, based on studies of biochemical signalling. Despite the fact that forces are involved in any kind of active cell motion, mechanical signalling has so far rarely been considered. Here we used atomic force microscopy to study the mechanical properties of developing brain tissue. Additionally, we exploited deformable cell culture substrates, traction force microscopy and calcium imaging to investigate how neurons respond to their mechanical environment. The tendency to grow in bundles, which neurons show in vivo, was significantly enhanced on soft substrates. Moreover, if grown on substrates incorporating linear stiffness gradients, neurons were repelled by stiff substrates. Calcium influxes through the activation of stretch-activated ion channels appear to be involved in neuronal mechanosensitivity. A comparison of our in vitro findings with the neurons' in vivo environment suggests that mechanical signalling is involved in neuronal pathfinding and constitutes a formerly unknown guidance mechanism.

15 min break

BP 2.7 Mon 11:30 H 1028

Inherently slow and weak forward forces of neuronal growth cones measured by a drift-stabilized Atomic Force Microscope — •Thomas Fuhs[1], Lydia Reuter[1], Iris Vonderhaid[1], Thomas Claudepierre[2], and Josef A. Käs[1] — [1]Universität Leipzig, Soft matter physics, Leipzig, Germany — [2]Universitätsklinikum Leipzig, Klinik und Poliklinik für Augenheilkunde, Leipzig, Germany

Previous results have convincingly shown that neurons prefer soft environments, such as glia cells. This assures that neurons are confined to the central nervous system and cannot wander off. Nevertheless, the question remains, whether or not growth cones have the ability to migrate in stiffer environments like glial scars, as required in nerve regeneration. We investigated the mechanical properties and force generation of extending retinal ganglion cells and NG108-15 growth cones using different AFM based methods. With our drift-stabilized AFM we could, for the first time, measure the forward pushing forces at

the leading edge of outgrowing neuronal growth cones. Our results demonstrate that growth cones have neither the required stability nor the ability to produce forces necessary to penetrate hard tissues.

BP 2.8 Mon 11:45 H 1028

Reconstruction of Cellular Forces During Migration Through Three-Dimensional Collagen Meshworks — •Julian Steinwachs, Claus Metzner, Nadine Lang, Navid Bonakdar, Stefan Münster, and Ben Fabry — Biophysics Group Universität Erlangen-Nürnberg

Reconstituted collagen gels are a widely used substitute of connective tissue to study cell migration in three dimensions. The importance of cellular traction forces needed for the cells to overcome the steric hindrance of the connective tissue is still unknown. We developed a method to quantify cell tractions in a highly nonlinear fibrous biopolymer 3-D network such as collagen. Using confocal reflection microscopy we image the 3-D fiber structure around cells as they migrate through the collagen gels. Cell forces are then relaxed using cytochalasin D, and the relaxed state of the gel is also imaged. Using a fiber pattern matching algorithm, we reconstruct the cell-induced deformation field around every cell. Matrix stresses are computed with a model for the elastic behavior of collagen gels in which the non-affine behavior (buckling, alignment and tautening of fibers) is approximated by a network of nonlinear elements that deform in an affine way. The model parameters are obtained from rheological measurements. We then optimize the cell tractions that best account for the measured deformation field with a least squared optimization routine. If the precise cell contour is unknown, it is still possible to reconstruct the stress field around the cell and to quantify the traction magnitude. Total computation time is less than 5 minutes per cell on an average desktop computer.

BP 2.9 Mon 12:00 H 1028

Traction Force Reconstruction based on Finite Element Methods — •Jérôme Soiné[1,2] and Ulrich Schwarz[1,2] — [1]Bioquant, Heidelberg University, Heidelberg, Germany — [2]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

Over the last decade, it has been established that tissue cells are able to sense the stiffness, geometry and topography of their adhesive environment by actively applying forces to the cell-matrix interface. Cellular forces can be reconstructed with *traction force microscopy*. This method combines cell culture experiments on soft elastic substrates with quantitative image processing and solution of the inverse problem of elasticity theory. Traditional approaches are based on the well-known exact Green's function for planar linear elastic materials known as *Boussinesq solution* [1-3]. For non-planar substrates or non-linear material laws, this approach fails due to the lack of exact solutions. In order to overcome these limitations, we have developed a force reconstruction technique that uses a numeric optimization approach based on finite element methods. It allows us to reconstruct cellular forces for arbitrary substrate geometry and different material laws with a resolution comparable to previous approaches.

[1] Dembo and Wang, Biophysical Journal, 1999
[2] Butler et al., Am. J. Physiol. Cell Physiol., 2002
[3] Sabass et al., Biophysical Journal, 2008

BP 2.10 Mon 12:15 H 1028

Probing PI3-kinase based cell reorientation in spatio-temporally controlled chemotactic gradient fields — Boern Meier and •Doris Heinrich — Center for Nanoscience (CeNS) and Faculty of Physics, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München

We developed a microfluidic chamber to manipulate cell migration in spatio-temporally controlled gradient fields. Bidirectional chemical gradients over a width of more than 300 um and timescales from seconds to several hours allow for parallel exposure of entire cell ensembles. This setup greatly facilitates statistical analysis of cellular migration properties in response to changing gradient directions and for genetic or pharmacological perturbation of the underlying regulatory network.

The long standing observation that actin polymerization, actuated by the phosphorylation of PIP2 by PI3-kinase, is primarily mediating chemotactic migration, has recently been challenged by the observation of Phospholipase A2 induced pseudopod splitting at the leading edge, which enhances persistence in directed cell migration. In Dictyostelium discoideum cells, we find that PI3-kinase based formation of new pseudopods is promoted by steep chemotactic gradients and reduced cellular starvation times, while reduction of the gradient steepness and ongoing starvation enhances persistent cell migration. Consecutive experiments with increased gradient switching frequencies promise further insight into the dynamic regulation of both parallel feedback loops.

BP 2.11 Mon 12:30 H 1028

Quantitative Investigations of Circular Dorsal Ruffling Dynamics — •Erik Bernitt[1,3], Malte Ohmstede[1], Pritpal Singh[2], Cheng-Gee Koh[2], and Hans-Günther Döbereiner[1,3] — [1]Institut für Biophysik, Universität Bremen, 28334 Bremen — [2]School of Biological Sciences, Nanyang Technological University, 639798 Singapore — [3]Mechanobiology Institute Singapore, National University of Singapore, 117411 Singapore

Circular dorsal ruffles (CDRs) are actin-based structures that, unlike peripheral ruffles, form on the dorsal side of cells. Upon initialization, a membrane sheet of vertical extension forms that propagates in a ring-like fashion over the cell. After formation CDRs enlarge, sometimes covering the complete dorsal side of the cell, propagate and collapse to one point. CDRs are known to occur, e.g., on fibroblast cells upon growth factor stimulation. Even though this has been known for decades, the underlying mechanisms leading to formation and propagation of these coherent solitary waves are not understood. Only recently models have been published that describe CDRs based on diffusion reaction processes in the cytosol and on the membrane.

We use DIC-based optical sectioning in conjunction with image processing for localisation and the three-dimensional reconstruction of CDR morphology. We are the first to describe the CDR dynamics in terms of morphology and propagation velocities in great detail. We correlate these data with fluorenscence data of the actin cytoskeleton, providing the first dynamic data on the onset of the migratory state, one hypothesized biological function of CDRs.

BP 2.12 Mon 12:45 H 1028

Viscosity-Sensing and Mechano-Transduction of Cells on Adhesive Lipid Bilayers — Lena Astrid Lautscham[1], Corey Yu-Hung Lin[2], •Daniel Minner[2], Wolfgang Goldmann[1], Christoph Naumann[2], and Ben Fabry[1] — [1]University Erlangen-Nuremberg, Department of Physics — [2]Indiana University-Purdue University, Department of Chemistry and Chemical Biology

Adherent cells have been shown to sense the mechanical properties of their extracellular matrix and to respond to it by altering their morphology, migration speed, and cytoskeletal organization. Previous studies focused on substrate elasticity to investigate cellular mechano sensing and transduction. Here, we altered the substrate viscosity as an alternative route to probe the influence of matrix mechanics on cell responses. Polymer-tethered multi-lipid bilayer systems on a solid support provide a method to tune the substrate viscosity over an extended range by altering the number of stacked bilayers. In contrast to elastic substrates where deformations come to a halt when cell tractions reach a steady state, cell adhesion ligands in viscous substrates remain mobile and thus provide a different mechanical stimulus. To maintain cell tractions, cells need to continuously reorganize their focal adhesions and associated cytoskeletal structures. We probed mechanical bilayer properties as well as cytoskeletal properties with magnetic tweezers. Our data indicate that mouse embryonic fibroblasts (MEF) are extremely susceptible to decreasing substrate viscosity and respond by altering their cytoskeletal and focal adhesion dynamics, cytoskeletal stiffness and spreading area.

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

Time: Monday 9:30–13:15 Location: MA 001

BP 3.1 Mon 9:30 MA 001

On various types of synchronization in networks of coupled neurons — •Philipp Hövel[1,2], Alexander Fengler[1], Alexander Heesing[1], and Eckehard Schöll[1] — [1]Technische Universität Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Germany

Research on complex networks continues to receive more and more attention since the last decades both from a data-driven and dynamics-driven perspective. In the latter case, collective and cooperative dynamics of coupled systems forms a central phenomenon that is of large interest in various fields. These range from social science and economics to biology, physics, and neuroscience and beyond.

In our contribution, we discuss the synchronization of coupled integrate-and-fire neurons with partial reset in various network topologies. These include all-to-all, ring, and scale-free networks. We find a transition from complete synchronization via cluster synchronization to desynchronization in dependence upon the reset parameter. Our results are based on numerical simulations, which we complement by analytical considerations.

BP 3.2 Mon 9:45 MA 001

Complex activation patterns in a simple deterministic model of excitable neural networks — •Guadalupe C. Garcia[1], Claus C. Hilgetag[2], and Marc Thorsten Hütt[1] — [1]School of Engineering and Science, Jacobs University, Bremen, Germany — [2]University Medical Center Eppendorf, Hamburg University, Hamburg, Germany

Understanding the interplay of topology and dynamics of excitable neural networks is one of the major challenges in computational neuroscience. Here we employ a simple deterministic model of excitation propagation to explore how network-wide activation patterns are shaped by neural network architecture.

The model consists of three discrete states for each node (susceptible S, excited E, refractory R), which are updated synchronously in discrete time steps according to a set of update rules allowing for signal propagation. In particular, an element returns to the susceptible state after r time steps. For small r, the network dynamics settle into an regular oscillatory behavior after a transient period. The set of nodes is thus partitioned into distinct groups of nodes, where two nodes are in the same group when they are simultaneously excited.

Two questions about this process are at the core of our investigation: (1) How does the dynamic partitioning into groups depend on network architecture (investigated by averaging the groupings over many different initial conditions)? (2) How does the length of the transient depend on network architecture? By exploring these deterministic excitation dynamics we aim at better understanding, which topological features facilitate self-sustained activity of neural networks.

BP 3.3 Mon 10:00 MA 001

Dynamics of inhomogeneous neural systems with nonlocal coupling — •Iryna Omelchenko[1,2], Philipp Hövel[1,2], and Eckehard Schöll[1] — [1]Technische Universität Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Germany

We investigate the cooperative dynamics of nonlocally coupled neural populations modeled by FitzHugh-Nagumo systems, which is a generic model for type-II excitability. The individual systems are considered to operate above a Hopf bifurcation, that is, they display oscillatory local dynamics. Furthermore, inhomogeneity of the local elements is introduced in the system via a distribution of threshold parameters. Varying the coupling parameters, i.e., coupling radius and strength, and in dependence on the inhomogeneous system's parameter distribution, we analyze spatio-temporal dynamics in the system. Coherent solutions, their stability and mechanisms of transition from coherence to incoherence are analyzed. Especially, we discuss the occurrence of chimera states that exhibit spatial coexistence of regular synchronized and irregular spatially incoherent regions.

BP 3.4 Mon 10:15 MA 001

Spiral-wave prediction in a lattice of FitzHugh-Nagumo oscillators — •Miriam Grace and Marc-Thorsten Hütt — Jacobs University Bremen, Bremen, Germany

In many biological systems, variability of the components can be expected to outrank statistical fluctuations in the shaping of self-organized patterns. The distribution of single-element properties should thus allow the prediction of features of such patterns. In a series of previous studies on established computational models of *Dictyostelium discoideum* pattern formation we demonstrated that the initial properties of potentially very few cells cells have a driving influence on the resulting asymptotic collective state of the colony [1,2]. One plausible biological mechanism for the generation of variability in cell properties and of spiral wave patterns is the concept of a "developmental path", where cells gradually move on a trajectory through parameter space. Here we review the current state of knowledge of spiral-wave prediction in excitable systems and present a new one-dimensional developmental path based on the FitzHugh-Nagumo model, incorporating parameter drift and concomitant variability in the distribution of cells embarking on this path, which gives rise to stable spiral waves. Such a generic model of spiral wave predictability allows new insights into the relationship between biological variability and features of the resulting spatiotemporal pattern.

[1] Geberth, D. and Hütt, M.-Th. (2008). Phys. Rev. E 78, 031917.

[2] Geberth, D. and Hütt, M.-Th. (2009). PLoS Computational Biology 5, e1000422.

BP 3.5 Mon 10:30 MA 001

Spatio-temporal dynamics of bumblebees foraging under predation risk — Friedrich Lenz[1], Thomas C. Ings[2], Lars Chittka[2], Aleksei V. Chechkin[3], and •Rainer Klages[1] — [1]Queen Mary University of London, School of Mathematical Sciences, UK — [2]Queen Mary University of London, School of Biological and Chemical Sciences, UK — [3]Inst, f. Theor. Physics, NSC KIPT, Kharkov, Ukraine

We study bumblebees searching for nectar in a laboratory experiment with and without different types of artificial spiders as predators. We find that the flight velocities obey mixed probability distributions reflecting the access to the food sources while the threat posed by the spiders shows up only in the velocity correlations. This means that the bumblebees adjust their flight patterns spatially to the environment and temporally to predation risk. Key information on response to environmental changes is thus contained in temporal correlation functions and not in spatial distributions.

[1] preprint arXiv:1108.1278 (2011)

BP 3.6 Mon 10:45 MA 001

Fluctuation-sensitive coarse-graining for stochastic dynamics — •Bernhard Altaner and Jürgen Vollmer — Max Planck Institut für Dynamik und Selbstorganisation, Göttingen

We consider Markov processes on a finite state space. Such stochastic processes can be viewed as a random walk on a network. Physically, the states represent a mesoscopic description as they summarize regions of phase space of an underlying microscopic dynamics. For non-equilibrium steady states, probability conservation gives rise to cyclic dynamics. Cycles connect the stochastic, mesoscopic description to the thermodynamic, macroscopic description. Here, we present a method for complexity reduction of the mesoscopic dynamics is where the new stochastic dynamics preserves the most important connections to the other scales. As an example, we consider the stochastic dynamics of the molecular motor protein kinesin.

BP 3.7 Mon 11:00 MA 001

The role of diffusion in the SIRS epidemic model — Fernando Peruani[1] and •Chiu Fan Lee[2] — [1]Lab. J.A.Dieudonné, Université de Nice - Sophia Antipolis — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In the well-mixed limit of the classical SIRS epidemic model, an initial epidemic outbreak will persist if the basic reproductive number is larger than 1. This quantity indicates the number of secondary cases caused by an infected individual and is believed to depend exclusively on the parameters relevant to the spreading of the disease. If the individuals in the system also diffuse, it is unclear how this epidemic threshold will be affected. In this work, we perform extensive lattice-based simulations to demonstrate that the epidemic threshold and the average number of infected individuals are in fact strongly affected by the diffusion coefficient, D, exhibited by the agents. We then support our numerical results with field-theoretic analysis.

15 min, break

BP 3.8 Mon 11:30 MA 001

Generalized Entropies for Clustering, e.g., in Molecular Evolution — •Kay Hamacher — TU Darmstadt, 64287 Darmstadt, Germany

Entropy is a key concept in information theory. Analysis of empirical data is often improved by relying on (relative) entropies. In this talk I want to describe current progress in clustering approaches by optimization techniques [1-2] applied to entropy distances via generalized entropy concepts [3], in phylogenies [4,5], finite-size effects in empirical data [6], and in molecular design [7].

[1] K. Hamacher. J.Comp.Phys., 227(2):1500-1509, 2007

[2] K. Hamacher. Europhys.Lett. 74(6):944, 2006

[3] R. Bose, G. Thiel, K. Hamacher. Variation in Local Entropy to Cluster Genomic Sequences, submitted, 2011.

[4] K. Hamacher. Proc. of BIOINFORMATICS 2010, p. 114-122, A. Fred, J. Filipe, H. Gamboa (eds.), ISBN 978-989-674-019-1

[5] K. Hamacher, Information Theoretical Dissection of the Holobiont - Host-Virus Interaction as an Example, Nova Acta Leopoldina, accepted, 2011

[6] P. Weil, F. Hoffgaard, K. Hamacher. Comp. Biol. Chem. 33:440-444, 2009

[7] K. Hamacher. J.Comp.Chem., 28(16):2576-2580, 2007

BP 3.9 Mon 11:45 MA 001

Stochastic description of birth and death processes governed by a mixture of exponential and non-exponential waiting times — •Stephan Eule — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

The dynamics of complex biological systems is significantly influenced by fluctuations originating from intrinsic as well as extrinsic sources. In general, the discrete nature of individual events, such as the birth and death of an individual in a population or the production and degradation of molecules in a chemical reaction, is the main source of intrinsic noise. The occurrence of such events is usually modeled by Poissonian statistics, implying that the probability per unit time for an event to happen is assumed to be constant. Many complex systems however exhibit deviations from elementary Poissonian statistics. Such deviations can arise for example in coarse-grained stochastic models of gene expression, where the waiting time distribution can be more general than the simple exponential distribution.

In this contribution we consider birth and death processes which are governed by both, exponential as well as non-exponential waiting times. We derive the corresponding master equation and present methods to approach this equation analytically. As an example we consider a reaction where the production of molecules is governed by a non-exponential waiting time distribution and the degradation follows regular Poissonian statistics.

BP 3.10 Mon 12:00 MA 001

Discriminating the effects of spatial extent and population size in cyclic competition among species — •David Lamouroux[1,2], Stephan Eule[1], Theo Geisel[1,2], and Jan Nagler[1,2] — [1]Max Planck Institute for Dynamics & Self-Organization, Göttingen, Germany — [2]Institute for Nonlinear Dynamics, Department of Physics, Univeristy of Göttingen, Göttingen, Germany

Quantifying and understanding the stability and biodiversity of ecosystems is a major task in biological physics as well as in theoretical ecology. From the perspective of game theory, this is highly relevant for questions pertaining to the emergence of cooperation or the coexistence of cyclically competing species. For the latter, it has recently been shown that the mobility of individuals can support the stability of biodiversity by the formation of spirals. In this contribution, we present a population model for species under cyclic competition that extends earlier lattice models to allow the single cells to accommodate more than one individual by introducing a per cell carrying capacity. We confirm that the emergence of spirals induce a transition from an unstable to a stable regime. This transition however does not appear to be sharp and we find a broad intermediate regime that exhibits an ambiguous behavior. The separation of the two regimes by the usual scaling analysis is thus hampered. The newly introduced carrying capacity offers an alternative way of characterizing the transition. We thus overcome the original limitations by separately analyzing the effect of spatial extent and population size.

BP 3.11 Mon 12:15 MA 001

Modelling of DNA-Hybridization — •Olaf Leidinger and Ludger Santen — Universität des Saarlandes

Bringing together two types of single-stranded DNA molecules (targets: perfect matching and those with one mismatch) in a aqueous solution and one type of surface-attached single-stranded DNA molecules (probes) one can observe hybridization of double stranded DNA molecules. The percentage of perfect matching (PM) strands at the surface is found to be independent of the concentration of those with one mismatch (MM). This dominance is not in agreement with a Langmuir adsorption kinetics in contrast to the adsorption of a single species. We introduce a theoretical approach to the competitive adsorption of DNA strands illustrating the prerequisites for the dominant adsorption of PM DNA strands.

BP 3.12 Mon 12:30 MA 001

A Statistical Analysis of Production in Cells: Flux Distributions, Enzyme Time Scales and Metabolic Network Properties — •Moritz E. Beber and Marc-Thorsten Hütt — School of Engineering and Science, Jacobs University Bremen, Germany

Numerous studies have addressed statistical properties of metabolic systems, both from the perspective of network structure and of dynamical systems. On a genome-wide scale, the considered dynamics were usually metabolic fluxes, i.e., material flow through biochemical reactions, either measured *in vivo* or computed using flux-balance analysis as a proxy for real behaviour.

In this study, we revisit and modify some of the existing results linking topology and dynamics: (1) We integrate timing information about the principal agents of catalysation of biochemical reactions, the enzymes, in a new way. (2) We carefully analyse the interplay of different network properties and re-compute metabolic network motifs, taking into account the fact that metabolic networks are bipartite, modular, layered, and contain different categories of bidirectional links. (3) Using a minimal model of evolved flow networks as a guideline, we explore, which network properties are correlated with metabolic robustness.

Our object of study is the metabolism of *Escherichia coli*. We use a manually curated metabolic network for topological information, a realistic model of its metabolism for flux balance analysis sampling diverse environmental conditions, and information on the mechanics of enzymes from a specialised database.

BP 3.13 Mon 12:45 MA 001

Active microswimmers with spatially varying self-propulsion — •Aljoscha Hahn[1], Giovanni Volpe[2,3], Clemens Bechinger[2,3], and Holger Stark[1] — [1]Technische Universität Berlin, Germany — [2]Max-Planck-Institut für intelligente Systeme, Stuttgart, Germany — [3]Universität Stuttgart, Germany

The statistical physics of active microswimmers, which are capable of propelling themselves through a viscous environment, is intensively investigated at the present time. Recently, Janus particles were studied in a subcritical mixture [1] and it was found that the speed of self-propulsion can be controlled by the strength of illumination. In particular, a spatially varying light intensity induces a spatially varying self-propulsion. Based on the Smoluchowski equation, we study how active particles with a position dependent swimming speed behave and speculate about a novel type of ratchet.

[1] G. Volpe et al, Soft Matter 7, 8810 (2011)

BP 3.14 Mon 13:00 MA 001

Continuous Dynamic Photostimulation - delivering defined, in-vivo-like fluctuating stimuli with Channelrhodopsins — •Andreas Neef[1,3], Achmed El Hady[1,2,3], Walter Stühmer[2,3], and Fred Wolf[1,3] — [1]MPI für Dynamik und Selbstorganisation, Göttingen — [2]MPI für Experimentelle Medizin, Göttingen — [3]BFNT

Central neurons typically operate in a noise driven regime: thousands excitatory and inhibitory synapses give rise to a constantly fluctuating conductance. Its statistic is similar to low-pass filtered white noise conductance that can be parameterized by is average, standard deviation and correlation time. An understanding of action potential (AP) generation and encoding in the noise driven regime requires the detection of AP times during stimulation with defined time dependent conductance. Using a light activated ion channel (ChIEF) under continuously fluctuating illumination, we achieve a defined, reproducible conductance modulation that mimicks the effect of the naturally occurring synaptic inputs. Cultured neurons subjected to this continuous

dynamic photostimulation (CoDyPs) generate seemingly random, but reproducible patterns of APs in experiments lasting several hours. The induced conductance waveform can be precisely predicted by convolution of the light signal with the light-conductance transfer function of ChIEF. Together with non-invasive AP detection by extracellular electrodes, CoDyPs lays the foundation for very long-lasting studies of action potential generation in a fluctuation driven regime. This will allow the measurement of dynamical response properties and the respective cut-off frequencies from individual neurons.

BP 4: Symposium SYXD: 100 years of X-ray diffraction: from the Laue experiment to new frontiers (with KR, CPP, DF, MA, MM, GP)

Time: Monday 15:00–17:30 Location: H 0105

Invited Talk BP 4.1 Mon 15:00 H 0105

Disputed discovery: The beginnings of X-ray diffraction in crystals — •Michael Eckert — Deutsches Museum, Forschungsinstitut, Museumsinsel 1, D-80538 München

The discovery of X-ray diffraction in crystals was based on misconceptions about the nature of X-rays. The background of "Laue's discovery" and its early repercussions are described from the perspective of contemporary views in 1912. The riddle concerned the origin of the monochromacy observed in the Laue spots.

Invited Talk BP 4.2 Mon 15:30 H 0105

Why are quasicrystals quasiperiodic? — •Walter Steurer — Laboratorium für Kristallographie, ETH Zürich, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Schweiz

It took more than two years until Dan Shechtman could publish his finding of a rapidly solidified Al-Mn phase with sharp Bragg reflections and icosahedral point group symmetry. His results were not accepted, initially, since they seemed to contradict fundamental laws of crystallography. A further twenty-seven years had to pass by until his discovery of quasicrystals was honoured by the Nobel Prize in 2011. This discovery was fundamental because quasiperiodic order represents a novel equilibrium state of solid matter fundamentally different from the common periodic one.

At present, stable quasicrystals have been found in more than fifty binary and ternary intermetallic systems. They show mostly decagonal or icosahedral diffraction symmetry contrary to soft quasicrystals. These are mainly qasiperiodic structures resulting from the self-assembly of either micelles in a liquid or of terpolymers with dodecagonal symmetry. The so far most promising applications of quasiperiodic structures seem to be in the field of photonic and phononic crystals.

The focus of the talk will be on the driving forces for the formation and stablization of quasiperiodic structures.

Invited Talk BP 4.3 Mon 16:00 H 0105

Coherent Diffraction Imaging with Free-Eletron Lasers — •Massimo Altarelli — European XFEL GmbH, 22607 Hamburg

One hundred years after the discovery of x-ray diffraction from crystals, spatially coherent, ultra-brilliant and ultra-short pulses of x-ray radiation from free electron lasers (FEL's) open the way to structure solution without the hurdle of crystallization. Biological objects such as cells, viruses, possibly down to individual macromolecules and to atomic resolution, and individual nanostructures in material sciences are eligible for these novel studies. An overview of the x-ray FEL sources and their basic physical principles and properties, of the strategies for sample handling and data collection and a glimpse of the necessary algorithms to phase the diffraction patterns are given. Example of results from the soft x-ray FLASH source in Hamburg and from the Linac Coherent Light Source in Stanford are illustrated. The perspectives and the challenges of the high repetition rate (up to 27 000 pulses/s) of the European XFEL, under construction in the Hamburg region, are also briefly discussed

Invited Talk BP 4.4 Mon 16:30 H 0105

X-ray free-electron lasers - emerging opportunities for structural biology — •Ilme Schlichting — Max Planck Institute for Medical Research, Heidelberg, Germany

X-ray crystallography is a mature yet still advancing method for structure determination of molecules with any molecular weight. Facilitated greatly by synchrotron X-ray sources, the method is limited only by the quality and size of the crystals and by radiation damage. Free-electron lasers (FELs) provide orders of magnitude brighter and shorter X-ray pulses than conventional synchrotron sources. It has been proposed that radiation damage, which limits the high resolution imaging of soft condensed matter, can be "outrun' by using ultrafast and extremely intense X-ray pulses that pass the sample before the onset of significant radiation damage [1]. Thus, one of the most promising scientific applications of XFELs is in sub-nanometer resolution imaging of biological objects, including viruses, macromolecular assemblies, and nanocrystals. The concept of "diffraction-before-destruction" has been demonstrated recently at the Linac Coherent Light Source (LCLS) [2], the first operational hard X-ray FEL, for protein micro- and nanocrystals [3] and single mimivirus particles [4]. These experiments and recent developments and progress will be presented.

[1]. Neutze et al., Nature 406, 752-757 (2000). [2]. Emma, Nature Photonics 4, 641-647 (2010). [3]. Chapman et al., Nature 470, 73-77 (2011). [4]. Seibert et al., Nature 470, 78-81 (2011).

Invited Talk BP 4.5 Mon 17:00 H 0105

Structure analysis by x-ray diffraction and x-ray imaging: beyond crystals, beyond averages, and beyond modeling — •Tim Salditt — Georg-August-Universität Göttingen, Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Classical x-ray diffraction has been based on three constraints: (i) averages over macroscopic accumulation time and sample sizes, which are many orders of magnitude larger than the structures to be resolved; (ii) homeogeneous "well ordered" samples which are - if not crystalline - characterized by well-defined correlation functions; (iii) data analysis by fitting to modeled diffraction data. However, many condensed matter problems, in particular in functional materials, soft matter and biomolecular samples, address non-equilibrium states with competing length scales, hierachical structures, and intrinsic dynamics. Progress in x-ray sources and optics has helped to meet these challenges. Conceptually often still close to the Laue experiment, far-field diffraction data can now be collected in controllable field of vies, with highly focused beams reaching the 10 nm range. Biomolecular diffraction signals can be recorded from hierachical structures such as a biological cells. Perhaps most importantly, fully coherent illumination enables data inversion without prohibitive model building. How these advances serve science, will be illustrated by examples in neuro-biophysics. We present experiments addressing different structural levels and bridging length scales, from proteins and lipid assemblies up to a complete organelle such as the synaptic vesicle, from an isolated axon up to an unsliced nerve, from tissue slice to the sensory organ.

BP 5: Statistical Physics of Biological Systems II (with DY)

Time: Monday 15:00–17:30 Location: H 1058

BP 5.1 Mon 15:00 H 1058

The probability of parallel evolution — •Joachim Krug[1], Ivan G. Szendro[1], Martijn F. Schenk[2,3], and J. Arjan G.M. de Visser[3] — [1]Institut für Theoretische Physik, Universität zu Köln, Germany — [2]Institut für Genetik, Universität zu Köln, Germany — [3]Laboratory for Genetics, Wageningen University, Netherlands

The question whether evolutionary processes are repeatable is of central importance in evolutionary biology and continues to be vigorously debated. In a simple version of this problem introduced by Orr, one considers a situation where n beneficial mutations are available to an

organism and asks for the probability P that the same mutation is fixed in two replicate populations. When the fitness values are drawn from a distribution that belongs to the Gumbel domain of attraction, Orr showed that $P = 2/(n+1)$, about twice the neutral expectation $1/n$ that would apply if all mutations were equally likely to fix. Motivated by recent experiments that observed a heavy-tailed distribution of fitness effects in an antibiotic resistance gene, we extend Orr's analysis to distributions of selection coefficients s of Pareto form, $f(s) \sim s^{-(\alpha+1)}$. Using an approach from the statistical physics of disordered systems, we show that the probability of parallel evolution is dramatically enhanced when $\alpha < 2$, with $P \sim n^{-(2-\alpha)}$ for $1 < \alpha < 2$ and $P = const.$ for $\alpha < 1$. We also briefly address the influence of population size on the probability of parallel evolution.

BP 5.2 Mon 15:15 H 1058

Evolution of cooperation in microbial biofilms - A stochastic model for the growth and survival of bacterial mats — •Johannes Knebel, Anna Melbinger, Jonas Cremer, and Erwin Frey — LMU Muenchen, Deutschland

Cooperating microbes are widespread in nature despite running the risk of being exploited by free-riders. This so-called dilemma of cooperation is especially important for microbial biofilms where diverse different strains interact in a complex community. The structure and composition of such a biofilm change over time and thereby influence the evolution of cooperation within the system. In turn, the level of cooperation affects the growth dynamics of the biofilm.

Here, we investigate this coupling for an experimentally well-defined situation in which mutants of the Pseudomonas fluorescens strain form a mat at the liquid-air interface by the production of an extra-cellular matrix [1]. We model the occurrence of cooperation in this bacterial population by taking into account the formation of the mat. The presence of cooperators enhances the growth of the mat, but at the same time cheaters can infiltrate the population and put the viability of the mat at risk. We find that the survival time of the mat crucially depends on its initial dynamics which is subject to demographic fluctuations [2]. More generally, our work provides conceptual insights into the requirements and mechanisms for the evolution of cooperation.

[1] P. Rainey et al., Nature 425, 72 (2003).
[2] A. Melbinger et al., PRL 105, 178101 (2010).

BP 5.3 Mon 15:30 H 1058

Meso-scale symmetries explain dynamical equivalence of food webs — •Helge Aufderheide[1,2], Lars Rudolf[2], and Thilo Gross[2] — [1]MPI für Physik komplexer Systeme, Dresden — [2]University of Bristol, Bristol

In complex networks much of the dynamics emerges from the complex interactions between its constituents. However, connecting the interaction topology with the final dynamics remains a hard and largely unsolved problem. Inspired by a recent result on the dynamical equivalence of food webs differing only by local symmetries in their trophic graph, we investigate the effects of such symmetries on the dynamics of food webs. Using generalized modeling to establish the food web Jacobian matrix near the steady states we can study entire classes of food web models instead of fixing specific functional dependencies between the interacting species. Thereby we find that food webs differing by local symmetries indeed carry identical dynamics up to effects localized inside the symmetric part. On one hand this result for equivalent dynamics provides a link between the topology and the dynamical properties of a food web. On the other hand the formalism should be applicable to identify classes of equivalent dynamics hidden to empirical observation in more complicated systems.

BP 5.4 Mon 15:45 H 1058

Geometrical trajectories of a Listeria-type actin-driven particle in 2D — •Fu-Lai Wen[1], Kwan-tai Leung[1,3], and Hsuan-Yi Chen[1,2,3] — [1]National Central University, Jhongli, Taiwan 32001, Republic of China — [2]Physics Division, National Center for Theoretical Sciences, Hsinchu, Taiwan 30113, Republic of China — [3]Institute of Physics, Academia Sinica, Taipei, Taiwan 11529, Republic of China

Self-propulsions have been a focus of the non-equilibrium statistical physics where an input energy is converted into the kinetic energy of motion. It is interesting that a deformable self-propelled domain is shown to generate a series of geometrical trajectories like circles, wiggles, etc. A similar result is also found in the motion of a bacterium Listeria which, although not deformable, moves in a geometrical trajectory by the polymerization of protein actin on its surface. Similar actin-driven motility was also shown in vitro studies on functionalized beads or disks. Here, a phenomenological model is constructed for the generation of geometrical trajectories of a Listeria-type actin-driven spherical particle in two dimensions. In our model, the evolutions of actin filament density and force on surface are coupled to the translation and rotation of the particle which in turn are determined by those densities. It is shown that this feedback can destabilize the straight trajectories and lead to the geometrical trajectories observed in experiments. It further shows that a straight trajectory transits to a circular one through a pitchfork bifurcation or to a wiggled one through a Hopf bifurcation on the distributions of those densities. This transition mechanism is generic and robust as indicated in our studies.

BP 5.5 Mon 16:00 H 1058

Mean Exit Time of a Brownian Particle from a Spherical Domain with Multiple Exit Sites on the Boundary — •Ronny Straube[1], Michael J. Ward[2], and Alexei F. Cheviakov[3] — [1]Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg — [2]University of British Columbia, Vancouver, Canada — [3]University of Saskatchewan, Saskatoon, Canada

In biological signal transduction a target molecule often has to find a small exit site on an otherwise impermeable boundary. Important examples of such **narrow escape** processes include diffusion through ion channels and trafficking through pores of the nuclear membrane. We have recently extended the calculation of the mean exit time (MET) from the case of a Brownian particle exiting from a spherical domain with a single exit site [1] to the case of multiple exit sites [2]. Using the method of matched asymptotic expansions we provide a three-term approximation of the MET which explicitly depends on the spatial configuration of the exit sites. We show that for a fixed surface fraction of exit sites the MET reaches a value close to its minimum already for 30-40 exit sites which suggests, for example, that cell nuclei have many more pores than would be needed if nuclear export was a purely diffusion-limited process.

[1] Singer A, Schuss Z, Holcman D, Eisenberg RS. Narrow escape, part I. J. Stat. Phys. 122, 437-463 (2006).
[2] Cheviakov AF, Ward MJ, Straube R. An asymptotic analysis of the mean first passage time for narrow escape problems: part II: The sphere. SIAM Multiscale Model. Simul. 8, 836–870 (2010).

BP 5.6 Mon 16:15 H 1058

Fractional Brownian Motion in Crowded Fluids — Dominique Ernst[1], Marcel Hellmann[2], Jürgen Köhler[1], and •Matthias Weiss[2] — [1]Experimental Physics IV, University of Bayreuth, D-95440 Bayreuth — [2]Experimental Physics I, University of Bayreuth, D-95440 Bayreuth

Diffusion in crowded fluids, e.g. in the cytoplasm of living cells, has frequently been reported to show an anomalous characteristics ('subdiffusion'). Several random walk models have been proposed to explain these observations, yet so far an experimentally supported decision in favor of one of these models has been lacking. Here, we show that experimentally obtained trajectories in a prototypical crowded fluid show an ergodic behavior and an asphericity that is most consistent with the predictions of fractional Brownian motion, i.e. an anti-correlated, antipersistent generalization of normal Brownian motion that is related to the fluid's viscoelasticity.

BP 5.7 Mon 16:30 H 1058

Time domain representation of active nonlinear cochlear waves — •Florian Fruth[1,2], Frank Jülicher[1], and Benjamin Lindner[2] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden — [2]Bernstein Center for Computational Neuroscience, Philippstr. 13, Haus 2, 10115 Berlin

The inner ear, the so called cochlea, can be modeled generically in terms of coupled critical oscillators, which has been done previously in the frequency (Fourier) domain. This one-dimensional model describes a nonlinear cochlear wave that is pumped by active oscillators. We extend and generalize this model by constructing a similar version in time domain, in order to include dynamical noise (originating, e.g. in the stochastic activity of outer hair cells) and static disorder (resulting from inhomogeneities of system parameters along the cochlea). We discuss the spontaneous oscillations in the model and also investigate its response to external stimuli such as clicks or pure tones.

BP 5.8 Mon 16:45 H 1058

The effects of temperature changes on the timing of cell division — •Federico Vazquez[1,2], Abigail Klopper[3], Maria Begasse[2], and Stephan Grill[1,2] — [1]Max Planck Institute for the

Physics of Complex Systems — [2]Max Planck Institute for Molecular Cell Biology and Genetics — [3]Nature Publishing Group

Accurate timing of early embryogenesis is crucial for the development of an organism, and is subject to sensitive dependence on fluctuations in temperature. We investigate how timing is affected by temperature using *C. elegans* as a model organism, which benefits from rapid early cell divisions and an inability to maintain a constant body temperature, independent of ambient conditions. Experiments show that cell division rates have an Arrhenius dependence on temperature in an intermediate range, but they continuously deviate from this law outside this range, that is, for high and low temperatures. We propose a simple model for cell division, in which the state of the cell performs a Brownian motion on a complex network with temperature-dependent hopping rates, and associate division rates to mean first-passage times. We obtain analytical expressions for simple topologies that fit the experimental data very well, showing that the fundamental mechanism behind the temperature dependence rates can be captured by a very low dimensional system. By comparing timings between different phases as a function of temperature, we are able to relate the lack of event coordination to the malfunction of the cell cycle at extreme temperatures. We also compare rates of *C. elegans* and *C. briggsae*, two closely related organisms known to differ in their optimal temperature range.

BP 5.9 Mon 17:00 H 1058

Spatial organization of the cell cytoplasm: Amplifying protein concentration gradient by phase separation — •Chiu Fan Lee[1], Clifford P. Brangwynne[2], Jöbin Gharakhani[1], Zdeněk Petrášek[3], Petra Schwille[3], Anthony A. Hyman[4], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Chemical and Biological Engineering, Princeton University, USA — [3]Biotechnologisches Zentrum, Dresden, Germany — [4]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Pattern formation in the cell cytoplasm plays an important role in a number of biological processes. During cell division, the cell cytoplasm undergoes dramatic spatial reorganization. In the case of asymmetric cell division, cytoplasmic components are segregated spatially. An intriguing example is the spatial organization of the cytoplasm during asymmetric cell division in the C. elegans embryo, which involves the generation of a concentration gradient of the protein Mex-5 that in turn localizes P granules to the posterior side. P granules are liquid drops consisting of RNA and proteins that are important for germline specification. Combining theory and quantitative experiments, we propose a simple scenario that describes how the Mex-5 concentration gradient controls the spatial profile of P granule formation and the localization of P-granules to the posterior of the cell. Furthermore, we demonstrate that with the help of phase separation based on the Flory-Huggins formalism, the P granule concentration gradient can be drastically amplified in comparison to the Mex-5 concentration gradient.

BP 5.10 Mon 17:15 H 1058

Molecular Force Response Characteristics from Power Spectral Analysis of Optical Tweezer Experiments — •Yann von Hansen[1,2], Alexander Mehlich[1], Benjamin Pelz[1], Michael Hinczewski[1,3], Matthias Rief[1], and Roland R. Netz[1,2] — [1]Physik Department, TU München — [2]Fachbereich Physik, FU Berlin — [3]IPST, University of Maryland, USA

The thermal fluctuations of micron-sized beads in dual trap optical tweezer experiments contain a wealth of dynamic information about the viscoelastic properties of the experimental object of study. Dynamic deconvolution theory relates the beads' power spectral densities (PSDs) and the mechanic force response of individual components in the mechanic network [1]. For the quantitative evaluation of the measured signals, a detailed understanding of instrumental characteristics and an accurate calibration of the setup are required. For a simple model system, a pair of unconnected, but hydrodynamically interacting spheres, we obtain excellent agreement between theoretical and measured self- and cross-PSDs over a wide range of inter-bead distances and frequencies, for motion parallel and perpendicular to the inter-bead axis. A comparison to theoretical predictions based on instantaneous hydrodynamics emphasizes the importance of hydrodynamic retardation effects. The viscoelastic response of the force-transducing element between the beads in more complex experimental constructs can be obtained applying a maximum likelihood method [2].

[1] M. Hinczewski et al., Proc. Natl. Acad. Sci. USA 107, 21493 (2010)
[2] Y. von Hansen et al., manuscript in preparation

BP 6: Physics of Cells II

Time: Monday 15:00–17:30 Location: H 1028

Invited Talk BP 6.1 Mon 15:00 H 1028

Intercellular Interactions and the Mystery of Growth Control — •Boris Shraiman — Kavli Institute for Theoretical Physics, UC, Santa Barbara, CA93106, USA

Despite their obvious importance in animal development and disease, the mechanisms that control cell proliferation and tissue growth, are poorly understood. This talk will review the facts, issues and current ideas focusing on the problem of size determination in fly wing development. In particular while proliferation is driven cell autonomously by morphogen growth factors, it appears that the inhibitory control of growth depends on the global tissue-wide profile and history of growth. This global *integration* of growth is likely to be mediated by intercellular interactions involving both mechanics and cell-contact signaling.

BP 6.2 Mon 15:30 H 1028

Optimal cellular mobility for synchronization arising from the gradual recovery of intercellular interactions — •Koichiro Uriu[1], Saul Ares[2], Andrew C. Oates[1], and Luis G. Morelli[1] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Spanish National Center of Biotechnology CNB-CSIC, Madrid, Spain

Intercellular communication enables the flow of information in living tissues. During embryonic development, tissues undergo massive reorganization involving cellular movements. These cellular movements can be beneficial for the flow of information, because cells get to see effectively more neighbors as they move. However, cells may need some time to establish and develop new communication channels with their new neighbors. Then, if the movement is too fast, they may fail to establish functional communication channels, and movement will be detrimental to information flow. Here we address these questions in the context of moving coupled oscillators, a model system motivated by genetic oscillations in the vertebrate segmentation clock. We find that there is an optimal moving rate for which synchronization is faster and stronger, and a critical moving rate above which synchronization is not possible. These features are the consequence of a competition between the time scale for cellular mobility and that for the recovery of intercellular interaction. Our study indicates that the competition between these two time scales is key to the flow of information in living tissues.

BP 6.3 Mon 15:45 H 1028

The Mechanobiology of *Physarum polycephalum* — •Christina Oettmeier[1,2], Erik Bernitt[1,2], and Hans-Günther Döbereiner[1,2] — [1]Institut für Biophysik, Universität Bremen, 28334 Bremen — [2]Mechanobiology Institute, National University of Singapore, 117411 Singapore

We characterize the mechanobiological properties of *P. polycephalum*. This amoeboid slime mold can reach large sizes and is one single, multinuclear cell. By using microplasmodia, we introduce a reliable and reproducible system for the study of network formation and individual cell motility. Microplasmodia are a special growth form, quasi-spherical in shape and 200-500 microns small. Created by cultivation in shaking culture, they exhibit the same actin-myosin based oscillations as the large plasmodia. We monitor cell dynamics in different ways: First, by observing area oscillations with bright-field microscopy, whereby the spatio-temporal dynamics of focal area and contour could be analyzed. Fast oscillations with a period of 1-2 min as well as a superimposed slow oscillation with a period of about 20 min were found.

The second method, calcium imaging with the ratiometric dye Fura-2-AM, was used to clarify the correlation between biochemical signalling and contractions. These correlate with a low local calcium concentration, corresponding to *Physarum*'s calcium-inhibited actin-myosin interaction. Third, the viscoelastic properties were investigated using a microindentation setup. In conclusion, we have shown that microplasmodia are very well suited to study the mechanobiology of *Physarum* due to the reliability, robustness and precision of the system.

BP 6.4 Mon 16:00 H 1028

Mutant cell dynamics in hierarchical organized tissues and resistance development to molecular targeted treatment strategies — •Benjamin Werner and Arne Traulsen — Max Planck Institut für Evolutionsbiologie, Plön, Germany

Most cancers are caused by either a single or more often an accumulation of mutations and thereby altered cell differentiation properties. Nowadays many of these mutations are known and in individual cases molecular targeted drugs were developed, converting ultimate life threatening into chronic diseases. Unfortunately cancer cells tend to develop resistance, leading to treatment failures. We analyze a resistance inducing experiment by applying a minimalistic mathematical model and are able to infer important system parameters, highlighting different resistance mechanism [1]. Translating these in vitro results into an in vivo dynamics is challenging, due to complex cell interactions in hierarchical organized tissues. A minimalistic individual based mathematical model allows us to describe basic properties of mutant cell dynamics in such tissues, most important the cell compartment of the mutant origin and the time development of the mutant population [2]. From this it is apparent that small differences in vitro can lead to important consequences in vivo.

[1] Werner B, Lutz D, Brümmendorf TH,Traulsen A, Balabanov S (2011) Dynamics of resistance development to imatinib. PLoS One .

[2] Werner B, Dingli D, Lenaerts T, Pacheco J, Traulsen A (2011) Dynamics of mutant cells in hierarchical organized tissues. PLoS Comput Biol .

BP 6.5 Mon 16:15 H 1028

Mechanical response of living cells to laser induced temperature shocks — •Anatol Fritsch, Tobias Kiessling, Roland Stange, and Josef Käs — Universität Leipzig, Leipzig, Germany

Living cells obtain mechanical stability from the cytoskeleton, a complex network of filamentous proteins, linkers and molecular motors. Alterations in cell mechanics to environmental stimuli, e.g. drug treatment, substrate stiffness, etc has been frequently investigated.

We developed a modified microfluidic Optical Stretcher setup able to adjust temperature during creep experiments on a millisecond timescale while automatically measuring thousands of cells. The features and reliability of this new tool are presented. A strong impact of temperature on single cell mechanics is revealed. Rarely investigated before, modulation of cell mechanics in response to temperature changes unexpectedly connects single cell mechanics to the rheology of polymer solutions.

BP 6.6 Mon 16:30 H 1028

Tailored Micro-Stencils for studying the impact of size and shape of migrating cell ensembles on their collective behavior — •Sebastian Rausch[1,2], Christian H. J. Böhm[1,2], and Joachim P. Spatz[1,2] — [1]Max Planck Institute for Intelligent Systems, Department of New Materials and Biosystems, Stuttgart — [2]Heidelberg University, Institute for Physical Chemistry, Heidelberg

Many fundamental biological processes, including morphogenesis, tissue repair and tumor invasion, require the collective motions of cells within groups, that are connected by cell-cell junctions.

The objective of our work is to elucidate and characterize the collective behavior of cell ensembles addressing the following key questions: To which extent are cell systems capable of developing multi-cellular collective patterns? How are collective properties established and controlled? We are thereby particularly interested in the formation of so called leader-cells and the specific impact of size and shape of a cell ensemble on its collective behavior and emergent properties.

Here, we introduce a tailored and adapted micro-stencil-technique based on soft-lithography, which allows us to create cell ensembles of arbitrary and well-defined shape and size. Our approach enables us to quantify the impact of these crucial boundary conditions. This technique enables us to improve the understanding of collective cell migration mode. Thorough knowledge of this fundamental migration behavior is a necessary prerequisite for a comprehensive understanding of morphogenesis or tumor metastasis via collective migration.

BP 6.7 Mon 16:45 H 1028

A theory of sarcomeric pattern formation by actin cluster coalescence — •Benjamin M Friedrich[1,3], Elisabeth Fischer-Friedrich[2,3], Nir S Gov[2], and Samuel A Safran[1] — [1]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel — [2]Department of Chemical Physics, Weizmann Institute of Science, Rehovot, Israel — [3]Current address: Max-Planck Institute for the Physics of Complex Systems, Dresden, Germany

Contractile function of striated muscle cells depends crucially on the almost crystalline order of actin and myosin filaments in myofibrils, but the physical mechanisms of myofibril assembly remains ill-defined. Passive diffusive sorting of actin filaments into sarcomeric order is kinetically impossible, suggesting a pivotal role of active processes in sarcomeric pattern formation. Using a computational model, we show that actin filament treadmilling in the presence of processive plus-end crosslinking provides a simple and robust mechanism for the polarity sorting of actin filaments. We propose that the coalescence of crosslinked actin clusters could be key for sarcomeric pattern formation. In our simulations, sarcomere spacing is set by filament length prompting tight length control already at early stages of pattern formation. The proposed mechanism could be generic and apply both to premyofibrils and nascent myofibrils in developing muscle cells as well as possibly to striated stress-fibers in non-muscle cells.

BP 6.8 Mon 17:00 H 1028

Probing the initial stages of phagocytosis with magnetic microparticles — •Matthias Irmscher[1], Arthur de Jong[1], Menno Prins[1,2], and Holger Kress[1] — [1]TU Eindhoven, Eindhoven, The Netherlands — [2]Philips Research, Eindhoven, The Netherlands

Phagocytosis, the uptake of external objects, such as bacteria is a key function of immune cells. It is a process that is driven by a deformation of the cell membrane with the aim of engulfing the target. The signaling pathways that drive phagocytosis have been extensively studied but little is known about the inherent mechanical aspects. We study the mechanics of phagocytosis by measuring the time-resolved changes of the membrane stiffness around a particle that acts as a phagocytic target. We use magnetic microparticles coated with immunoglobulin G to trigger phagocytosis upon binding. To quantify the translational and rotational motion of the magnetic particles, we tag them with fluorescent fiduciary markers. We exert a mechanical torque on the particles by applying a modulating magnetic field and simultaneously measure the rotational and translational particle displacements to quantify the mechanical properties of the binding site. Our measurements show an irreversible stiffening of the contact site by at least a factor five within a time span of a few hundred seconds. We hypothesize that the observed increase in stiffness originates from the cell membrane wrapping around the particle. By considering the energy of a deformed membrane, we describe the size of the phagocytic cup as a function of the measured stiffness. Our technique provides a new tool to quantitatively study the dynamics of membrane processes such as phagocytosis.

BP 6.9 Mon 17:15 H 1028

Mechanosensing of Type IV Pilus mediated Force in Epithelial Cells — •Enno Rainer Oldewurtel, Dirk Opitz, and Berenike Maier — Biozentrum, Universität zu Köln, Zülpicher Str. 47b, 50674 Köln

Mechanical stimuli can act as important cues in triggering signalling of cellular functions. The human pathogen *Neisseria gonorrhoeae* produces thin polymeric cell appendages called type-IV-pili (T4P). Retraction of these T4P can generate remarkably high forces and has been shown to be required for cytoskeletal changes (cortical plaques) in the host cell during infection.

Here, laser tweezers are used with T4P coated beads to mimic the mechanical stimulus of *N. gonorrhoeae* and to detect the forces required for the response. Cytoskeletal changes are monitored via fluorescent confocal imaging. We demonstrated a rapid cytoskeletal response to force generated by T4P. Both actin-EGFP and ezrin-EGFP accumulate beneath T4P-coated beads when force is applied exceeding controls without force or without pili within minutes.

Investigating possible mechanisms underlying this response we infected epithelial cells with *N. gonorrhoeae* and observed the distribution of other proteins tagged to fluorescent markers beneath bacterial micro-colonies. Vinculin, a typical focal complex protein, did not accumulate in cortical plaques. When adding RGD peptides in order to

decrease a potential interaction between T4P and integrins, the formation of cortical plaques does not appear to be hindered. These results suggest a mechanism differing to the formation focal complexes.

BP 7: Posters: Proteins

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

BP 7.1 Mon 17:30 Poster A

Conformational energy hierarchy of benchmark polyalanine based peptides with secondary structure — •Sucismita Chutia, Mariana Rossi, Volker Blum, and Matthias Scheffler — Fritz-Haber Institute, Berlin, Germany

An important challenge for the theoretical study of peptides and proteins is a faithful representation of the most stable conformations and their energy hierarchy. We here address the accuracy of a first-principles based conformational search approach for two polyalanine-based peptides that are well studied in vacuum experiments and can thus be considered "benchmark cases". We use a force-field based prescreening of the astronomically large number of possible conformers, followed by thousands of post-relaxations using density functional theory (PBE) with corrections for van der Waals terms [1]. This approach yields good agreement with experiment for the polyalanine based peptide Ac-Ala_5-$LysH^+$ [2]. However, in the case of the equally well studied peptide Ac-Phe-Ala_5-$LysH^+$ [3], the experimentally observed structures at low temperature are not simply the lowest (potential) energy ones. By varying the density functional, we show that its accuracy could partially account for the discrepancy, but in addition, much better agreement with experiment would result by including room-temperature vibrational free energy contributions. We suggest that the predominance of the experimental conformers is affected by selection/freezing at room temperature. [1] A.Tkatchenko and M.Scheffler, PRL **102**, 073005 (2009). [2] M. Rossi *et al.*, J. Phys. Chem. Lett. **1**, 3465 (2010). [3] J.A. Stearns *et al.*, PCCP **11**, 125 (2009).

BP 7.2 Mon 17:30 Poster A

Characterization and Application of the redox-sensitive GFP-mutant roGFP — •Sebastien Peter[1], Sebastian Wierer[3], Kirstin Elgass[4], Stefan Bieker[1], Alfred Meixner[2], Ulrike Zentgraf[1], and Frank Schleifenbaum[1] — [1]Zentrum für Molekularbiologie der Pflanzen, Universität Tübingen, Deutschland — [2]Institut für physikalische und theoretische Chemie, Universität Tübingen, Deutschland — [3]Protein Crystallography and Molecular Bioinformatics, Universität Konstanz, Deutschland — [4]Biochemistry Department, La Trobe University, Bundoora, Australia

For the quantitative analysis of molecular processes in living (plant) cells new combinatorial approaches in optical and spectroscopic technologies are required. The use of green fluorescent protein (GFP) and its variants has revolutionized the in vivo analysis of cell biological processes. More recently, fluorescent proteins have been designed and adapted for targeted sensing of cellular metabolites. Recent progress has been made in generating a redox- sensitive mutant of GFP (roGFP). Here, we characterize the optical properties of roGFP in dependence on the environmental redox state including a comprehensive comparison of different spectral analysis approaches in vitro. Furthermore, we demonstrate several applications of roGFP in living plants such as long-term redox potential readout in plant cells.

BP 7.3 Mon 17:30 Poster A

Simulating the infrared spectra of solvated molecules — •Jonathan Brox, Sebastian Waltz, Maja Kobus, and Gerhard Stock — Biomolecular Dynamics, Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg

Advances in time-dependent two dimensional infrared spectroscopy (IR) give the possibility to resolve structural dynamics peptides and proteins in real time. In particular, the spectrum of the amide I mode is a sensitive probe for conformational dynamics. To model IR spectra, we need to calculate the instantaneous vibrational frequency. We simulate small peptides in water to estimate the intra- and intermolecular contributions to the frequency shift. Established models describe the influence of the solvent during the simulation to the amide I band in different ways. In this talk, we will compare first results from a force-field based ansatz by D. Oxtoby [1] with an ab initio based method [2] and an empirical map [3].

[1] D. Oxtoby, Annu. Rev. Phys. Chem. **32**, 77 (1981)
[2] R. Gorbunov, D. Kosov and G. Stock, J.Chem. Phys. 2005, **122**, 224904
[3] L. Wang, C. Middleton, M. Zanni and J. Skinner, J. Phys. Chem. B 2011, **115**, 3713

BP 7.4 Mon 17:30 Poster A

Macromolecular unfolding properties in presence of compatible solutes — •Jens Smiatek[1], Hans-Joachim Galla[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, WWU Münster, D-48149 Münster, Germany — [2]Institut für Biochemie, WWU Münster, D-48149 Münster, Germany

We present Molecular Dynamics simulations of Chymotrypsin inhibitor II and PEO in presence of compatible solutes. Our results indicate that the native compact state of the studied macromolecules is stabilized in presence of hydroxyectoine. We are able to explain the corresponding mechanism by a variation of the solvent properties for higher hydroxyectoine concentrations. Our results are validated by detailed free energy calculations.

BP 7.5 Mon 17:30 Poster A

Dynamic disorder in enzyme catalyzed reactions: a general phenomenon? — Tatyana Terentyeva[1], Hans Engelkamp[2], Alan E. Rowan[2], Tamiki Komatsuzaki[3], Johan Hofkens[1], Chun-Biu Li[3], and •Kerstin Blank[2] — [1]Katholieke Universiteit Leuven, Department of Chemistry, Leuven, Belgium — [2]Radboud University Nijmegen, Institute for Molecules and Materials, Nijmegen, The Netherlands — [3]Hokkaido University, Research Institute for Electronic Science, Sapporo, Japan

Single molecule fluorescence experiments allow the recording of the sequence of individual enzymatic turnover reactions. Experiments with different enzymes have shown that the waiting times between turnovers follow a stretched exponential distribution interpreted as dynamic disorder. Although easily explained with the existence of several enzyme conformations with different activity the question remains if dynamic disorder is a general property of enzymes. Studying the enzyme chymotrypsin we observe deviations from a stretched exponential distribution. Moreover, we see obvious differences in the shape of the waiting time distributions depending on the data analysis method used. Comparing the performance of the most widely employed binning and thresholding approach with change point analysis we observe that the underlying on- and off-histograms are not necessarily extracted from the "signal" buried in noise. When using the more accurate change point analysis for data of chymotrypsin no characteristics of dynamic disorder can be found. In light of these new results, dynamic disorder might not be a general characteristic of enzymatic reactions.

BP 7.6 Mon 17:30 Poster A

Molecular Dynamics Simulations of Hydrated Proteins: Possible Origins of a Logarithmic Protein Relaxation. — •Kerstin Kämpf and Michael Vogel — TU Darmstadt, Institut für Festkörperphysik, 64289 Darmstadt

Biological function is the consequence of protein fluctuations in a complex energy landscape. An unresolved puzzle of protein dynamics is the origin of a strongly nonexponential relaxation observed over several orders of magnitude in time.

In order to elucidate this phenomenon, we perform molecular dynamics simulations of hydrated elastin and myoglobin. It is observed that the orientational and translational correlation functions of the protein backbone are well described by a power law [1] or a logarithmic decay [2]. Assuming a heterogeneous origin of the power-law decay, we analyze the temperature dependent mean relaxation rates. An Arrhenius behavior with an activation energy $E_a \approx 0.25$ eV is obtained, corresponding to the energy necessary to break a hydrogen bond. Fitting to a logarithmic decay, we tested whether the predictions of the mode-coupling theory are fulfilled. We investigate further how far the dynamics of hydrated proteins resemble that of other complex systems.

Finally, we calculate multi-time correlation functions to determine the relevance of homogeneous and heterogeneous contribution to the

strongly nonexponential decay. This analysis allows to characterize the complex energy landscape and thus to shed light on the nature of the microscopic processes underlying protein function.

[1] Iben et al. PRL 62, 1916. [2] Lagi et al, PRL, 103, 108102.

BP 7.7 Mon 17:30 Poster A

How cations change peptide conformation: First principles simulations and infrared spectroscopy — •Carsten Baldauf[1], Kevin Pagel[1], Volker Blum[1], Stephan Warnke[1], Gert von Helden[1], Beate Koksch[2], Gerard Meijer[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institut für Chemie und Biochemie, FU Berlin

Turns are the hinges arranging periodic secondary structure elements (helices and strands) to form compact protein tertiary folds. Li^+ alters protein backbone conformation. We investigate this effect on structure and dynamics of turns Ac-Ala-{Ala,Asp}-Pro-Ala-NMe by theoretical conformational analyses and experimental vibrational spectroscopy. As standard force fields apparently lack accuracy for ion-peptide interactions, we demonstrate a trustworthy description of the potential-energy surface of these systems by van der Waals corrected density-functional theory (PBE+vdW) and compare to gas-phase infrared spectroscopy, both approaches in the exact-same clean-room environment. We predict canonical turn conformations for the peptides alone. Li^+ and Na^+ adsorb to C=O groups, induce unusual backbone conformations, and prevent H bond formation. By including free-energy contributions, essential for consistent theory-experiment comparison, we show that multiple conformers coexist at room temperature. First-principles molecular dynamics simulations lead to theoretical spectra (including anharmonic effects) which indicate low-energy conformers do not equally contribute to the experimental spectra. They also give insights into backbone motion patterns (peptide bond crankshaft rotation).

BP 7.8 Mon 17:30 Poster A

Chloroplast fluorescence excitation and emission spectroscopy in live plant cells — •Sebastien Peter[1], Martina Zell[5], Christian Blum[3], Kirstin Elgass[4], Veronica Maurino[5], Alfred Meixner[2], Vinod Subramaniam[3], and Frank Schleifenbaum[1] — [1]Zentrum für Molekularbiologie der Pflanzen, Universität Tübingen, Deutschland — [2]Institut für physikalische und theoretische Chemie, Universität Tübingen, Deutschland — [3]Biophysical Engineering, University of Twente, Enschede, The Netherlands — [4]Biochemistry Department, La Trobe University, Bundoora, Australia — [5]Botanisches Institut, Universität zu Köln, Deutschland

Statistical analysis of chloroplast fluorescence spectra recorded at room temperature enables for drawing conclusions about the relative PSI/PSII ratio in wild type and carbon deficient plant cells. Leaf cells exhibit fluorescence from chloroplasts whose spectra show two bands assigned to the photosystems. Changes in a plant's environmental conditions are reflected by an altered efficiency of photosynthesis. Fluorescence excitation spectra of plants grown under different conditions show three peaks assigned to different carotenoids. The spectra not only differ in the intensity ratios between different pigments but also in the broadth of their distributions revealing a higher adaptation flexibility of wild-type plants. Therefore, fluorescence excitation and emission spectroscopy at room temperature enables for live read-out of the photosynthesis adaption to external conditions without generating artifacts from extensive sample preparation and low temperatures.

BP 7.9 Mon 17:30 Poster A

Ab initio Molecular Dynamics & NMR Spectra of Phycocyanobilin in the α-C-Phycocyanin binding pocket — •Hossam Elgabarty and Daniel Sebastiani — Freie Universität Berlin Fachbereich Physik Arnimallee 14 14195 Berlin

Biliproteins are ubiquitous photoreceptors. On exposure to red light the bound bilin chromophore exhibits a very quick photoisomerization within a few picoseconds [1]. Interactions between the bilin and its binding pocket play a crucial role in this process. We have performed ab-initio QM/MM molecular dynamics simulations of phycocyanobilin bound to the C-subunit of α-C-phycocyanin. Our results provide insight into the nature of the local interactions around the chromophore. Calculations of ^{14}N and ^{1}H NMR shifts are in good agreement with experimental spectra and demonstrate that the chromophore is stably protonated in acccord with experimental findings [2]. Our results pave the way to further investigation of the photocycle by exploiting the sensitivity of NMR spectra to local environment [3].

1 Ulijasz, A. T., Vierstra, R. D. Curr. Opin. Plant Biol., 14, 498-506. (**2011**)

2 Hahn, J., Kühne, R., Schmieder, P. ChemBioChem, 8, 2249-55. (**2007**)

3 Elgabarty, H., Röben, M., Schmieder, P., Sebastiani, D. (Submitted)

BP 7.10 Mon 17:30 Poster A

Many-Body study of the excited-state properties of the Retinal Protonated Schiff Base of Rhodopsin — •Adriano Mosca Conte[1], Leonardo Guidoni[2], Daniele Varsano[3], and Olivia Pulci[1] — [1]MIFP, NAST, ETSF,CNR INFM-SMC, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, Roma, Italy — [2]University of L'Aquila, Dipartimento di Chimica, Ingegneria Chimica e Materiali, Via Campo di Pile, 67100, L'Aquila, Italy — [3]University of Rome "La Sapienza" , P.le Aldo Moro 2, Rome, Italy

The first step of the mechanism of vision in living creatures is the photo-isomerization of the rhodopsin chromophore: the protonated Schiff base of the 11-cis retinal. We investigate the optical properties of the tZt-penta-3,5-dieniminium cation, a simplified model for the retinal, along the isomerization pathway by ab-initio calculations based on Many-Body Perturbation Theory (GW method and the Bethe-Salpeter equation), and by TDDFT. Our excitation energies are qualitatively in agreement with previous Quantum Monte Carlo and Post-Hartree Fock calculations. We then investigate the effect of the protein environment on the optical absorption spectra of the 11-cis retinal, in gas phase and in the rhodopsin. We follow a Quantum-Mechanics/Molecular-Mechanics scheme in which the retinal is treated by quantum Many-Body methods (DFT+GW+BSE), while the surrounding atoms of the protein are treated according to a classical model. Our results show that the effect of the rhodopsin on the retinal produces a geometrical distorsion of the retinal and a blueshift on the absorption spectrum in good agreement with the experiments.

BP 7.11 Mon 17:30 Poster A

A method to construct the free energy landscape of peptide aggregation from molecular dynamics simulations. — •Laura Riccardi, Phuong H. Nguyen, and Gerhard Stock — Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, 79104 Freiburg, Germany

A broad range of diseases are associated with the conversion of polypeptide chains from their normally soluble form to insoluble fibrillar aggregates. One of the most studied pathogenic peptides is the Alzheimer β-amyloid peptide, and its fragment $A\beta_{16-22}$ appears to be a perfect model system as it is among the shortest fragments which are able to form fibrils [1]. We propose a new method to identify and characterize the different conformational states occurring during the aggregation process. This method is general as no *a priori* knowledge of the dynamics of the process or the structure of the encounter complex is required. In the different steps, intramolecular and intermolecular interactions are considered as well as the degeneracy of the multi-molecule system. The obtained states are used to construct a network which reflects the free energy landscape of the process and helps to identify the aggregation pathways.

[1] P.H. Nguyen et al, Monomer adds to preformed structured oligomers of $A\beta$-peptides by a two-stage dock-lock mechanism. PNAS 104, 111 (2007)

BP 7.12 Mon 17:30 Poster A

***Ab initio* conformation trends across 20 amino acids, dipeptides, and their interaction with divalent ions** — •Matti Ropo, Carsten Baldauf, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Ion-protein interactions are of tremendous importance in cellular signalling of all organisms. For instance, the binding properties of Ca^{2+} can be mimicked by heavy metals like Pb, thus disturbing Ca-dependent functions[1]. We have constructed an exhaustive, first-principles based conformational (*in vacuo*) database of the 20 proteinogenic amino acids, their dipeptides, and of their interactions with the divalent cations of Ca, Sr, Ba, Cd, Pb, and Hg. The database was established using all-electron density functional theory with the van der Waals-corrected PBE functional.[2] We here use it to discuss trends of biological interest, for example: (i) a uniform binding order of ions relative to Ca^{2+}—Sr^{2+} and Ba^{2+} bind weaker, Pb^{2+} binds similar, Cd^{2+} and Hg^{2+} stronger. (ii) Dipeptides bind cations stronger than

amino acids alone. (iii) Interestingly, Ca^{2+} binds strongest to Arg and Tyr, not to Asp or Glu (assuming the neutral protonation state for the amino acids). (iv) We evaluate backbone conformations by means of Ramachandran plots and atomic distribution function and compare these data sets to experimental structural data from the RCSB protein data bank. Finally, we address the impact of density functionals beyond the generalized gradient approximation. [1] H.A. Godwin, Curr. Opin. Chem. Biol. **5**, 223 (2001); [2] A. Tkatchenko and M. Scheffler, PRL **102**, 73005 (2009).

BP 7.13 Mon 17:30 Poster A

Lactoferrin: dynamics of a flexible protein in solution investigated by neutron scattering — •Clemens Sill[1], Ralf Biehl[1], Bernd Hoffmann[2], and Dieter Richter[1] — [1]JCNS-1 & ICS-1, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]ICS-7, Forschungszentrum Jülich, 52425 Jülich, Germany

The understanding of the functionality of proteins started with a rigid model, namely the Lock and Key analogy, in 1894. Meanwhile, a more dynamic and flexible picture of these macromolecules has evolved to explain protein function like catalyzing biochemical reactions, transport, regulation, storage or defensive tasks. The importance of thermodynamically driven, internal motions for the functioning of proteins is subject of ongoing research.

We will present recent investigations of protein dynamics on Lactoferrin, a protein with antimicrobial activity which is part of the innate immune system. It consists of two binding sites, each is capable of binding and releasing one iron ion. The crystallographic structures show that the binding sites have open and closed conformations, assumedly depending on the presence of iron. We are analyzing the internal dynamics of different binding states to elucidate the binding mechanism with neutron scattering. Our unique method includes large scale structural characterization with small angle neutron scattering and the observation of internal motions of subdomains with neutron spin echo spectroscopy on nanosecond scale. This combination provides the opportunity to investigate the link between binding mechanism, internal dynamics and conformational change.

BP 7.14 Mon 17:30 Poster A

The class IIa Water soluble chlorophyll binding protein (WSCP) from cauliflower can be described by an electronically strongly coupled dimer bound to two different protein configurations — •Franz-Josef Schmitt[1], Jörg Pieper[2], Christoph Theiss[1], Inga Trostmann[3], Harald Paulsen[3], Thomas Renger[4], Hans Joachim Eichler[1], Thomas Friedrich[1], and Gernot Renger[1] — [1]Berlin Institute of Technology, Germany — [2]University of Tartu, Estonia — [3]Johannes Gutenberg University Mainz, Germany — [4]Johannes Keppler University Linz, Austria

Spectroscopic studies on pigment-pigment and pigment-protein interactions of chlorophyll (Chl) a and b bound to the recombinant protein of class II a WSCP from cauliflower were performed with absorption and fluorescence spectroscopy in the time domain of fs and ps, respectively, providing evidence for spectral inhomogeneity in these samples even if the WSCP contains only homodimers. In class II a WSCP two Chls form a strongly excitonically coupled open sandwich dimer within the tetrameric protein matrix. A modulation of the electronic states of the coupled Chl dimer by the protein environment with a typical time constant of 100 ps at 10 K is inferred to be responsible for a fast and strongly temperature dependent fluorescence component. This idea is in line with refined theoretical models and results of complementary studies of hole burning and fluorescence line narrowing spectroscopy. We show that the time resolved fluorescence spectra can be simulated with rate equation models based on results obtained with recent FLN and hole burning studies.

BP 7.15 Mon 17:30 Poster A

Determination of the hydrodynamic radius of GFP-tagRFP FRET-Constructs with Fluorescence Correlation Spectroscopy — •Patrick Hätti[1], Franz-Josef Schmitt[2], Cornelia Junghans[2], Marco Vitali[2], and Thomas Friedrich[2] — [1]Institute of Optics and Atomic Physics, Berlin Institute of Technology, Germany — [2]Max Volmer Laboratory for Biophysical Chemistry, Berlin Institute of Technology, Germany

Fluorescence correlation spectroscopy (FCS) is suitable to determine the hydrodynamic radius of single molecules and protein chromophors by taking the $G(\tau)$ autocorrelation function and calculating the diffusion time. FCS and fluorescence lifetime measurements were done simultaneously with a novel Fluorescence Lifetime Imaging Microscopy setup (FLIM) with an integrated Single-Photon-Avalanche-Diode (SPAD). We determined the hydrodynamic radius of Green Fluorescent Protein to 3.2 nm. A FRET-construct consisting of the GFP-tagRFP fusion protein was observed with a much larger hydrodynamic radius of 12.6 nm, which might be explained by a more complex geometrical structure of the molecule that has more degrees of freedom. GFP and tagRFP are linked via a 5 amino acid-long linker that connects the two single, barrel-shaped fluorescent proteins. In addition to FCS, the setup allows the determination of the fluorescence lifetimes and therefore the calculation of the center-to-center distance of the molecular transition dipoles according to the theory of Förster Resonance Energy Transfer, which is compared with the hydrodynamic radius.

BP 7.16 Mon 17:30 Poster A

Characterization of novel bimolecular fluorescence complementation (BiFC) protein complexes by single-molecule spectroscopy — •Sven zur Oven-Krockhaus[1], Sebastien Peter[1], Alfred Meixner[2], Klaus Harter[1], and Frank Schleifenbaum[1] — [1]Zentrum für Molekularbiologie der Pflanzen, Tübingen, Deutschland — [2]Institut für physikalische und theoretische Chemie, Tübingen, Deutschland

The identification and characterization of protein-protein interaction networks in living organisms is of major importance in current proteome sciences. Bimolecular fluorescence complementation (BiFC) constitutes an innovative method to visualize interaction partners in living cells. As this technique utilizes molecular markers, a competent knowledge of their photophysical properties is essential. In the case of multicolor BiFC, two nearby fragments of different GFP mutants can spontaneously recombine to a functional fluorescent protein complex. Even though they only differ in few amino acids, differently composed complexes show a significant diversity in their spectroscopic properties. As many photophysical features are concealed in bulk measurements, a single molecule approach has been employed to characterize model systems of these BiFC complexes. Several hundred single molecule spectra and fluorescence intensity time traces were accumulated in order to identify the spectroscopically most relevant amino acids in the protein shell structure - uniquely revealing their influence on the shells' mechanical flexibility.

BP 7.17 Mon 17:30 Poster A

Calculation of the CD spectrum of a peptide from its conformational phase space — •Zlatko Brkljača[1], Karmen Čondić-Jurkić[1], David M. Smith[2], and Ana-Sunčana Smith[1] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Computer Chemie Centrum, Universität Erlangen-Nürnberg, Erlangen, Germany

Met-enkephalin (Tyr-Gly-Gly-Phe-Met) and its unnatural analogue Ada-enkephalin are opioid peptides which act as inhibitors of tumorcells in a receptor-mediated fashion. We have investigated the structural preferences of these peptides in 2,2,2-trifluoroethanol in an attempt to calculate their respective CD spectra. To this end, we have characterized the conformational preferences of the zwitterionic and neutral forms of Met-enkephalin and of both the *R*- and the *S*-epimers of Ada-enkephalin, as obtained by replica exchange molecular dynamics. The CD spectrum for each peptide was subsequently obtained with a procedure of successive averaging, which accounts for the sidechains and the backbone variations of the peptides and the effect of the solvent on the CD spectra. To make a proper comparison with the experiment, we have produced composite spectra that account for the appropriate contributions of the zwitterionic and neutral forms of the peptides as well as the expected epimeric ratio. Such a procedure results in theoretically obtained CD spectra that successfully reproduce the most important features of the experimentally measured spectra. Consequently, the link between the CD spectra and the conformational phase space of flexible peptides can be established for the first time.

BP 7.18 Mon 17:30 Poster A

Combined time-resolved and integrated analysis of FRET efficiency in genetically expressed GFP-tagRFP fusion proteins — •Jörn Weissenborn[1], Franz-Josef Schmitt[2], Patrick Hätti[1], Cornelia Junghans[2], Oliver Schöps[1], Ulrike Woggon[1], and Thomas Friedrich[2] — [1]Institute for Optics and Atomic Physics, Berlin Institute of Technology, Germany — [2]Max Volmer Laboratory for Biophysical Chemistry, Berlin Institute of Technology, Germany

Förster resonance energy transfer (FRET) was investigated in constructs consisting of GFP-tagRFP fusion proteins with varying dis-

tance between donor and acceptor. In the short and long construct, GFP and tagRFP are linked via a 5 and 13 amino acid-long linker, respectively, that connects the two single, barrel-shaped fluorescence proteins. Interestingly, a strong donor quenching of the short-linker FRET construct does not lead to a concomitant rise of the acceptor fluorescence (RFP) with the same amplitude. An accurate analysis of 2-dimensional photoluminescence excitation spectroscopy (PLE) and time-and wavelength resolved fluorescence decay showed congruent results. The data analysis reveals that only 50 % of the GFP molecules are coupled to tagRFP via excitation energy transfer (EET). The efficiency of the EET in the coupled GFP-tagRFP pairs calculates to about 65 %. According to our experiments and the FRET theory, the long-linker construct should show virtually no EET. The overall transfer efficiency (coupled and uncoupled species) is calculated to 30 % and < 1 % in the short- and long-linker FRET construct, respectively.

BP 7.19 Mon 17:30 Poster A

Ribonuclease A: A Model System to Study Structure and Dynamics of Disordered Proteins — •Jennifer Fischer[1], Ralf Biehl[1], Bernd Hoffmann[2], and Dieter Richter[1] — [1]Forschungszentrum Jülich, ICS-1, Jülich, Germany — [2]Forschungszentrum Jülich, ICS-7, Jülich, Germany

Up to know structure and dynamics are believed to play the key role in protein function. Now it is evident that roughly 30% of eukaryotic proteins are partially or even completely unfolded [1]. Nevertheless, intrinsically unfolded proteins are functional and involved in several biological processes. To get further insight into disordered structures and their dynamics, we use Ribonuclease A (RNase A) as a model system, as it is a well known protein denaturing reversibly upon heating. Additionally, by varying the buffer conditions such as pH values and by reducing the disulfide bonds, several states can be prepared. A detailed study of the structure and dynamics using Small Angle Neutron and X-ray Scattering (SANS, SAXS) as well as Neutron Spin Echo Spechtroscopy (NSE) and Circular Dichroism Spectroscopy is presented. The combination of these techniques allows us to observe large-scale internal dynamics of subdomains or of unfolded protein strands that operate on the same length scale as rotational diffusion. However, the timescale can be different and depends on the protein structure and internal interactions. [1] A. L. Fink, Current Opinion in Structural Biology 2005, 15:35-41

BP 7.20 Mon 17:30 Poster A

Probing peptide structure prototypes with first-principles replica exchange: Ac-Ala$_{19}$-LysH$^+$ vs. Ac-LysH$^+$-Ala$_{19}$ — •Franziska Schubert, Mariana Rossi, Carsten Baldauf, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut der MPG, D-14195 Berlin

Predicting the structure of peptides requires a method with high accuracy for "weak" interactions. We here focus on the predominant structure types of two alanine-based peptides under "clean-room" conditions in the gas phase from first principles and in comparison to experimental IR spectroscopy [1]: Ac-Ala$_{19}$-LysH$^+$, which is α-helical [2,3], in contrast to Ac-LysH$^+$-Ala$_{19}$, where mostly globular monomers and a small amount of helical dimers and helices with non-standard protonation sites are expected [3]. Despite supposedly very different conformers, Ac-LysH$^+$-Ala$_{19}$ and Ac-Ala$_{19}$-LysH$^+$ yield very similar experimental IR spectra in the $\approx$1000-2000 cm^{-1} wavenumber range. We suggest plausible candidates for all likely structure prototypes generated by a two-step structure search: On top of force-field based replica exchange molecular dynamics (REMD) scans we follow up with further REMD scans based on density functional theory with the van der Waals corrected [4] PBE functional. Helix-turn-helix motifs emerge as the most likely candidates and explain a subtle peak shift in experiment. [1] IRMPD experiments: G. von Helden, P. Kupser, K. Pagel, F. Filsinger, G. Meijer, Department of Molecular Physics, Fritz-Haber-Institut; [2] M. Rossi *et al.*, JPCL **1**, 3465 (2010); [3] M. Jarrold, PCCP **9**, 1659 (2007); [4] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).

BP 7.21 Mon 17:30 Poster A

Solvent induced isomerization in phycocyanobilin — •Tobias Watermann, Hossam Elgabarty, and Daniel Sebastiani — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Phytochromes belong to the family of light detecting proteins, that are responsible for the reaction of biological systems to light. Their central functional part is a chromophore, which isomerizes upon excitation and initializes the signaling process of the protein. Recent NMR experiments [1] on the isolated chromophore phycocyanobilin show differing spectroscopic properties for different solvents. We investigate the underlying conformational space by means of ab-initio molecular dynamics and free energy calculations as well as ab-initio spectroscopy [2]. It turns out that it is of crucial importance to include the explicit solvent and its interaction with the chromophore. In our ab-initio molecular dynamics simulations, we observe specific preferences for certain conformations as a function of the polarity of the solvent. These computational results are confirmed by comparing ab-initio NMR chemical shifts in the different situations to corresponding experiments. This solvent dependent effect can be traced back to a change in the equilibrium between intra- and intermolecular hydrogen bonds of the chromophore and the solvent.

1 M. Röben, P. Schmieder, Magn. Reson. Chem., 49, 543-548 (**2011**)

2 T. Watermann, H. Elgabarty, M. Röben, P. Schmieder, D. Sebastiani (Submitted)

BP 7.22 Mon 17:30 Poster A

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

Tip-enhanced Raman spectroscopy (TERS) combines high spatial resolution of atomic force microscopy (AFM) with structural sensitivity of surface-enhanced Raman spectroscopy (SERS). Using a gold-coated AFM tip, it is possible to measure Raman signals with a spatial resolution up to 30 nm.

AFM allows imaging, measuring (e.g.: single-molecule force spectroscopy), and manipulating matter at the nanoscale. The information is gathered by "feeling" the surface with a mechanical probe.

Raman spectroscopy provides information about the molecular structure of proteins. In order to detect a monolayer of molecules we use surface-enhanced Raman spectroscopy (SERS). The SERS signal is enhanced in the vicinity of (usually) silver- or gold-coated surfaces (up to a factor of $10^9 - 10^{12}$ compared to conventional Raman).

Up to now, this technique is mainly applied to surfaces modified with inorganic samples. However, TERS is a promising tool to investigate membrane proteins since single molecules could be studied by Raman spectroscopy under biological conditions.

Here, we introduce the experimental setup and discuss the application of TERS to the investigation of membrane proteins.

BP 7.23 Mon 17:30 Poster A

Investigation of the PhoB-Interaction with the DNA - minor groove by Single Molecule Force Spectroscopy — •Adeline Bieker[1], Volker Walhorn[1], Gesa Niemann[2], Markus Ritzefeld[2], Norbert Sewald[2], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanoscience, University of Bielefeld, Germany — [2]Organic and Bioorganic Chemistry, University of Bielefeld, Germany

Interactions between proteins and DNA are essential for the regulation of cellular processes in all living organisms. In this context, it is of special interest to investigate and quantify the sequence-specific molecular recognition between transcription factors and their cognate DNA sequences [1].

We investigated point mutated proteins originating from the DNA-binding domain (DBD) of the Escherichia coli transcription factor PhoB. By means of AFM-based Single Molecule Force Spectroscopy (SMFS) we acquired binding forces and molecular elasticities to elucidate the complex stability. Based on the Bell-Evans-Modell [2] we estimated the thermal dissociation rate constants (k_{off}) and the molecular interaction length (x_β), that allowed a structure related interpretation of the physical binding mechanisms involved.

[1] Small. 2009 Apr;5(4):484-495.

[2] Biophys. J. 1997;72:1541-1555.

BP 7.24 Mon 17:30 Poster A

A Coarse-Grained Model for Protein Backbone Dynamics — Andreas Wagenmann and •Tihamer Geyer — Zentrum f. Bioinformatik, Universität des Saarlandes, Saarbrücken

When one wants to simulate the folding of proteins or the dynamics of intrinsically disordered proteins, atomistic simulations very soon become prohibitively expensive. This is even more so when multiple proteins are considered as for example in the case of amyloid formation. For these scenarios coarse-grained models are required. Here we present a newly developed hierarchic coarse-grained model which

builds upon Langevin Dynamics. Using this very efficient solvent-free simulation technique allows for more freedom in the modeling than a united-atom-approach with its still spherical super-atoms. Here we show how we base the model of the protein backbone on non-spherical building blocks with off-center bonds. By construction, the allowed regions in the Ramachandran angle space are reproduced. Non-local steric interactions, electrostatics, and hydrogen bonds form a second layer and modify the secondary structure propensities according to the residue types. We also demonstrate that poly-peptides form alpha-helical or beta-strand structures according to their amino-acid composition even when we start from random initial configurations. This model can be used to efficiently simulate the folding and association of unfolded proteins like Amyloid-β or α-synuclein.

BP 7.25 Mon 17:30 Poster A

Using Dynamic Graphs to Quantitatively Visualize Agglomeration in Spatial Simulations — •Tihamer Geyer[1], Florian Lauck[2], and Volkhard Helms[1] — [1]Zentrum für Bioinformatik, Universität des Saarlandes, Saarbrücken — [2]Dept. of Bioengineering and Therapeutic Sciences, UCSF, San Francisco, USA

The usual approaches to analyze many-particle simulations of association processes either focus on time-averaged measures for the degree of binding like radial distribution functions or cluster sizes, or movies are generated which in principle provide all the details but in an only qualitative way. Here we show how dynamic graphs can be used to visualize quantitatively the time dependent events of complex formation and breaking. For this, a simple distance criterion is used to set up a time dependent graph from the snapshots of the spatial simulation [1]. Some examples highlight how even simple graph measures like the degree distribution or the clustering coefficient can be used to follow the dynamics, to unambiguously identify complexes in a sea of monomers and partially assembled fragments, or to quantify how regular or amorphous an aggregate is [2]. In a further step the spatial simulation and the dynamic graph will be combined such that the simulation can make use of the connectivity encoded in the graph by, e.g., defining temporary pseudo-particles or different diffusion coefficients based on how many neighbors are actually bound.

[1] F. Lauck, V. Helms, T. Geyer, *J. Chem. Theor. Comput.* **5** (2009) 641

[2] T. Geyer, *BMC Biophys.* **4** (2011) 7

BP 7.26 Mon 17:30 Poster A

Investigations of the Dynamics of Protein Hydration Water, Water in an amorphous Ice Confinement and bulk Water, performed with molecular dynamics Simulations — •Felix Klameth and Michael Vogel — Institut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt

The hydration water of proteins is essential for the biological function of proteins. For Myoglobin, large fluctuations of the protein structure enable oxygen diffusion to the protein heme-group. It was proposed, that water dynamics slave the protein motion [1], but till now the explicit mechanisms of protein water coupling are not understood. In order to clarify the protein-water interaction we study the dynamics of protein hydration water. We perform molecular dynamics simulations in a temperature range from 180 K up to 300 K. To unravel specific effects at the protein surface, we compare the results for the protein hydration water with that of bulk water and of water confined in amorphous ice. There are differences observed in the water-dynamics in this systems. The temperature dependence of the α-relaxation shows an Arrhenius-behaviour for the protein-hydration water, whereas a Vogel-Fulcher-Tammann-behaviour was observed for the bulk- and the confined water. Near both surfaces, protein and ice, the relaxation times of water are increased, compared to that of bulk. The mechanisms for this characteristics are not understood so far.

[1] Frauenfelder et al, PNAS 106 (2009)

BP 7.27 Mon 17:30 Poster A

The Impact of Salt and Pressure on the Interaction Potential of Proteins in Solution — •Johannes Möller[1], Martin A Schroer[1], Mirko Erlkamp[2], Sebastian Grobelny[2], Michael Paulus[1], Andre Steffen[1], Sebastian Tiemeyer[1], Florian J Wirkert[1], Metin Tolan[1], and Roland Winter[2] — [1]Fakultät Physik/DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44227 Dortmund — [2]Physikalische Chemie, TU Dortmund, Otto-Hahn-Str. 6, 44227 Dortmund

The fabrication of crystals from protein solution has become the defining task in obtaining high resolution protein structures by X-ray diffraction. Here, the use of salt in the solution is commonly known to increase attractive interactions and therefore *salting out* the proteins. Nevertheless, the fabrication of high quality crystals is still a challenging task, due to the many different influences on the interactions in the protein solution, e.g. temperature, ionic strength, protein concentration, and pressure. We present the results of Small Angle X-ray Scattering experiments, which reveal the combined influence of hydrostatic pressure and ionic strength on the interaction potential of dense protein solution. Here, a more precise knowledge about the interaction between proteins in solution can help to predetermine possible crystallization conditions, which is even more important when only a small amount of protein is available.

BP 7.28 Mon 17:30 Poster A

Aggregation of Human Antimicrobial Peptide Fragments at Interfaces — •Claudia Dannehl[1], Thomas Gutsmann[2], and Gerald Brezesinski[1] — [1]Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam — [2]Research Center Borstel, Center for Medicine and Biosience, 23845 Borstel

Antimicrobial peptides (AMPs) are short, amphiphilic proteins and part of the host immune defense. They protect organisms against bacteria, viruses and fungi simply by disrupting their membrane. In our work, we focus on two fragments of the human cathelicidin and lipid monolayers as model membranes to get insight into this peptide-lipid interaction. It was shown by XR and IRRAS, that both peptides adopt an alpha-helical conformation, when adsorbed to lipid monolayers, but differ in their way of action. Both peptides lead to a fluidization of a negatively charged DPPG monolayer, indicated by an increased transition pressure from a liquid-like to a liquid-condensed phase (seen by GIXD and IRRAS), but the increase in surface pressure and the change in the amide band upon adsorption is peptide specific. We assume that the stronger peptide-lipid interaction of one peptide is accompanied by a peptide aggregation at the interface, as studied by IRRAS on monolayers and CD spectroscopy with SDS in bulk (above the CMC). No changes in the spectra were recorded with IRRAS for zwitterionic lipids (DPPC, DOPC) and CD for the cationic CTAB , which means that the aggregation of the peptide is dominated by the charge density of the target.

BP 7.29 Mon 17:30 Poster A

CD-spectroscopy as a tool for characterizing protein-polymer complexes — •Sven Brandt[1], Krystin Krauel[1], Kay E. Gottschalk[2], Christiane A. Helm[3], and Stephan Block[1] — [1]ZIK HIKE - Zentrum für Innovationskompetenz Humorale Immunreaktionen bei kardiovaskulären Erkrankungen„ Fleischmannstr. 42-44, D-17487 Greifswald, Germany — [2]Institut für Experimentelle Physik, Universität Ulm, D-89069 Ulm — [3]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany

Aggregates of platelet factor 4 (PF4), a highly positively charged protein that is stored in platelet alpha-granules, and natural or artificial polyanions are formed. Changes in the proteins secondary structure are monitored with circular dichroism (CD) spectroscopy, while the polyanion concentration is varied systematically. We observe pronounced structural changes of the PF4 during the interaction with highly charged polyanions. At a specific protein/monomer ratio the structural changes of the protein are most pronounced, suggesting that all proteins are incorporated into PF4-polyanion complexes. Only minor or no changes are found for weakly charged and neutral polymers. Interestingly, the most striking changes are observed for those PF4-polyanion complexes which are known to be immunogenic, such as aggregates with heparin, which can induce the life-threatening immune disorder called heparin-induced thrombocytopenia (HIT).

BP 7.30 Mon 17:30 Poster A

Probing the Transport of Ionic Liquids in Aqueous Solution through Nanopores — •Niraj Modi, Pratik Raj Singh, Kozhinjampara R. Mahendran, Robert Schulz, Mathias Winterhalter, and Ulrich Kleinekathöfer — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

The temperature-dependent transport of the ionic liquid 1-butyl-3-methyl-imidazolium chloride (BMIM-Cl) in aqueous solution is studied theoretically and experimentally. Using molecular dynamics simulations and ion-conductance measurements, the transport is examined in bulk as well as through a biological nanopore, i.e., OmpF and its mutant D113A. This investigation is motivated by the observation

that aqueous solutions of BMIM-Cl drastically reduce the translocation speed of DNA or antibiotics through nanopores in electrophysiological measurements. This makes BMIM-Cl an interesting alternative salt to improve the time resolution. In line with previous investigations of simple salts, the size of the ions and their orientation adds another important degree of freedom to the ion transport, thereby slowing down the transport through nanopores. An excellent agreement between theory and conductance measurements is obtained for wild-type OmpF and a reasonable agreement for the mutant. Moreover, all-atom simulations allow an atomistic analysis revealing molecular details of the rate-limiting ion interactions with the channel[1].

[1] N. Modi et al., J. Phys. Chem. Lett. 2, 2331 (2011).

BP 7.31 Mon 17:30 Poster A

Computersimulation of protein adsorption on polyelectrolyte brushes — •Cemil Yigit[1] and Joachim Dzubiella[2] — [1]Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin — [2]Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin

We investigate the adsorption of proteins on a partially-charged and end-grafted polyelectrolyte brush using explicit-water and coarse-grained computer simulations and Poisson-Boltzmann theory. The effects of the salt concentration, grafting density, and the charge fraction of the brushes on brush profiles and protein adsorption free energies are calculated and compared to approximative analytical theories.

BP 7.32 Mon 17:30 Poster A

Divalent cation force field optimization based on thermodynamic properties

— •Shavkat Mamatkulov[1], Maria Fyta[2], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany
— [2]Physik Department, Technische Universität München, 85748 Garching, Germany

In this work we develop force field parameters of the divalent cations Mg^{2+}, Ca^{2+}, Ba^{2+}, and Sr^{2+}. We perform Molecular Dynamics simulations with explicit water, using the SPC/E water model. The scheme we propose for the derivation of the ionic force fields is based on a simultaneous optimization of single-ion and ion-pair properties. The solvation free energy and the effective radius of the divalent cations are the single ion properties used in our approach. As a probe for the ion pair properties we compute the activity derivatives of salts in aqueous solutions. The optimization of the ionic force fields was done in two distinct steps. First, the solvation free energy and the first maximum in the ion-water radial distribution function (RDF) were determined as a function of the Lennard-Jones (LJ) parameters used in the simulations. Second, knowledge of the combinations of the LJ parameters which reproduce the exact solvation free energy and the first peak in the RDF of the divalent cations allowed us to compute the activity derivatives of the electrolytes such as MgY_2, CaY_2, BaY_2, SrY_2, where Y=Cl^-, Br^-,I^-.

BP 7.33 Mon 17:30 Poster A

Single Peptide Desorption from Solid Surfaces — •Susanne Liese[1], Nadine Schwierz[2], and Roland Netz[1] — [1]FU Berlin, Germany — [2]TU Munich, Germany

The desorption of single homopeptides from solid surfaces is examined by molecular dynamic (MD) simulations and analytical calculations. To investigate the role of the surface hydrophobicity on peptide desorption, the relation between the hydrophobicity of a self-assembled monolayer (SAM) with non-polar terminal groups and the force necessary to desorb different homopeptides from such surfaces is investigated by MD simulations. For the purely non-polar surfaces the desorption force decreases with increasing surface hydrophobicity and increases with increasing peptide hydrophobicity. Additionally, the equilibrium and non-equilibrium effects of the finite polymer length on the forced desorption of single polymers by AFMs, is examined in the framework of a freely jointed chain and a worm-like chain-model. With these rather simple models experimental observations from the group of Prof. Thorsten Hugel at TU Munich are successfully described, such as the dependency between rupture length and desorption force. Furthermore, the question, to which extent the desorption process is reversible, is addressed.

BP 7.34 Mon 17:30 Poster A

Single molecule force spectroscopy of desmoglein-2-homocomplexes — •Verena Mohaupt[1], Volker Walhorn[1], Anna Gärtner[2], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience, Bielefeld University, Germany — [2]E. & H. Klessmann Institute for Cardiovascular Research & Development, Heart and Diabetes Centre NRW, Ruhr-University Bochum, Bad Oeyenhausen, Germany

Desmosomes are molecular complexes of cell-adhesion molecules and linking proteins that form the junction between adherent cells like heart muscle cells. These domains exhibit a high density of Ca^{2+}-dependent cell adhesion proteins like desmoglein (DSG) or desmocollin (DSC). Notably, mutations in desmosomal proteins are often associated with inherent heart muscle disease like arrhythmogenic right ventricular cardiomyopathy (ARVC), which is the major cause of sudden cardiac death in adolescent and athletes.

We use atomic force microscopy (AFM) and AFM single molecule force spectroscopy (AFM-SMFS) to investigate and quantify the Ca^{2+}-dependent bond strength of single DSG2-homocomlexes. Furthermore binding kinetics and reaction lengths can be deduced according to the Kramers-Bell-Evans model. The analysis and comparison of wildtype and mutant DSG2 with respect of insights to the processes of ARVC related heart muscle degeneration will be discussed.

BP 7.35 Mon 17:30 Poster A

Peptide Dynamics Simulations in Light and Heavy Water: Zooming in on Internal Friction — •Julius Christoph Friedrich Schulz Schulz[1], Lennart Schmidt[1], Joachim Dzubiella[2], and Roland Netz[1] — [1]Fachbereich Physik, Freie Universitaet Berlin, 14195 Berlin, Germany — [2]Helmholtz Zentrum Berlin fuer Materialien und Energie, 14109 Berlin, Germany

Frictional effects due to the chain itself, rather than the solvent, may have a significant effect on protein dynamics. Experimentally, such "internal friction" has been investigated by studying folding or binding kinetics at varying solvent viscosity; however the molecular origin of these effects is hard to pinpoint. We consider the kinetics of disordered glycine-serine and alpha-helix forming alanine peptides, and a coarse-grained protein folding model in explicit-solvent molecular dynamics simulations. By varying the solvent mass over more than two orders of magnitude, we alter only the solvent viscosity and not the folding free energy. Folding dynamics at the near-vanishing solvent viscosities accessible by this approach suggest that solvent and internal friction effects are intrinsically entangled. This finding is rationalized by calculation of the polymer end-to-end distance dynamics from a Rouse model that includes internal friction. An analysis of the friction profile along different reaction coordinates suggests a connection between friction and the formation of hydrogen bonds upon folding.

BP 7.36 Mon 17:30 Poster A

Free Energy Landscape for Entrance Pathway of CoA into the Active Site of Pyruvate-Formate-Lyase — •Karmen Čondić-Jurkić[1,2], Ana-Sunčana Smith[1], and David M. Smith[2,3] — [1]Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Rudjer Bošković Institute, Zagreb, Croatia — [3]Computer-Chemie-Centrum, Universität Erlangen-Nürnberg, Erlangen, Germany

Knowledge of how free energy of a certain process changes along the reaction coordinate has always been of great interest, both in chemistry and physics. Therefore, a lot of effort has been made in the direction of developing methods and computational tools to estimate potential of mean force. Several such methods implemented in the AMBER software package were used in the search of the possible entrance pathways of a ligand (CoA) into the active site of the protein (Pyruvate-Formate-Lyase). The conformational space of the system was explored by the umbrella sampling method and its variation, so called targeted MD. The latter method allows somewhat greater flexibility in the choice of the possible pathway by defining the reaction coordinate as structural RMS deviation between the final and initial conformation and could give rise to alternative pathways. As a complementary approach to these equilibrium methods, we have used steered dynamics to study the process by exposing it to non-equilibrium conditions, i.e. by doing the pulling experiments and using Crooks fluctuation theorem to extract the information about the free energy profile. Finally, the PMF obtained from all three approaches will be compared and discussed.

BP 7.37 Mon 17:30 Poster A

Investigation of desmin intermediate filament assembly by atomic force microscopy — •Mareike Dieding[1], Volker Walhorn[1], Andreas Brodehl[2], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience,

Bielefeld University, Germany — [2]E. & H. Klessmann Institute for Cardiovascular Research & Development, Heart and Diabetes Centre NRW, Ruhr-University Bochum, Bad Oeynhausen, Germany

Intermediate filament (IF) proteins form extended filamentous networks in metazoan cells. Desmin IF is a vital structural component of the cytoskeleton in myocytes. In line with the functional importance of desmin, we investigated several desmin mutants associated with the inherited heart muscle disease arrhythmogenic right ventricular cardiomyopathy (ARVC), which is a major cause of sudden cardiac death in adolescent and athletes.

Using atomic force microscopy (AFM), we studied desmin oligomers at different stages of the *in vitro* assembly process. Thereby we were able to reveal various mutation specific structural defects at distinct stages of the filament assembly. These findings are nicely supported by complementary methods like cell transfection studies [1,2].

[1] A. Brodehl et al., *Dual-color photoactivation localization microscopy of cardiomyopathy associated desmin mutants*, submitted.

[2] B. Klauke et al., *De novo desmin-mutation N116S is associated with arrhythmogenic right ventricular cardiomyopathy*, Hum. Mol. Genet. 19(23), 2010.

BP 7.38 Mon 17:30 Poster A

SMS - FRET spectroscopy has emerged as a versatile tool in life sciences. — •Phillip Kroehn and Jörg Enderlein — Drittes Physikalisches Institut Göttingen

The applications range from protein-protein interactions and imaging microscopy to fast dynamic processes such as protein folding.

For SMS-FRET measurements in protein folding studies, site specific labelling of the protein with a donor and acceptor dye is limited to the reaction of cystein and lysine residues. Depending on the site of the protein two approaches overcome the uncertainty of random labelling.

1)*For small proteins or peptides up to 50 aa, solid phase peptide synthesis (SPPS) is the method of choice. By using aa with different protective groups site specific coupling to virtual all residues is possible.

2)*For larger proteins two new evolving methods enable the site specific coupling of dyes: a) the so called orthogonal-system allows the insertion of unnatural aa via bacterial expression in the polypeptide chain, the dye is then specifically coupled to the functional side chain of the unnatural aa. (Schulz et al J Am. Chem. Soc., 2008). b) Intein mediated protein ligation can be used to efficiently fuse short peptides with attached fluorophores to expressed proteins (Grant et al, Biol. Chem., 2006).

BP 7.39 Mon 17:30 Poster A

Structural properties of Salvinorin A, an entheogenic substance which may become a psychotherapeutic compound — •Davoud Pouladsaz[1], Azadeh Ebrahimi[2], and Hermann Schluesener[2] — [1]Department of Biological Physics, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Neuropathology, Faculty of Medicine, University of Tübingen, Tübingen, Germany

Salvinorin A is the main active psychotropic compound in Salvia divinorum, a Mexican plant which has a long history of use as an entheogen by indigenous Mazatec shamans in Oaxaca and has gained popularity as a recreational hallucinogen for the inhalation of its pyrolyzed smoke. The potent psychotropic effects of Salvinorin A, unlike many other hallucinogenic compounds that are mediated by the serotonin receptor 5-HT_{2A}, are exerted through the activation of κ-Opioid receptors which are widely distributed throughout the central and peripheral nervous systems and in other tissues. The basic mechanisms behind these effects are particularly remarkable, because Salvinorin A is a non-nitrogenous κ-Opioid receptor agonist. Since the structural properties of Salvinorin A play an important role in ligand affinity and selectivity of κ-Opioid receptor, we use molecular docking techniques to identify and study the active sites of the κ-Opioid receptor in interaction with Salvinorin A. The results may improve our understanding of how novel compounds for treatment of perceptual distortions may be derived from Salvinorin A.

BP 7.40 Mon 17:30 Poster A

Biological applications for nano-mechanical detection of molecular recognition — •Andreas Mader[1], Kathrin Gruber[1], Roberto Castelli[2], Peter H. Seeberger[2], Joachim O. Rädler[1], and Madeleine Leisner[1] — [1]LMU München, Fakultät fuer Physik — [2]Department of Biology, Chemistry and Pharmacy, Freie Universität Berlin

Advances in carbohydrate sequencing technologies have revealed the tremendous complexity of the glycome. Understanding the biological function of carbohydrates requires the identification and quantification of carbohydrate interactions with biomolecules. The increasing importance of carbohydrate-based sensors able to specifically detect sugar binding molecules or cells, has been shown for medical diagnostics and drug screening. Our biosensor, with a self-assembled mannoside sensing layer, specifically detects carbohydrate-protein binding interactions (mannoside - ConA), as well as real time interaction of carbohydrates with different E. coli strains in solution. Binding to the cantilever surface causes mechanical surface stress, that is transduced into a mechanical force and cantilever bending. The degree and duration of cantilever deflection correlates with the interaction's strength. In this study we present carbohydrate-based cantilever biosensors as a robust, label-free, and scalable method to analyze carbohydrate-protein and carbohydrate-bacteria interactions. The cantilevers thereby exhibit specific and reproducible deflection with a high sensitivity range of over four orders of magnitude.

BP 7.41 Mon 17:30 Poster A

Dynamic force spectroscopy on fluorescence labeled tau-peptides and monoclonal antibodies measured by using Optical Tweezers — •Tim Stangner, Carolin Wagner, David Singer, Christof Gutsche, Olaf Ueberschär, Ralf Hoffmann, and Frierich Kremer — Uni Leipzig, Leipzig, Germany

Since humans become older and older with the fast evolution of medicine, degenerative diseases edge ever closer to focus of research. Especially Alzheimer's disease is the most common form of dementia. Each Alzheimer patient shows two commonly known changes in the brain: senile plaques of β-amyloid-peptide and tangles of hyperphosphorylated tau proteins. Dynamic force spectroscopy (DFS) is performed by using optical tweezers on the level of single receptor-ligand-interactions. Here we report about the specific binding of two anti-human tau-monoclonal antibodies (mAbs), HPT-104 and HPT-110, interacting with synthetic (non-)fluorescence-labeled tau-peptides with different phosphorylation pattern. The fluorescent tagged tau-peptides, anchored on Melanmin-resin beads, are presorted with the fluorescence activated cell sorting (FACS) method in order to achieve homogenous surface coverage. Specific binding events between peptide and mAbs are described according to the Dudko-Hummer-Szabo-model [1]. A comparison between labeled and non-labeled tau-peptide and their interactions with mAbs shall show the influence of the linker-(PEG-spacer) and the fluorescein-molecule on the parameters, obtained by the Dudko-Hummer-Szabo-model [1].

References: [1] Dudko et al.; PNAS 2008 vol. 105 no. 41 15755-15760

BP 7.42 Mon 17:30 Poster A

Modeling the Light-Dependent Repression of Photosynthesis Genes by the AppA/PpsR System in Rhodobacter sphaeroides — •Rakesh Pandey[1], Dietrich Flockerzi[1], Marcus J. B. Hauser[2], and Ronny Straube[1] — [1]Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg — [2]Institute of Experimental Physics, Otto-von-Guericke University, Magdeburg

Purple bacteria derive energy from aerobic respiration or photosynthesis (PS) depending on the availability of oxygen and light. Under aerobic conditions, PS genes are specifically repressed by the PpsR protein. In R. sphaeroides, the repressive action of PpsR is antagonized by the blue-light sensitive flavoprotein AppA which forms transcriptionally inactive complexes with PpsR under anaerobic conditions. However, under semi-aerobic conditions blue-light excitation of AppA causes the AppA-PpsR complexes to dissociate leading, again, to PS gene repression. We have recently proposed a simple mathematical model [1] which suggests that this phenotype arises from the formation of a maximum in the response curve of PpsR at intermediate oxygen levels. Here, we present an extended model which incorporates a more realistic mechanism for the light regulation. Its predictions compare favorably with experimental results on the light-dependent repression of PS genes under semi-aerobic conditions. We also identify potential kinetic and stoichiometric constraints that the interplay between light and redox regulation imposes on the functionality of the AppA/PpsR system, especially with respect to a possible bistable response. [1] Pandey R, Flockerzi D, Hauser MJB, Straube R. Biophys. J. 100, 2347 (2011).

BP 8: Posters: Biopolymers and Biomaterials (with CPP)

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

BP 8.1 Mon 17:30 Poster A

Sample preparation of softwood with cryo-microtome and focused ion beam for X-ray nano-diffraction studies - a comparison — •Selina Storm[1,2], Malte Ogurreck[1], and Martin Müller[1] — [1]HZG, Geesthacht — [2]IEAP, University of Kiel

The cell structure of softwood has been investigated to understand the exceptional mechanical strength of this biological material. X-ray diffraction with nano-focused synchrotron radiation beam allows a spatial resolution of below 100 nm so that the transition zones between different cell wall layers as well as the cell wall layers themselves can be investigated in previously unknown quality.

A crucial point in this context is the sample preparation and the knowledge of its orientation. Thin sample slices (d<10 μm) can be cut out with a cryo-microtome or a focused ion beam. The use of a cryo-microtome has the disadvantage that the sample is easily damaged, e.g. splintering of the cell wall which leads to misleading results in the diffraction patterns. The achievable accuracy of the sample alignment is only in the order of several degrees which is insufficient for a detailed analysis. To overcome these disadvantages a focused ion beam is a promising alternative. Here, the results will be discussed and compared.

BP 8.2 Mon 17:30 Poster A

A Dielectrophoresis Study on the Frequency-Dependent Behaviour of Sepsis Pathogens in Media with Different Conductivities — •Ulrich-Christian Schröder[1,2], Uwe Glaser[1,2], Christian Leiterer[2], Andrea Csâki[2], Wolfgang Fritzsche[2], Uwe Hübner[2], Jürgen Popp[2,3], Michael Bauer[1], and Ute Neugebauer[1,2] — [1]Center for Sepsis Control and Care, Jena University Hospital — [2]Institute of Photonic Technology Jena e.V. — [3]Institute for Physical Chemistry and Abbe Center of Photonics, University Jena

Sepsis is a heavy inflammatory response of the human body due to the invasion of pathogenic organisms, which leads to high mortality rates. To ensure a start of early therapy, we are developing a highly sensitive, rapid, label-free and culture independent Lab on Chip method to estimate the resistance of sepsis pathogens towards antibiotics. Dielectrophoresis makes use of the interaction of high frequency non-uniform electrical fields with dielectric nano- and microparticles and can be used to manipulate sepsis pathogens within microsized regions. In the presented work the dielectrophoretic behaviour of the sepsis pathogens is studied for different frequency ranges as well as for different medium conductivities to trap and collect these organisms for further non-invasive optical characterization and furthermore to use dielectrophoresis as a diagnostic tool to distinguish between living and dead bacteria. Acknowledgement: The financial support of the BMBF (FKZ 01EO1002) is highly acknowledged.

BP 8.3 Mon 17:30 Poster A

The nacre protein perlucin - homology model and properties — •Malte Launspach[1], Martin Zacharias[2], and Monika Fritz[1] — [1]Institute of Biophysics, University of Bremen — [2]Biomolecular Dynamics (T38), Technical University Munich

The natural composite nacre is known for its iridescence as well as high fracture toughness. Both properties emerge from a well defined microstructure of nacre. Aragonite - a calcium carbonate polymorph - polygonal platelets with a diameter in the micrometer range and a height of about 500 nanometer are embedded in an organic layer comprised of proteins and chitin. One of these proteins of the organic layer is perlucin. This protein seems to be the most abundant one in nacre and it influences the growth of calcite as it was shown by AFM measurements. Currently we try to characterise this protein and its function in nacre formation.

Here we present a model of the C-type lectin perlucin derived from comparative modelling and tested with molecular dynamics simulations. Further we use common gelfiltration techniques and a computer docking program to investigate the perlucin-perlucin interaction. To probe the mineral interaction capabilities of perlucin we perform AFM imaging of aragonite and calcite surfaces in supersaturated calcium carbonate solutions in presence of perlucin.

BP 8.4 Mon 17:30 Poster A

Ab-initio characterization of potential siderophore-mediated metal transport systems — •Angelica Zacarias[1], Mabel Moreno[1,2], Mato Knez[1], Luis Velasquez[2], Andrea Porzel[3], and E.K.U. Gross[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale) — [2]CEDENNA and Universidad de Santiago de Chile, Avda. Ecuador 3493, Estación Central, Santiago, Chile — [3]Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Weinberg 3, 06120 Halle (Saale)

The high affinity of enterobactin for iron has a wide range of biological applications (such as the treatment of bacterial diseases) as it allows its use for complex-mediated iron transport.

We present preliminary results that analyze the electronic and spectroscopic properties of the bare enterobactin as well as other metal-enterobactin systems.

We will show that the computer aided characterization of the products synthesized via Atomic Layer Deposition (ALD) techniques allows a better understanding not only of the iron-enterobactin association but also the further affinity of the enterobactin and iron-enterobactin for other metals. The extensive knowledge of this relationship and the use of ALD as synthetic technique has potential uses of the enterobactin complex in the treatment of bacterial diseases as well as in the area of environmental contamination.

BP 8.5 Mon 17:30 Poster A

Systematic investigation of lipids on a titanium layer on the incubation time in water and in growth medium via x-ray reflectometry — •Anahita Shahin[1], Dieter Lott[1], Regine Willumeit[1], Bérengère Luthringer[1], Alexander Grünwald[2], and Andreas Schreyer[1] — [1]Helmholtz-Zentrum Geesthacht, Max-Planck-Str. 1, 21502 Geesthacht — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln

Soft matter is increasingly investigated with x-ray scattering during the last years for the detailed structural characterization of this important class of samples. In particular it provides a valuable contribution to the area of medical physics, for instance for the optimization of implants. In this work in-situ x-ray reflectometry and diffraction under small angles is used to analyze the structural properties of lipid bilayers under a variety of conditions. Particular attention is paid to a solid-supported membrane system in which a 70 nm titanium layer deposited on a silicon substrate is coated by lipids. The main objective is to analyze how many lipid bilayers can be attached to the solid titanium layer and how the number of layers changes upon the incubation time in growth medium (Dulbecco's Modified Eagle's Medium (DMEM)) and in water. Here we concentrate on time-dependent measurements to find the optimal incubation time for the lipids in the different media. The combination of experiments and simulation of the scattering data is a valuable tool to understand the ordering and time dependence.

BP 8.6 Mon 17:30 Poster A

Tissue growth as mass generation in a linear elastic medium — •Niko Komin, Lars Ole Schwen, and Tobias Preusser — Fraunhofer MEVIS, Bremen, Germany

The liver as a major metabolic organ fulfils a huge variety of vital metabolic tasks in a mammalian organism. Its great ability to regenerate after injury allows for the transplantation of a large part of the organ from a living donor to a recipient in need. Liver mass and function is restored within a matter of months after operation.

In the talk we will present the regeneration process as the generation of mass (tissue) within a linear elastic medium. Cell proliferation depends on nutrition via the regrowing vascular structure and the topology of the vascular structure is governed by optimization criteria. We will present modelling techniques and results.

BP 8.7 Mon 17:30 Poster A

Basic investigation of skin under Plasma treatment — •Marcel Marschewski[1], Joanna Hirschberg[2], Tarek Omairi[2], Oliver Höfft[3], Steffen Emmert[4], Wolfgang Viöl[2], and Wolfgang Maus-Friedrichs[1] — [1]IEPT, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Fakultät Naturwissenschaft und Technik Hochschule für angewandte Wissenschaft und Kunst Hildesheim/Holzminden/Göttingen, Von-Ossietzky-Str. 99, 37085 Göttingen, Germany — [3]IMV, TU Clausthal, Arnold-Sommerfeld-Str.

6, 38678 Clausthal-Zellerfeld, Germany — [4]Department of Dermatology, Venerology and Allergology Georg-August-University Göttingen, Robert-Koch-Strasse 40, 37075 Göttingen, Germany

The lipids of the stratum corneum loom large for the barrier function of human skin. Recently several important findings related to mutations of the fillaggrin-gen and according to this, diseases like ichthyose and atopic dermatitis were made but not yet completely understood. Cold plasma treatment on e.g. skin diseases causes in an abatement of diseases by the assured disinfected effect of plasma [1]. Here, we present our first results on the basic investigation of skin, studied with X-ray photoelectron spectroscopy. We have prepared our samples by using current skin glue which is usually used for cut closure. Furthermore we have investigated the change in plasma treated skin samples to understand the basic effects of plasma treatment of biological systems.

[1] Morfill G E, Shimizu T, Steffes B and Schmidt H-U 2009 Nosocomial infections - a new approach towards preventive medicine using plasmas New Journal of Physics 11, 115019

BP 8.8 Mon 17:30 Poster A

Moderate Swelling of Type I Collagen Fibrils in Humid Air — •Eike-Christian Spitzner, Stephanie Röper, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz, Germany

We investigate purified type I collagen extracted from bovine hide. In aqueous solution, triple helices of collagen molecules (tropocollagens) form fibrils driven by hydrogen bonding processes. Single collagen fibrils, deposited on a silicon substrate, were exposed to air with controlled relative humidity (RH). We used in-situ multi-setpoint intermittent contact mode atomic force microscopy for imaging the collagen fibrils at 20% RH, during moderate swelling at 80% RH, as well as dried again at 20% RH. Changes in the mechanical properties of the characteristic D-band structure were observed. At 20% RH, the typical 67 nm spacing appears in the shape of the fibril, whereas at moderate swelling (80% RH) it is visible as a periodic variation of local material properties. Furthermore, in parts of the fibrils, where no D-band structure was observed in the initial state, reconfigurations take place during swelling, which we attribute to a phase transition in the liquid crystalline alignment of the tropocollagen units.

BP 8.9 Mon 17:30 Poster A

Characterization of Protein Films on Dental Materials — •Fabian Kratz[1], Nils Körber[1], Christine Müller[1], Natalia Umanskaya[2], Matthias Hannig[2], and Christiane Ziegler[1] — [1]Department of Physics and Research Centre OPTIMAS; University of Kaiserslautern; D-676632 — [2]Clinic of Operative Dentistry, Clinic of Operative Dentistry, Periodontology and Preventive Dentistry, University Hospital, Saarland University, D-66424

In dentistry a greater knowledge of protein film establishment processes is of high concern, because protein films are the basis for bacterial adhesion. Especially in the human mouth caries is a consequence of a biofilm. The ambition is to characterize protein films on model materials and continuative on dental relevant materials like titanium, gold, natural enamel, PMMA and PTFE under the influence of dental relevant parameters (like pH and the roughness of the material) by using different surface science methods in combination with biochemical assays. The thickness of the protein films, measured by ellipsometry and scanning force microscopy (SFM), corresponds to the size of the protein molecules. This hypothesizes a monolayer adsorption process.. The combination with biochemical methods like BCA assay and enzymatic activity determines the adsorbed amount of protein and its activity in the case of lysozyme. An influence of the surface roughness, the pH value and the surface material on the adsorbed amount is observed by BCA assay. As a function of the surface material and the pH (thus carious conditions) the enzymatic activity differs.

BP 8.10 Mon 17:30 Poster A

Influence of subsurface properties on proteins, bacteria and geckos: Is adhesion superficial? — •Peter Loskill[1], Hendrik Hähl[1], Jonathan Puthoff[2], Kellar Autumn[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]Department of Biology, Lewis & Clark College, Portland, OR 97219, USA

Understanding and controlling the adhesion of biological objects to inorganic surfaces are important tasks that find application in various topics such as in the development of antimicrobial surfaces or artificial adhesives. To characterize biological adhesion, most studies describe a substrate solely by its surface properties. The composition of the material beneath the surface is frequently overlooked. That way, long-range van der Waals (vdW) interactions are disregarded. Previous studies revealed that microscopic biological objects such as proteins are affected by vdW interactions. We could show now that mesoscopic and even macroscopic objects are also influenced by differences in the microscopic interface potential. By using tailored silicon wafers with variable silicon dioxide layer thickness, we were able to tune the vdW part of the interface potential independently of the surface properties. On these substrates, we performed adhesion measurements with bacteria of the Staphylococcus genus and with a species of tropical gecko. The bacterial adhesion was explored via atomic force microscopy in the forces spectroscopy mode, using cantilevers on which living bacteria were immobilized. To characterize the gecko adhesion, we mimicked the typical gecko movement with a custom mechanical testing platform.

BP 8.11 Mon 17:30 Poster A

Understanding the Basis of Nacre Formation: Instabilities and Pattern Formation in Growing Polymer Brushes — •Björn Nadrowski[1], Ingrid Weiss[2], and Karsten Kruse[1] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Leibniz-Institut für Neue Materialien, 66123 Saarbrücken, Germany

Nacre is strong, resilient and beautiful. It is a composite material consisting of layers of biominerals such as aragonite and organic molecules such as chitin. It is thought that the particular mechanical properties of nacre are due to its composite nature and the microstructure of the arrangements of aragonite platelets and the softer organic layers in-between those platelets[1]. Formation of nacre starts with the secretion of chitin into the extrapallial space[2]. The secretion process itself might be of importance for the ensuing microstructure of the nacre-in-being. Inspired by this biological-physical background, we study instabilities and pattern formation in growing polymer brushes. Using analytical and computational approaches, we study the different structures and instabilities that can be observed depending on polymer growth velocity, pore density, bending rigidity, and monomer interaction strength.

[1] Currey, J. D. et al.,Proc Biol Sci **268** (2001) 107.
[2] Weiss, I. M., Chembiochem **11** (2010) 297.

BP 8.12 Mon 17:30 Poster A

Preparation of dense hydroxyapatite samples for surface science application — •Christian Zeitz[1], Deniz Kahraman[2], Samuel Grandthyll[1], Frank Müller[1], Jörg Schmauch[1], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]KIT, Ceramics in Mechanical Engineering, D - 76131 Karlsruhe, Germany

Hydroxyapatite (HAP) is a conflicting material: On the one hand, HAP is greatly available in nature as bone or tooth mineral material, but, on the other hand, these natural samples only hardly fulfill the needs of science concerning chemical composition or structural simplicity. Therefore and because the material has important influence in physiology, this study aims for a preparation method for artificial HAP samples of high density. In order to make available the basic interactions, best possible homogeneity and chemical purity is achieved as well as structural smoothness. A thorough characterization of the samples is presented together with some results of an investigation of the effects of fluoridation.

BP 8.13 Mon 17:30 Poster A

Microrheology in syncytial Drosophila embryos — •Alok D. Wessel[1], Takuma Kanesaki[2], Jörg Grosshans[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Zentrum für Biochemie und Molekulare Zellbiologie, Universitätsmedizin, Georg August-Universität, Göttingen

In early development, Drosophila melanogaster embryos are in a syncytial stage, i.e. multiplying nuclei are not yet separated by membranes, but are interconnected by cytoskeletal polymer networks consisting of actin and microtubules. Between division stages 9 and 13, nuclei and the cytoskeletal network form a 2D cortical layer. We characterize the mechanical properties of this composite network and spatial variations across nuclear compartments as well as temporal variations over the nuclear division cycles via high-speed video-microrheology. We record position fluctuations of injected micron-sized beads with a high-speed camera at sampling frequencies up to tens of kHz. From single-particle dynamics and from multi-particle correlations we can

compute viscoelastic material properties.

BP 8.14 Mon 17:30 Poster A

Mechanically Tunable Composite Hydrogels as Biomimetic Matrices — •Christina Jayachandran[1], Christoph Schmidt[2], and Florian Rehfeldt[3] — [1]3rd Institute of Biophysics,Georg-August Universität,Göttingen,Germany — [2]3rd Institute of Biophysics,Georg-August Universität,Göttingen,Germany — [3]3rd Institute of Biophysics,Georg-August Universität,Göttingen,Germany

In vivo cells face various micro-environments which differ significantly both in their physical and biochemical properties and the extra cellular matrix (ECM) plays a key role in providing these cues. Mimicking these diverse environments in vitro, is necessary to understand the fundamental processes that govern cell matrix interactions and also of paramount importance for medical applications, e.g. regenerative medicine. The standard methods of preparing elastic matrices employ homogenous polyacrylamide (PA) gels or PDMS rubber substrates coated with extracellular matrix proteins to facilitate adhesions.

Our strategy is based on hybrid matrices composed of an isotropic hyrdogel and a fibrous protein scaffold to better mimic the in vivo niche. Contrary to the conventional substrates which exhibit a linear response, these matrices show non- linear elastic behaviour characteristic of biopolymers and tissues. We study the mechanical properties of these novel substrates by bulk rheology and atomic force microscopy and also discuss the differential cellular response of cells to them compared to conventional PA gels.

BP 8.15 Mon 17:30 Poster A

Untersuchungen zur Biostabilität eines implantierbaren Glucosesensors — •Marlen Froehlich, Karl-Ernst Ehwald, Philipp Kulse, Oksana Fursenko, Jens Katzer und Mario Birkholz — IHP - Leibniz-Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder)

Es wurde ein Biosensorchip, der für die Verwendung in einem implantierbaren Glucosemonitor vorgesehen ist, in Hinblick auf seine Stabilität in biologischen Milieus untersucht. Der Sensorchip wurde in der Pilotlinie des IHP in einer CMOS/BiCMOS-Technologie gefertigt. Er arbeitet mit einem mikroelektromechanischen System und funktioniert nach dem Prinzip der Affinitätsviskosimetrie. Die Untersuchungen erfolgten durch Exposition der Chips in verschiedenen Modell-Lösungen und Vorher-Nachher-Vergleiche, wobei die auftretenden Schadensprofile mit optischer Mikroskopie, Ellipsometrie und AFM bestimmt wurden. Es erfolgten in vitro und in vivo Tests, wobei die ersten der Methodenentwicklung dienten. Dazu wurden Waferbruchstücke für den Zeitraum von Wochen in körpermilieuartigen Lösungen eingebracht. Eine in vivo Untersuchung an einem menschlichen Probanden ermöglichte eine dem Einsatzgebiet entsprechende Analyse der Teile des Mikroviskosimeters, die der Körperflüssigkeit ausgesetzt waren. Es wurden nur geringe Änderungen von Schichtdicke und Rauheit beobachtet. Der stärkste Effekt betraf die SiON-Passivierung mit einer Abbaurate von rund 50 nm/Monat. TiN zeigte keinen Abbau durch Biokorrosion. Danach ist zu erwarten, dass die Sensorchips für einen Zeitraum von mindestens zwölf Monaten stabil im menschlichen Gewebe arbeiten.

BP 8.16 Mon 17:30 Poster A

Lipid-Coated Implant Materials under Load — •Martin Kreuzer[1,2], Matthias Reinhardt[2], Markus Strobl[3], Jochen Stahn[4], Maksym Golub[5], Regine Willumeit[5], Reiner Dahint[1], and Roland Steitz[2] — [1]Universität Heidelberg, Deutschland — [2]Helmholtz-Zentrum Berlin, Deutschland — [3]European Spallation Source, Schweden — [4]Paul-Scherrer Institut, Schweiz — [5]Hemholtz-Zentrum Geesthacht, Deutschland

In the last decade, the search for biocompatible materials has become a major topic in medical research. In that context coating of implants by lipid layers seems an obvious strategy for achieving better acceptance of the implant in the human organism. The combination of suitable metallic implants with lipid coverage is most promising for forthcoming implant modifications. Here, one of the fundamental requirements is the reliable preparation of stable lipid coatings on the implant surfaces. We investigated the stability of oligolamellar lipid bilayers prepared by spin coating on silicon discs and titanium-coated silicon substrates against an excess water phase under shear load by neutron reflectivity. We evaluated a critical temperature region at which a stack of DMPC lipid bilayers detaches from titanium-coated and bare silicon surfaces, respectively, against heavy water under shear load. The critical temperature region coincides with the main phase transition temperature of DMPC in excess heavy water. The experimental setup made it possible to follow the unbinding process on a molecular scale. Our experiments did not show a significant difference between the lipid coatings on bare silicon and titanium coated silicon supports.

BP 9: Focus: Systems Biology of Bacteria (with jDPG)

Time: Tuesday 9:30–12:30 Location: E 020

Invited Talk BP 9.1 Tue 9:30 E 020

Stochastic gene regulation strategies in bacteria — •Ulrich Gerland — LMU, Munich, Germany

The regulatory circuits that control the processing of signals and the transcription of genes in bacterial cells are fascinating nonlinear stochastic systems. They often appear to be optimized by evolution, but they are only beginning to be explored on a quantitative level. I will briefly review some of the developments in this field, and then focus on a small regulatory circuit that controls the production of the machinery required to import and digest a specific sugar in E. coli bacteria. In a population of cells, this remarkably simple circuit leads to heterogeneous dynamic behavior that appears to implement an optimal strategy to deal with unpredictable environments.

Invited Talk BP 9.2 Tue 10:00 E 020

The evolutionary advantage of being round — •Oskar Hallatschek — Max Planck Research Group for Biophysics and Evolutionary Dynamics, MPI-DS, Goettingen, Germany

Bacterial species display an astonishing variety of shapes, such as round, rod-like, comma- or spiral-shaped. Shape is thought to influence several biological functions, such as nutrient take-up, swimming and the attachment to surfaces. Here, we study a possible impact of cell shape on adaptation. We show that, due to a biophysical buckling instability, rod-like bacteria exhibit much higher levels of random number fluctuation (genetic drift) in growing colonies than round microbes. Consequently, the establishment of beneficial mutations is strongly suppressed in colonies of rod-like bacteria. Our experiments and model thus support the hypothesis that shape strongly influences adaptability of growing biofilms.

Invited Talk BP 9.3 Tue 10:30 E 020

Optimal control strategies in living cells — •Markus Kollmann — Department Biologie, Universität Düsseldorf, Germany

Unicellular organisms have evolved an astonishing repertoire to survive in fluctuating environments. To ensure high reproductive success, microorganisms adapt sufficiently fast to new living conditions, such as nutrient availability, osmolarity, and ambient temperature. Such phenotypic adaptation is coordinated by the activity of cellular circuits, whose components are regulated on the level of DNA, RNA, and protein. The question arises whether the observed regulatory strategies of microorganisms can be explained by an optimal tradeoff between precision, timing and resource efficiency of cellular response. Strong evidence for such optimized cellular control can be found within bacteria and the evolved control strategies show striking similarities to predictions from optimal control theory. We give several examples for highly optimized bacterial circuits, their proposed objective functions, and their molecular realizations.

Invited Talk BP 9.4 Tue 11:00 E 020

Bacterial communication systems — •Ilka Bischofs — ZMBH, Heidelberg, Germany

Bacteria interact with each other in multiple ways, e.g. via diffusible signaling molecules. In a process called quorum sensing bacteria produce, secrete, sense and respond to signals, which accumulate with cell density. This allows them to control gene expression in a cell density-dependent manner. For example, frequently they launch spe-

cific responses, which are executed more efficiently collectively, upon reaching a "quorum". Interestingly, in nature there exists a variety of different quorum sensing network architectures. In particular, cell density information enters into cellular decision making processes in various ways. By means of simple theoretical models we compare different quorum sensing network architectures. Based on this analysis we begin to derive network design principles that may explain the significance of certain architectural features found in natural networks and we make predictions on how to build synthetic networks with optimized functions.

BP 9.5 Tue 11:30 E 020

A Plausible Mechanism for the Generation of Ultrasensitivity and Bistability in Bacterial Two-Component Systems — •Ronny Straube — Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Two-component systems are the simplest signal processing units mostly found in bacteria. They consist of a histidine kinase (HK) and a cognate response regulator (RR) which often acts as a transcription factor. Upon stimulation the HK undergoes autophosphorylation and, subsequently, transfers the phosphate group to the RR. In addition, many HKs also exhibit phosphatase activity towards the phosphorylated form of the RR. The relative activity between autophosphorylation, kinase and phosphatase mode is often regulated by small allosteric effectors. Using a simple mathematical model I show that if the kinase and phosphatase activities are regulated in a reciprocal fashion two-component systems can generate highly sigmoidal responses (ultrasensitivity) quite similar to covalent modification systems in eukaryotes [1]. Under proper kinetic conditions the response can even become hysteretic with an intermediate bistable regime. Hence, despite the bifunctional nature of the HK switch-like all-or-none responses could already be generated at the protein-protein level without genetic regulation. [1] Goldbeter A, Koshland, DE Jr. An amplified sensitivity arising from covalent modification in biological systems. Proc. Natl. Acad. Sci USA 78, 6840-6844 (1981).

BP 9.6 Tue 11:45 E 020

A model for sigma factor competition in bacterial cells — •Marco Mauri and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Bacteria respond to changing environment conditions by switching the global pattern of transcribed genes, making only those products essential for their survival. In response to specif environmental stresses the cell activates several stress-specific molecules called sigma factors. They bind the core RNA polymerase (RNAP) - the machinery of transcription - and direct it towards the appropriate stress response genes. Since more than one sigma species could be present in the cell at the same time, it is believed that the modulation of their availability and competition among them for core RNAP provide important mechanisms for the global switch of the transcriptional program.

To analyze this competition, we have developed a theoretical model based on earlier work from the Gross lab [1]. The model shows that competition occurs only when the number of free sigmas exceeds the number of free cores. Within this framework, we analyzed the effects of some factors that modulate the competition such as anti-sigma factors, small RNA and active transcription. We applied the model to in vitro sigma competition experiments [2] and obtained good agreement. We also used the model to examine under which conditions a stop of transcription of ribosomal RNA as in the stringent response can passively up-regulate transcription driven by alternative sigmas.

[1] Grigorova et al., PNAS. 103, 5332 (2006)
[2] Jishage et al., Genes & Dev. 16, 1260 (2002)

BP 9.7 Tue 12:00 E 020

Unified description of Min protein patterns in vivo and in vitro — •Mike Bonny[1], Elisabeth Fischer-Friedrich[2], Martin Loose[4], Petra Schwille[3], and Karsten Kruse[1] — [1]Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [3]Biophysics, BIOTEC, TU Dresden, Tatzberg 47/49, 01307 Dresden, Germany — [4]Harvard Medical School, Department of Systems Biology, 200 Longwood Avenue, Warren Alpert Building, Boston, MA 0211

The bacterial proteins MinD and MinE self-organize into a variety of fascinating patterns in the presence of a membrane. In vivo, standing and traveling waves as well as bistable stationary states are observed. In vitro they form plane and spiral waves. Several models explain Min protein pattern formation by cooperative attachment of MinD to the membrane and MinE-induced detachment from the membrane. However, a description reproducing all observed patterns is missing. We have found that MinE can bind by itself transiently to the membrane [1,2]. Analyzing mean field and stochastic models of Min protein dynamics, we find that our description shows all observed in vivo and in vitro patterns if we include the transient membrane interaction of MinE.

[1] M. Loose et al., Struct. Mol. Biol., 18, 577 (2011).
[2] K. Park et al., Cell, 146, 396 (2011).

BP 9.8 Tue 12:15 E 020

Quorum sensing of motile bacteria in spatial confinement — •Jan Ribbe and Berenike Maier — Institut für theoretische Physik, Universität zu Köln, Köln, Germany

Microscopic structures influence the direction of swimming bacteria through hydrodynamic interaction. Thus we hypothesize that the concentration of bacteria in spatially structured environments is heterogeneous and can potentially lead to local accumulation of bacteria. Bacteria in groups often have different lifestyles than individuals. Controlled by quorum sensing and nutrient limitation, a well-defined fraction of cells differentiates into the competent state at high cell density.

Here, we intend to test the hypothesis whether the state of motility impacts on bacterial lifestyle. First we addressed the question whether competence and motility are mutually exclusive. We found that cells of *Bacillus subtilis* that have decided to become competent do not necessarily abolish motility. The rate of motility of competent cells decreases, but remains at 20±10 %. Next, we generated asymmetric microfluidic channels with volumes of 30 pl. We found that motile cells accumulate in the dead ends of the asymmetric channels and exhibit a pronounced concentration gradient. Active swimming promoted accumulation significantly. Using fluorescence reporters for the master regulator of competence, we found that the number of competent cells is strongly increased in dead ends where cell concentration is high. In future experiments we will characterize the spatio-temporal development of competence in microhabitats of different dimensions.

BP 10: Biopolymers and Biomaterials (with CPP)

Time: Tuesday 9:30–13:00 Location: H 1058

Invited Talk BP 10.1 Tue 9:30 H 1058

Surface topology effect on cell interaction at the nanoscale — •Giuseppe Battaglia — Department of Biomedical Science, The University of Sheffield, Sheffield, UK

One of the most important classes of synthetic systems for creating self-assembled nanostructures is amphiphilic block copolymers. By controlling the architecture of individual molecules, it is possible to generate nanostructures either in an undiluted melt or in solution. These ordered nanostructures are tunable over a broad variety of morphologies, ranging from discrete micelles and vesicles to continuous network structures. Their synthetic nature allows the design of interfaces with different chemical functional groups and geometrical properties. This, in combination with molecular architecture, determines the levels of ordering in self-organizing polymeric materials. Such an effective control is extremely beneficial when it comes to design materials that have to interact with biological systems. I will be discussing how block copolymers can be used for the design of nanoscopic vectors that go across different biological barriers from the thick tissues to the very cell interior to deliver therapeutic agents and/or diagnostic probes. Similarly exploiting the facile interface engineering of block copolymers I will show how these can be used to design functional interfaces for polymeric scaffolds for cell and tissue engineering.

BP 10.2 Tue 10:00 H 1058

Molecularly imprinted conductive polymers for controlled

trafficking of neurotransmitter at solid-liquid interfaces — •Neelima Paul[1,2], Markus Mueller[1], Amitesh Paul[3], Elke Guenther[4], Iver Lauermann[1], Peter Müller-Buschbaum[2], and Martha Ch. Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85747 Garching, Germany — [3]TU München, Physik-Department, LS Neutronenstreuung, James-Franck-Str. 1, 85748 Garching, Germany — [4]Natural and Medical Sciences Institute at the University of Tübingen, Markwiesenstr. 55, 72770 Reutlingen, Germany

The state of the art approach to restore sight in certain cases of blindness is the replacement of the damaged photoreceptors by a subretinal implant consisting of light-sensitive photodiodes . We suggest to chemically stimulate the neurons by replacing the photodiodes in the subretinal implant by a molecularly imprinted polymer (MIP), imprinted with a neurotransmitter, such as glutamate. By controlling the neurotransmitter trafficking across a solid-liquid interface with voltage, we show the possibility of using this MIP for chemical stimulation of retinal neurons. ATR-FTIR spectroscopy and XPS has been used to chemically confirm the imprint of neurotransmitter in the MIP at the solid-liquid and the solid-air interface respectively. Fluorescence spectroscopy using the dye, fluorescamine, has been used to monitor the changes in neurotransmitter concentration in various solvents.

BP 10.3 Tue 10:15 H 1058

Excitation energy transfer processes in coupled phycobiliprotein complexes of A. marina and semiconductor nanocrystals forming hybrid structures — •Franz-Josef Schmitt[1], Evgeny Maximov[3], Patrick Hätti[2], Vithiya Jeyasangar[2], Jörn Weissenborn[2], Vladimir Paschenko[3], Hans Joachim Eichler[2], Thomas Friedrich[1], and Gernot Renger[1] — [1]Max Volmer Laboratory for Biophysical Chemistry — [2]Institute of Optics and Atomic Physics, Berlin Institute of Technology, Germany — [3]Department of Biophysics, M.V. Lomonosow Moscow State University, Russia

Pigment-protein complexes isolated from the photosynthetic apparatus provide functionally optimized nanoscaled devices for the construction of light driven operational units. The present work describes results obtained on hybrid systems consisting of CdSe quantum dots (QDs) with ZnS shell and different phycobiliproteins (PBPs) like hexameric phycoerythrin (PE), phycocyanin (PC), allophycocyanin (APC) and rod shaped PBP antenna complexes from the cyanobacterium Acaryochloris marina. The surface of the QDs is functionalised by covering with anionic and cationic groups leading to electrostatic contact with PBP. Excitation energy transfer (EET) from QDs to PBPs occurs with varying efficiency of up to 90 % for coupled QD/PBP hybrid complexes and is highly dependent on the temperature. The study with different QDs shows that the Förster Integral crucially determines the efficiency of EET while the electrostatic surface charge is of secondary relevance. Highly efficient EET and fluorescence enhancement of the acceptor was observed for particular stoichiometric ratios between QDs and PBPs.

BP 10.4 Tue 10:30 H 1058

Neutron radiography study of water migration into casein micellar films — •Ezzeldin Metwalli[1], Helen E. Hermes[2], Elbio Calzada[3], Stefan U. Egelhaaf[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany — [2]Physik der weichen Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz, TU München, 85747 Garching, Germany

Casein, a milk protein, forms micelles with a radius of about 100-300 nm. Casein-protein based films are widely used as an adhesive for labeling glass bottles and other containers because of their superior mechanical stabilities in different humidities at temperatures between 2 and 40 C. This study demonstrates the use of neutron radiography as a viable method for the determination of the diffusion profile of water in casein films. The dry casein film is contacted with water and neutron radiographs are collected as function of elapsed time. Profiles of the water concentration are successfully measured by imaging. Two diffusion processes are observed: (a) fast diffusion with a decaying diffusion constant, resulting from water exchange with the hydration water bound to the casein proteins, and (b) slow and constant diffusion due to Fickian water transport into the voids and holes between the casein micelles and their aggregates in the porous film. Time evolution of the later diffusion process is compared with our recent GISANS investigation [1] of hydration behavior of casein thin films in water vapor.

[1] Metwalli et al., Langmuir 25, 4124 (2009)

BP 10.5 Tue 10:45 H 1058

Study of lipid and protein coatings on titanium surfaces by neutron scattering — •Maksym Golub[1], Regine Willumeit[1], Berengere Luthringer[1], Frank Feyerabend[1], Eric Watkins[2], Dieter Lott[1], Vasyl Haramus[1], Boris Toperveg[3], and Andreas Schreyer[1] — [1]Helmholtz Zentrum Geesthacht, Geesthacht, Germany — [2]ILL, Grenoble, France — [3]Ruhr-University Bochum, Germany

Permanent implants, e.g. using titanium and its alloy, are widely used and successfully implemented in medicine. To improve their performance lipid*s covering is applied. The study of the structure of the phospholipid (palmitoyl-oleoyl-sn-glycero-3-phosphoethanolamine - POPE) layering under liquid conditions in presence of growth medium and Human Serum Albumin (HSA), which is the favourable condition for cell adhesion, would provide key parameters to understand the interaction between cells and lipid coated implants. Such a system was measured by neutron reflectivity. Silicon crystals with a Ti layer (36 nm) on the top were covered by POPE lipids and measured at different conditions: D2O, D2O based growth medium and growth medium with protein i.e., HSA. A 2D detector was used for the data collection which allowed us to detect also the diffuse scattering which provides information about the lateral correlations in these films. The neutron reflectivity experiments enabled us to see the changes of layer structure due to adhesion of the protein and will be discussed here in detail.

BP 10.6 Tue 11:00 H 1058

Adhesion of gecko setae reflects nanoscale differences in subsurface energy — •Peter Loskill[1], Jonathan Puthoff[2], Matt Wilkinson[2], Kellar Autumn[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]Department of Biology, Lewis & Clark College, Portland, OR 97219, USA

Surface energies are commonly employed to determine the adhesive forces between materials. However, the component of surface energy derived from long-range forces, such as van der Waals forces, depends on the material's structure below the outermost atomic layers. Prior theoretical results and indirect experimental evidence suggest that the van der Waals energies of subsurface layers will influence interfacial adhesion forces. We discovered that nanometerscale differences in the oxide layer thickness of silicon wafers result in significant macroscale differences in the adhesion of isolated gecko setal arrays. Si/SiO_2 bilayer materials exhibited stronger adhesion when the SiO_2 layer is thin (approx. 2 nm). To further explore how layered materials influence adhesion, we functionalized similar substrates with an OTS monolayer and again identified a significant influence of the oxide layer thickness on adhesion. Our theoretical calculations describe how variation in the silicon dioxide layer thickness produces differences in the van der Waals interaction potential, and these differences are reflected in the adhesion mechanics. Setal arrays employed as tribological probes provide the first empirical evidence that the 'subsurface energy' of inhomogeneous materials influences the macroscopic surface forces.

15 min break

BP 10.7 Tue 11:30 H 1058

Biocompatibility of $Fe_{70}Pd_{30}$ ferromagnetic shape memory films for cell actuation — •Uta Allenstein[1], Yanhong Ma[2], Ariyan Arabi-Hashemi[2], Stefan G. Mayr[2], and Mareike Zink[1] — [1]Division of Soft Matter Physics, Institute for Experimental Physics I, University of Leipzig, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Translationszentrum für Regenerative Medizin and Fakultät für Physik und Geowissenschaften, Universität Leipzig, Germany

Ferromagnetic shape memory alloys (FSMAs) are a very promising and highly applicable class of smart functional materials which show various interesting features, such as the induction of large reversible strains of several percent due to an external magnetic field at a moderate stress. These properties support the application as actuators or valves in biomedical devices, as well as bone prostheses. Of course in vivo implantation demands good biocompatibility and adhesion of different tissues to the material. Thus, our study investigated the cellular response in contact with single crystalline $Fe_{70}Pd_{30}$ FSMA films on MgO substrates. The adhesive properties as well as the viability and proliferation of different cell types where tested on the substrates and tuned by coating the substrates with different adhesive materials,

such as Fibronectin, Laminin and Poly-L-Lysin. Tests were carried out with NIH 3T3 mouse fibroblasts, MCF 10A human epithelial cells and primary HOB human osteoblasts. We show that these three cell types obtain the ability to adhere and proliferate well on $Fe_{70}Pd_{30}$ FSMA substrates, demonstrating good biocompatibility of the films.

BP 10.8 Tue 11:45 H 1058

Direct Laser Writing for Three-dimensional Biological Application — •Benjamin Richter[1,2], Alexandra Greiner[1], Clemens Franz[1,2], Martin Wegener[2,3,4], and Martin Bastmeyer[1,2] — [1]Zoologisches Institut, Karlsruher Institut für Technologie, 76131 Karlsruhe — [2]DFG-Center for Functional Nanostructures (CFN), Karlsruher Institut für Technologie, 76131 Karlsruhe — [3]Angewandte Physik, Karlsruher Institut für Technologie, 76131 Karlsruhe — [4]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76021 Karlsruhe

Direct laser writing (DLW) is a versatile technique to fabricate tailored three-dimensional (3D) cell-culture scaffolds in the micrometer to nanometer range. By sequential DLW of two different photoresists, composite-polymer scaffolds with distinct protein-binding properties are fabricated and selectively bio-functionalized thereafter. Cells cultured in these scaffolds selectively form cell-adhesion sites with the functionalized parts, allowing for controlling cell adhesion and cell shape in 3D * forming the basis for future designer tissue-culture scaffolds. To go one step further photoactivation of 3D scaffolds might play an important role in the future. One application realized by using these two-component polymer scaffolds is measuring forces of cells in a three-dimensional environment. With our technique we can control the number, size, and geometry of adhesive cubes. The forces induced by a single cell onto the scaffolds are proportional to the bending of the beams.

BP 10.9 Tue 12:00 H 1058

Superparamagnetic Iron Oxide Nanoparticles as Radiosensitizer for Radiation Therapy — •Anja Sommer[1], Stefanie Klein[1], Luitpold Distel[2], and Carola Kryschi[1] — [1]Department of Chemistry and Pharmacy, Institute of Physical Chemistry I, University of Erlangen, Egerlandstr. 3, 91058 Erlangen, Germany — [2]Department of Radiation Oncology, University of Erlangen, Universitaetsstr. 27, 91058 Erlangen, Germany

Superparamagnetic iron oxide nanoparticles (SPION) have been widely used experimentally for numerous in vivo applications such as magnetic resonance imaging (MRI) contrast enhancement, hyperthermia and targeted drug delivery. we present the synthesis of surface-stabilized ultrasmall superparamagnetic iron oxide nanoparticles. In this contribution, we will report on functionalized SPION with sizes between 4 and 15 nm which were synthesized by alkine coprecipitation or thermal decomposition and subsequently coated with biocompatible acids. The differently stabilized SPION were fully characterized using HRTEM, XRD, SQUID, FTIR and Raman spectroscopy, XPS, TGA-MS and TGA-IR coupling and zeta potential measurements. Furthermore we present studies about their biocompatibility for cancer cell lines and their potential as radiosensitizer in radiation therapy.

BP 10.10 Tue 12:15 H 1058

X-ray diffraction on biocomposite materials at high hydrostatic pressure — •Christina Krywka[1], Roxana Ene[2], Shin-Gyu Kang[3], and Martin Müller[3] — [1]Christian-Albrechts-Universität zu Kiel, Institut für Experimentelle und Angewandte Physik, Leibnizstr. 19, D-24098 Kiel — [2]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Linnéstr. 5, 04103 Leipzig — [3]Helmholtz Zentrum Geesthacht, Max-Planck-Str. 1, D-21502 Geesthacht

The anisotropic compressibilites of the crystalline fractions of biocomposite materials (spider silk, silkworm silk, cellulose etc.) were analysed using wide angle X-ray scattering (WAXS) at moderate high pressure (0.01 to 0.5 GPa) using a hydrostatic high pressure cell. With this method, the compression moduli of the biocomposite materials were determined for the first time with high pressure resolution in a pressure range that corresponds to loads as they occur under natural conditions. Exemplarily, for spider silk the compression modulus of the nanocrystals is proven to be highest in the direction of intra-sheet hydrogen bonds. In addition, it is found that the applied pressure may increase the organization of the amorphous phase, indicated by a pressure enhanced diffraction ring.

BP 10.11 Tue 12:30 H 1058

Subspecies of nacre protein "perlucin" favors binding to aragonite over binding to calcite microcrystals — •Hanna Rademaker, Malte Launspach, and Monika Fritz — Institute for Biophysics, University of Bremen, Germany

Nacre is a compound material of calcium carbonate platelets and organic layers of chitin and proteins. The outstanding mechanical properties of nacre make it desirable to understand the details of the biomineralizing process. The calcium carbonate platelets in nacre show the crystal structure of aragonite and not of calcite. Therefore we are especially interested in proteins which favor binding to aragonite over binding to calcite. We adapted a simple detection method from Suzuki et al. [1] for this purpose.

In this work [2] biomineralizing proteins were chemically removed from the acid-insoluble matrix of nacre from *Haliotis laevigata* and incubated with aragonite and calcite microcrystals, respectively. The crystals were washed and then dissolved. SDS-PAGE of these solutions showed that one protein, a subspecies of perlucin, favors binding to aragonite crystals. This might be a hint that perlucin plays a key role in the biomineralization process.

[1] M. Suzuki et al., Science, **325** (5946), 1388-1390, 2009

[2] H. Rademaker and M. Launspach, Beilstein J. Nanotechnol., **2**, 222-227, 2011

BP 10.12 Tue 12:45 H 1058

Assessment of swelling driven actuation in a two-phase cellular material — •Lorenzo Guiducci[1], Yves J. M. Brechet[2], Peter Fratzl[1], and John W. C. Dunlop[1] — [1]Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Am Mühlenberg 1, Science Park Golm, Potsdam, Germany — [2]SIMaP-Grenoble Institute of Technology, Saint Martin d'Hères, France

Natural systems that are able to actuate -that is, generate stress/strain- have recently drawn the attention of scientific community. Examples include the seed dispersal unit of the wild wheat and stork's bill awn, which are able to crawl on the ground following the daily humidity cycle and the hydro-actuated unfolding of the ice-plant seed capsule.

In natural actuators, the extent of max elongation/forces depends on underlying microstructure, and swelling properties of the constituents: here we present a finite element (FE) simulation study that aims to assess the actuation performance -eigenstrains and effective stiffness at a certain swelling level- of an ideal two-phase cellular material. The eigenstrains assessment is rigorously performed simulating a tessellation of the bidimensional space with given unit cell. As observed in preliminary simulations of a finite patch of material with free boundaries, the resulting two-phase material deforms in a highly anisotropic way. For each value of swelling pressure, we get an equilibrated configuration of the unit cell that becomes the starting point for the calculation of the effective mechanical properties. Finally, we show that the FE results can be understood in terms of a simpler lattice spring model.

BP 11: Focus: Statistics of Cellular Motion (with DY)

This topical session brings together theoretical and experimental researchers working on statistical descriptions of cell motility, which is an emerging theme in the rapidly growing field of cell motility. (Organizers Carsten Beta, Peter Dieterich, Rainer Klages and Lutz Schimansky-Geier)

Time: Tuesday 9:30–13:30 Location: H 1028

Topical Talk BP 11.1 Tue 9:30 H 1028 **Data-driven modeling of cell trajectories: a do-it-yourself kit**

— •Henrik Flyvbjerg — DTU Nanotech, Kongens Lyngby, Denmark

Resent results in data-driven modeling of cell trajectories are reviewed. A do-it-yourself toolkit is presented. Technical points are discussed, such as how to glean mathematical properties of a model-to-be-found from appropriate model-independent experimental statistics, and how such statistics are affected by finite sampling frequency of time-lapse recordings and experimental errors on recorded positions.

Topical Talk BP 11.2 Tue 10:00 H 1028

The statistics of eukaryotic chemotaxis — •Eberhard Bodenschatz — MPI Dynamics and Self-Organization, Goettingen, Germany

The directed motion of eukaryotic cells in a chemoattractant gradient depends on the the steepness of the gradient as well as the average concentration surrounding the cell. It was recently theoretically predicted that for a given situation the chemotactic efficacy is determined by the stochastic fluctuations of a two step process: first the binding of the signaling molecule to the transmembrane receptor and second the intracellular unbinding of a second messenger. It was suggested that the signal to noise ratio of this two stage process is sufficient to explain the chemotactic behavior. In this talk we will first introduce eukaryotic chemotaxis and the experimental micro-fluidic system for controlled chemical signals. Then we shall present the data on the random directed motion of cells and will describe it with a 2D Langevin equation. Then we show that the stochasticity of the two step process can indeed describe the experimentally observed behavior.

Topical Talk BP 11.3 Tue 10:30 H 1028

Dynamics of directed cell migration — •Albrecht Schwab[1], Otto Lindemann[1], and Peter Dieterich[2] — [1]University of Münster, Germany — [2]University of Dresden, Germany

Directed migration (chemotaxis) is the prerequisite for an efficient immune defense. The chemical signal is transduced to the cell migration machinery via complex intracellular signaling cascades that also include the activation of plasma membrane Ca2+ channels of the TRPC family. Chemotaxis involves a cellular motor for migration and a steering mechanism. Here, we aim to determine which of these two components are controlled by TRPC channels. Their contribution is assessed with time-lapse video microscopy of single neutrophils from wildtype and TRPC knockout mice exposed to chemoattractants. Since raw velocities or straightness indices calculated from the experimental cell paths provide only a coarse interpretation of the migratory behavior, we analyze all data within the concept of stochastic processes. The cell is regarded as an object driven by internally correlated stochastic forces and external fields generated by chemoattractants. Anomalous properties that we previously identified in cells migrating without external stimuli and described with a fractional Klein-Kramers equation are maintained during chemotaxis. This enables a modeling based quantification of correlations and allows to disentangle the influence of the chemoattractants on the motor strength (thermal velocity) and directed migration (drift) of the cells under different conditions. Our statistical analyses show that TRPC channels are primarily involved in controlling the steering mechanism of chemotacting neutrophils.

Topical Talk BP 11.4 Tue 11:00 H 1028

Medley swimming of sleeping sickness parasites — •Vasily Zaburdaev[1], Sravanti Uppaluri[2], Thomas Pfohl[3], Markus Engstler[4], Rudolf Friedrich[5], and Holger Stark[6] — [1]Harvard University, Cambridge, USA — [2]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [3]University of Basel, Basel, Switzerland — [4]University of Würzburg, Würzburg, Germany — [5]University of Münster, Münster, Germany — [6]Technical University of Berlin, Berlin, Germany

Though cell locomotion has been examined almost since the discovery of the cell itself, advances in microscopy and biochemical studies have paved the way to a more fundamental understanding of cell motility. This work is a detailed, quantitative characterization of trypanosome motility. Trypanosomes, parasites responsible for deadly disease in humans and cattle, swim with the aid of an appendage called a flagellum. The flagellum, produces rapid undulatory movements that result in cell locomotion. We followed single trypanosomes in a homogeneous environment and found that cells that swim faster also exhibit stronger fluctuations in velocity. Statistical analysis allowed us to develop a mathematical model that could reproduce the diverse trajectories followed by the trypanosomes. Finally, we were able to show that the rapid movements of the body (with time scales on the order of 0.1s) are a result of an active process and thus cannot be described as simple thermal fluctuations. On the whole, such studies provide insight into basic mechanisms of motility, allow for modeling of cell movement, and may eventually even provide design ideas for artificial microswimmers.

15 min break

BP 11.5 Tue 11:45 H 1028

Describing Run and Tumble Motion with Alternating Random Walks — •Felix Thiel, Lutz Schimansky-Geier, and Igor M. Sokolov — Institut für Physik der Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

Run and tumble motion is the motile behaviour of flagellated bacteria like E.Coli. Much effort has been made in order to understand and describe such motion. Continuous time random walks (CTRW) are a common tool for description, but lack the possibility of incorporating different kinds of motion. In order to fill this gap, we present a modification of the usually considered CTRW: the alternating random walk. We explicitly distinguish between the run and the tumble phase. By using the techniques of CTRW – integral transforms and asymptotic analysis – we are able to obtain the short-time as well as the long-time behaviour of the mean squared displacement of the process. The main free parameters of the process governing the diffusive behaviour are the waiting-time-PDFs describing the dwelling time in run resp. tumble mode. It is shown that models constructed as above may exhibit a transition in diffusive behaviour from normal to superdiffusion and a change of the effective diffusion coefficient. They may thus be suitable to describe other situations which are known for those phenomena.

BP 11.6 Tue 12:00 H 1028

Swimming of microorganisms in a microchannel flow. — •Adam Wysocki, Roland G. Winkler, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich

We consider an active suspension – motile microorganisms dispersed in a fluid – under flow in a microchannel. We use a coarse-grained model of an active suspension, where the microorganisms are modeled as spherical particles with a prescribed tangential surface velocity, and the fluid is described by multiparticle collision dynamics approach, a particle-based, mesoscopic simulation method, which includes thermal fluctuations. Our model of a swimmer can easly be tuned to be a puller or a pusher, which generate thrust in the front or at the back of the body, respectively. At low swimmer concentrations, far from the walls and for external flow fields u small compared to the propulsion velocity U_0, puller and pusher swim upstream following on average a sinusoidal trajectory. Near the walls, where hydrodynamic interactions are significant, pullers and pushers show a qualitatively different behaviour. Individual pushers swim upstream near the wall for $U_0/u > 1$, while pullers swim downstream for $U_0/u \gg 1$ and change to upstream swimming with increasing flow field u. The collective behaviour at higher concentrations of microorganisms will be discussed.

BP 11.7 Tue 12:15 H 1028

Self-propelled rod-like microswimmers near surfaces — •Kristian Marx and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems, Forschungszentrum Jülich

Self-propelled microswimmers (e.g. sperm, E. coli and the alga Chlamydomonas) are biological organisms that propel themselves through fluid. In future applications, microswimmers may also be used as biosensors on lab-on-a-chip devices. They can be classified as having *pusher* or *puller polarity*, which are driven from the rear or the front, respectively. We study the behavior of a general polar rod model at high swimmer densities in three dimensions, in particular close to walls, including hydrodynamics and volume-exclusion interactions. We employ hydrodynamics simulations using a mesoscale particle based technique (*multi-particle collision dynamics*) implemented on GPU hardware. The swimmer behavior is found to strongly depend on the swimmer polarity: Pushers experience parallel alignment with the walls and strongly aggregate near them. Due to mutual hydrodynamic attraction the rods form motile clusters at the walls. Interacting clusters can form swirls, destroying long-range nematic order. Pullers aggregate into giant immotile clusters that span the entire system at high densities. While they are overall isotropic, the puller clusters show a typical hedgehog structure at the walls, with most of the swim-

mers pointing towards the walls. Finally, *unpolar driven* rods interact only weakly via hydrodynamics and show an isotropic-nematic phase transition at critical densities much lower than passive rod systems.

BP 11.8 Tue 12:30 H 1028

Collective Dynamics of swimming bacteria and surface attached clusters during biofilm formation — •Matthias Theves and Carsten Beta — Universität Potsdam, Potsdam, Germany

Biofilms (BFs) are communities of sessile bacteria, embedded in an extracellular polymeric structure (EPS), which form at solid-liquid or liquid- air interfaces. We use biocompatible microfluidic channels and high speed time lapse microscopy to study the recruitment of cells from the bulk fluid to a glass surface. During this early stage of BF-formation, bacteria from the swimming phase coexist with surface attached cells that cluster together and form the cores of growing colonies. We analyze the growth dynamics of both populations. After a continuous increase in cell density and cluster size, we observe a sudden increase in the number of swimming cells. Furthermore, we analyze the random walk of isolated swimmers and perform a statistical analysis that allows us to identify changes in the migration patterns of swimming cells in the presence of different obstacles in the microchannel and during experiments with different medium availability.

BP 11.9 Tue 12:45 H 1028

Rotationally induced polymorphic transitions of a bacterial flagellum — A full model of swimming *Rhodobacter sphaeroides* — •Reinhard Vogel and Holger Stark — Institute of Theoretical Physics, TU Berlin

The bacterium *Rhodobacter sphaeroides* swims by rotating a helical filament also called flagellum. The filament is driven by a rotary motor. Depending on the speed of the motor, the flagellum assumes different configurations characterized by its pitch and radius (polymorphism). If the motor stops, the flagellum relaxes into a coiled form with large radius and small pitch, whereas if the motor runs it assumes a helical state with large pitch better suited for swimming. Due to the switch between running and stopping, the bacterium changes its direction randomly.

The bacterial flagellum consists of three parts; the rotary motor embedded in the cell membrane, a short proximal hook that acts as a universal joint and couples the motor to the third part, the long helical filament. The helical shape of the filament converts rotational motion into a thrust force that pushes a bacterium forward. We present our approach to mimic the rotary motor and hook within a continuum model of the flagellum. We use the elastic theory for flagellar polymorphism, developed in Ref. [1], to investigate how an applied motor torque induces a transition between two polymorphic configurations. We attach the bacterial flagellum to a load particle and thereby model the locomotion of the bacterium *Rhodobacter sphaeroides*.

[1] R. Vogel and H. Stark, Eur. Phys. J. E **33**, 259–271 (2010).

BP 11.10 Tue 13:00 H 1028

Hydrodynamic Simulation of Bacteria Swimming — •Shang Yik Reigh, Roland G. Winkler, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Juelich, 52425 Juelich

Locomotion of bacteria such as E. coli or Salmonella is achieved by rotation of helical flagella, which are randomly distributed on the cell body. A directional running motion is attained by bundle formation of multiple flagella, while tumbling motion is achieved by the reverse rotation of one of the flagella. Alternating running and tumbling phases allow the bacteria to perform a directed random walk, and play an important role in their chemotaxis. During bacterial swimming, the pitch and the radius of flagella are changed (polymorphic transformations) and the cell body counter-rotates against the flagella to conserve angular momentum. To gain insight into the bacterial swimming behavior, hybrid mesoscale simulations are performed, which combine molecular dynamics simulations for the bacterium with the multiparticle collision (MPC) method for the solvent. The flagella are constructed by a sequence of mass points interacting by bond, bending, and torsional potentials. Such a model can efficiently be coupled to the MPC fluids. Results are presented for the synchronization and the bundle formation of several flagella. The synchronization and bundling times are analyzed in terms of the applied torque, the separation distances, and the number of flagella. The role of counter-rotating cell body for synchronization and bundling will be discussed.

BP 11.11 Tue 13:15 H 1028

Pili-induced clustering of *Neisseria gonorrhoeae* bacteria — •Johannes Taktikos[1,2], Vasily Zaburdaev[2], Nicolas Biais[3], David A. Weitz[2], and Holger Stark[1] — [1]Technische Universität Berlin — [2]Harvard University, USA — [3]Columbia University, USA

The attachment of *Neisseria gonorrhoeae* bacteria, the causative agent of the gonorrhea disease, to human epithelial cells constitutes the first step of colonization. The attachment of *N. gonorrhoeae* to surfaces or other cells is primarily mediated by filamentous appendages, called type IV pili. Cycles of elongation and retraction of these pili are responsible for a common form of bacterial motility called twitching motility which allows the bacteria to crawl over surfaces. Experimentally, *N. gonorrhoeae* cells initially dispersed over a surface agglomerate into round microcolonies within hours. It is so far not known whether this clustering is driven entirely by the pili dynamics or if chemotactic interactions are needed. Thus, we investigate whether the agglomeration may stem solely from the pili-mediated attraction between cells. By developing a model for pili-taxis, we try to explain the experimental measurements of the mean cluster size, number of clusters, and area fraction covered by the cells.

BP 12: Focus: Nonlinear Dynamics of the Heart (with DY)

Time: Wednesday 9:30–12:00 Location: MA 001

Invited Talk BP 12.1 Wed 9:30 MA 001

Modelling Excitation Contraction Coupling — •Martin Falcke — Max Delbrück Centrum für Molekulare Medizin Berlin

We present an efficient but detailed approach to modelling Ca^{2+}-induced Ca^{2+} release in the diadic cleft of cardiac ventricular myocytes. We developed a spatial resolved Ca^{2+} release unit (CaRU), consisting of the junctional sarcoplasmic reticulum and the diadic cleft. Individaul channels are modelled by Markov chains. By taking advantage of time scale seperation, the model could be finally reduced to only one ordinary differential equation for describing Ca^{2+} fluxes and diffusion. Additionally the channel gating is described in a stochastic way. The resulting model is able to reproduce experimental findings like the gradedness of SR release, the voltage dependence of ECC gain and typical spark life time.

Invited Talk BP 12.2 Wed 10:00 MA 001

Modeling of electrical and mechanical function of the heart — •Alexander Panfilov — Department of Physics and Astronomy, Gent University, Krijgslaan 281, S9, 9000 Gent, Belgium

Cardiac arrhythmias and sudden cardiac death is the leading cause of death accounting for about 1 death in 10 in industrialized countries. Although cardiac arrhythmias has been studied for well over a century, their underlying mechanisms remain largely unknown. One of the main problems in studies of cardiac arrhythmias is that they occur at the level of the whole organ only, while in most of the cases only single cell experiments can be performed. Due to these limitations alternative approaches such as mathematical modeling are of great interest. From mathematical point of view excitation of the heart is described by a system of non-linear parabolic PDEs of the reaction diffusion type with anisotropic diffusion operator. Cardiac arrhythmias correspond to the solutions of these equations in form of 2D or 3D vortices characterized by their filaments. In my talk I will briefly report on main directions of our research, such as development of virtual human heart model, and study organization of ventricular fibrillation due to dynamical instabilities in cardiac tissue and due to tissue heterogeneity. I will also report on modeling mechano-electric feedback in the heart using reaction-diffusion mechanics systems and ventricular fibrillation mechanisms due to deformation of cardiac tissue.

Invited Talk BP 12.3 Wed 10:30 MA 001

Mechanisms for calcium alternans — •Blas Echebarria, Enric

Alvarez-Lacalle, Carlos Lugo, Angelina Peñaranda, and Inma R. Cantalapiedra — Departament de Física Aplicada, Universitat Politècnica de Catalunya, 44-50 Av. Dr. Marañón, 08028 Barcelona, Spain

Alternans is a well-known cardiac pathology, in which the duration of the action potential (AP) alternates at consecutive beats. Due to its proarrhythmic effects it is important to understand the mechanisms underlying its genesis. It has been amply studied the case where alternans appears due to a steep relationship between the duration of an action potential and the time elapsed since the end of the previous AP. However, now it is widely accepted that alternans often appears due to instabilities in the dynamics of intracellular calcium cycling (itself an important messenger for the contraction of the cell). This instability can be due to a steep relationship between the amount of calcium released to the cytosol, and the calcium loading of the sarcoplasmic reticulum (SR), but also due to a slow recovery of the channels that regulate the release from the SR.

Invited Talk BP 12.4 Wed 11:00 MA 001

Synchronization as a mechanism of chaos control; Applications to cardiac arrhythmias. — •Flavio H. Fenton[1], Stefan Luther[1,2], Philip Bittihn[2], Daniel Hornung[2], Eberhard Bodenschatz[2], and Robert F. Gilmour Jr[1] — [1]2Department of Biomedical Sciences, Cornell University, Ithaca, New York, USA — [2]1Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

The heart is an excitable system, with electrical waves propagating in a coordinated manner to initiate a mechanical contraction. In pathologic states, normal electrical wave propagation can be disrupted, resulting in the development of spiral and scroll waves that repetitively excite the tissue. These waves are often unstable and break into multiple waves, a chaotic state that underlies cardiac fibrillation.

In this talk, we will discuss experimental and theoretical approaches for the control and termination of arrhythmias using low energy pulses. We will show how naturally occurring discontinuities in cardiac tissue conductivity can produce internal electrical activations following an electric field and how this *virtual electrode activations* can be used to synchronize and terminate arrhythmias with just 10% the energy of a standard defibrillation shock. Numerical simulations as well as experimental data from in vivo experiments will be presented along with a theory for the mechanism.

Invited Talk BP 12.5 Wed 11:30 MA 001

Cardiac dynamics from a nonlinear system's perspective - from basic science to applications — •Stefan Luther — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — Department of Biomedical Sciences, Cornell University, Ithaca, NY

Self-organized complex spatial-temporal dynamics underlies cardiac arrhythmias, a significant cause of mortality and morbidity worldwide. The term dynamical disease was coined, suggesting that they can be best understood from a dynamical system's perspective. The systematic integration experimental data from sub-cellular, cellular, tissue, and organ level to the in-vivo organism into mathematical models is key to the understanding of this complex biological system. The talk will provide an introduction to the biophysics and nonlinear dynamics of the heart, and discuss mechanisms that induce, sustain, and control life-threatening cardiac arrhythmias.

BP 13: DNA/RNA and Related Enzymes

Time: Wednesday 9:30–13:00 Location: H 1058

Topical Talk BP 13.1 Wed 9:30 H 1058

Chemo-mechanics of a ring-shaped helicase during unwinding — •Michael Schlierf[1,2], Ganggang Wang[3], Xiaojiang Chen[3], and Taekjip Ha[1,4] — [1]University of Illinois at Urbana-Champaign, Physics Department and Center for Physics of Living Cells, Urbana, Illinois — [2]B CUBE - Center for Molecular Bioengineering, TU Dresden — [3]University of Southern California, Department of Biological Sciences — [4]Howard Hughes Medical Institute, Urbana, Illinois

Most replicative helicases are hexameric ring-shaped enzymes and are essential for cell survival. Despite extensive biochemical, structural and single-molecule investigations, how the translocation activities are utilized in the mechanical process of dsDNA unwinding are poorly understood. We investigated DnaB-family helicase G40P using a single molecule fluorescence-based unwinding assay with a single base pair resolution. The high-resolution assay revealed that G40P is an ultraweak helicase that stalls at barriers as small as a single GC base pair and is a motor that moves with the step size of a single base pair. We directly observed the long-postulated activity of helicase slippage that is markedly enhanced under conditions that slow forward progression, but is fully suppressed by the primase DnaG.

BP 13.2 Wed 10:00 H 1058

The Speed of Ribosomes — •Sophia Rudorf, Angelo Valleriani, and Reinhard Lipowsky — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Am Mühlenberg 1, 14476 Potsdam

To synthesize a protein a ribosome moves along the codons of a messenger RNA (mRNA) and takes up corresponding aminoacylated transfer RNAs (aa-tRNAs). During this process called translation elongation the ribosome does not always proceed at the same speed. Here we present an analytical model to calculate codon-specific elongation rates based on aa-tRNA concentrations and codon usages. The model takes into account non-cognate aa-tRNAs that compete with cognate aa-tRNAs as well as the number of translating ribosomes. Using available in vivo data and codon usages obtained from mRNA Deep Sequencing we computed the elongation rates for Escherichia coli. Results of stochastic simulations based on these elongation rates coincide well with experimental data. We found that increasing the number of translating ribosomes strongly decreases the availability of frequently used aa-tRNAs. This leads to comparably low elongation rates of some abundant codons, in contrast to the generally high correlation of elongation rates and codon usages.

BP 13.3 Wed 10:15 H 1058

Nematic ordering due to intrinsic chain stiffness causes DNA molecules packed in phage capsids to preferentially form torus knots — Daniel Reith[1], Andrzej Stasiak[2], Peter Cifra[3], and •Peter Virnau[1] — [1]Department of Physics, Uni Mainz — [2]Center for Integrative Genomics, UNIL, Lausanne, Switzerland — [3]Polymer Institute, Slovak Academy of Sciences, Bratislava, Slovakia

When mature bacteriophages such as P2 or P4 are assembled in infected cells, a long linear DNA molecule is loaded into the phage capsid and arranges itself in a toroidal, nematic phase. Intriguingly, experiments show that the DNA is not only highly knotted, but also exhibits a rather uncommon knot spectrum. Observation that DNA molecules in bacteriophage capsids preferentially form torus knots provide a sensitive gauge to evaluate various models of DNA arrangement in phage heads. We demonstrate with computer simulations of a simple bead-spring model that an increasing chain stiffness not only leads to nematic ordering and a (somewhat counter-intuitive) increase of knottedness, it is also the decisive factor in promoting formation of DNA torus knots in phage capsids.

BP 13.4 Wed 10:30 H 1058

The binding of monoclonal antibodies and tau-peptides - how two binding sites add up to form a stable specific bond — •Carolin Wagner, David Singer, Tim Stangner, Christof Gutsche, Olaf Ueberschär, Ralf Hoffmann, and Friedrich Kremer — Leipzig University, Leipzig, Germany

Optical tweezers-assisted dynamic force spectroscopy (DFS) is employed to investigate specific receptor/ligand interactions on the level of single binding events [1]. Here, the specific binding of the anti-human tau monoclonal antibody (mAb), HPT-101, to synthetic tau-peptides is analyzed. Amongst others, the massive accumulation of tangles that mainly consist of hyperphosphorylated tau-proteins is characteristic for Alzheimer*s disease. The sorts of tau-peptides, which are used in this study, contain either one phosphorylation, at Thr231 and Ser235, respectively, or they are phosphorylated at both sites. From measurements using ELISA it is known, that the HPT-101 binds only specifically to the double-phosphorylated tau-peptide. The results obtained by DFS show, that HPT-101 binds also to each

sort of the mono-phosphorylated peptides. By analyzing the measured rupture-force distributions characteristic parameters like the lifetime of the bond without force t0, the characteristic length xts and the free energy of activation Delta G are determined for all interactions. Thereby it can be shown how the attachments of HPT-101 with the mono-phosphorylated peptides add up in the case of the double-phosphorylated peptide in order to form the strong specific binding.

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

BP 13.5 Wed 10:45 H 1058

Electrophortic mobility of DNA-grafted single colloids as studied by optical tweezers — •Ilya Semenov, Christof Gutsche, Mahdy M. Elmahdy, Olaf Ueberschär, and Friedrich Kremer — Institute for Experimental Physics I, University of Leipzig, Linnéstrasse 5, 04103 Leipzig, Germany

The electrophoretic mobility of single particles grafted with double stranded (ds) DNA is studied by use of optical tweezers (OT) accomplished with fast position detection (Single Colloid Electrophoresis [1, 2]). Parameters to be varied are the concentration (0.01 mMol/l - 1 Mol/l) and valency (KCl, $CaCl_2$, $LaCl_3$) of the ions in the surrounding aqueous medium, but as well the contour length (250, 1000 and 4000 base pairs) of the grafted chains. For the DNA-grafted colloids a pronounced decrease of the electrophoretic mobility is observed in comparison to blank particles under identical conditions. The findings are discussed in terms of the Standard Electrokinetic Model [3]. The electrophoretic mobility of a ds-DNA-grafted single colloid at high ionic strength can be understood quantitatively within the limits of the linearized Poisson-Boltzmann equation.

[1] I. Semenov et al., Journal of Physics: Condensed Matter 22, 494109 (2010).

[2] I. Semenov et al., Journal of Colloid and Interface Science 337, 260 (2009).

[3] R. W. O'Brien, and L. R. White, JCS, Farad. Trans. 2 74, 1607 (1978).

BP 13.6 Wed 11:00 H 1058

RNA folding dynamics studied with a structure-based model — •Michael Faber and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces Potsdam

RNA molecules form three-dimensional structures as complementary bases form bonds and the molecule coils. These structures determine the function and biochemical activity of the molecule. For example, the presence or absence of a specific RNA structure can invoke transcriptional pauses or terminate the transcription altogether. We have developed a structure-based model for studying the folding dynamics of RNA secondary structures. To simulate the dynamics, we use a Monte-Carlo method with Metropolis rates, where the basic steps are the closing or opening of one native contact. We apply this model to the folding and unfolding of simple RNA structures in the presence and absence of an external force.

15 min break

BP 13.7 Wed 11:30 H 1058

Computer simulation of chromatin: Effects of nucleosome positioning on chromatin structure — •Oliver Müller[1], Robert Schöpflin[1], Nick Kepper[2], Ramona Ettig[2], Karsten Rippe[2], and Gero Wedemann[1] — [1]CC Bioinformatics, University of Applied Sciences Stralsund, Zur Schwedenschanze 15, 18435 Stralsund, Germany — [2]Deutsches Krebsforschungszentrum & BioQuant, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany

The three-dimensional structure of chromatin is a key factor for DNA accessibility, replication and repair. Most theoretical models of chromatin imply a static, periodical positioning and uniform occupancy of nucleosomes. However, recent studies suggest a dynamic nucleosome positioning, which is both actively regulated by chromatin-remodeling complexes and passively influenced by thermal fluctuations. In turn, nucleosomes deviating from regular positions can introduce changes into chromatin fiber structure. To investigate the effects of nucleosome repositioning, we carried out Monte Carlo simulations with a coarse-grained chromatin model incorporating elastic fiber properties as well as electrostatic and internucleosomal interactions. We created fiber models based on experimental results and modified these by repositioning nucleosomes by a range of base pairs. After simulation, the chromatin energy landscape and fiber shape were analyzed. We observed a significant energy barrier against nucleosome repositioning which is larger than thermal fluctuations but within the range of ATP-dependent biological processes. Moreover, the region proximate to a repositioned nucleosome revealed an increased kinking susceptibility.

BP 13.8 Wed 11:45 H 1058

Confinement Driven Spatial Organization of Semiflexible Ring Polymers — Miriam Fritsche and •Dieter Heermann — Universität Heidelberg, Institut für Theoretische Physik, Philosophenweg 19, D-69120 Heidelberg

We investigate conformational properties of a semiflexible ring polymer in confined spaces. Taking into account the competing interplay between configurational entropy, bending energy and excluded volume, we elucidate the role that different geometrical constraints can play in shaping the spatial organization of biopolymers. While elongated, rod-like geometries reduce the amount of chain overcrossings and induce a pronounced ordering with respect to the long axis of the surrounding envelop, there exists no preferred orientational axis in case of spherical confinement. Upon increasing the system density and rigidity of the chain, the polymer migrates from the center of the accessible space towards the surrounding surface forming a spool-like structure known for DNA condensation within viral capsids. The existence of distinguished loop sizes for different confining geometries might influence co-localization in biopolymers necessary for the genome-wide coordination of gene expressed. Thus, the advantages of certain geometric constraints such as spherical confinement of viral DNA in a capsid or the rod-shaped envelop of the circular chromosome in Escherichia coli could be one driving force for controlling proper biological functioning.

BP 13.9 Wed 12:00 H 1058

Towards chromatin mimics: DNA self-assembly with linker histone H1 - a combined study of X-rays and microfluidics — •Adriana Cristina Toma[1], Rolf Dootz[2], and Thomas Pfohl[1,2] — [1]Chemistry Department, University Basel, Klingelbergstrasse 80, Basel, Switzerland — [2]Max Planck Institute of Dynamics and Self-Organization, Göttingen, Germany

Inspired by the nature of DNA packing we have investigated how linker histone H1influence the local structures of the formed DNA self-assemblies. Despite the key role of the linker-histone H1 in chromatin dynamics, its interactions with nucleosomal DNA are not fully understood. We have used the combination of in situ microfluidics and small angle X-ray microdiffraction in order to analyze the real-time dynamics and structural evolution of assemblies resulted from the binding of linker-histones H1 to DNA. Our results indicate that the mechanism of H1 interactions with DNA is a two-step process: at first H1 binds non-specifically to DNA and secondly the protein molecules rearrange inside the formed self-assemblies, distorting the columnar phase of DNA.

BP 13.10 Wed 12:15 H 1058

The partially closed conformation of DNA polymerase I provides a decision point for nucleotide selection — •Johannes Hohlbein[1], Catherine Joyce[2], and Achillefs Kapanidis[1] — [1]Biological Physics Research Group, Dept. of Physics, University of Oxford, UK — [2]Dept. of Molecular Biophysics and Biochemistry, Yale University, New Haven, CT, U.S.A.

The high fidelity of many DNA polymerases depends largely on conformational changes that precede the chemical step of phosphoryl transfer and serve as checkpoints to reject inappropriate substrates early in the reaction. One of these conformational changes is the fingers-closing transition, during which the fingers subdomain moves from an open to a closed conformation.

Here, we use single-molecule FRET to resolve conformational changes within the bacterial DNA polymerase I with sub-nanometre resolution. We compared the wild-type polymerase to derivatives bearing single amino-acid substitutions at residues E710 and Y766, both which are invariant within the A family of DNA polymerases.

Our results show that these derivatives have decreased affinity for the complementary dNTP, and do not perform efficient fingers-closing. Instead, intermediate FRET states are populated, which are likely to correspond to a fidelity-associated partially closed state of the fingers.

These differences in the interactions and conformations formed along the reaction path reduce discrimination between complementary and non-complementary nucleotides, and provide a basis for the reduced fidelity of the derivatives.

BP 13.11 Wed 12:30 H 1058

Stability of double-stranded oligonucleotide DNA with a

bulged loop: a microarray study — •Christian Trapp — Universität des Saarlandes, Biologische Experimentalphysik

The hybridization process, the formation of the DNA double-helix from single-strands of complementary sequences, is important for all living organisms. It is at the basis of many high throughput nucleic acid based technologies such as high throughput sequencing or DNA microarrays. The latter consist of surface bound ssDNA (probes), which can selectively bind to complementary strands (targets) in solution resulting in highly parallel measurements. The underlying physical mechanisms of the hybridization process are poorly understood. We have shown that the binding to DNA microarrays can be easily modeled when the length of probe and targets match [1-2]. Here we investigate the binding of longer targets to microarrays, which hybridize to the probes forming bulged loops. We systematically vary loop position and loop size and show that the result can be reproduced with simple theoretical models at thermal equilibrium, which also apply to solution-phase experiments.

[1] Naiser T, Kayser J, Mai T, Michel W, Ott A: Stability of a Surface-Bound Oligonucleotide Duplex Inferred from Molecular Dynamics: A Study of Single Nucleotide Defects Using DNA Microarrays, Phys. Rev. Lett. 2009, 102, 218301

[2] Naiser T, Kayser J, Mai T, Michel W, Ott A: Position dependent mismatch discrimination on DNA microarrays - experiment and Model, BMC Bioinformatics 2008, 9:509

BP 13.12 Wed 12:45 H 1058

Nucleobase adsorbed at graphene devices: enhance biosensorics — •Bo Song[1], Gianaurelio Cuniberti[2], Stefano Sanvito[3], and Haiping Fang[1] — [1]Laboratory of Physical Biology, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, P.O. Box 800-204, Shanghai 201800, China — [2]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [3]School of Physics and CRANN, Trinity College, Dublin 2, Ireland

Graphene as a good material for sensing single small molecules, is hardly believed to identify bio-molecules via electrical currents. This is because bio-molecules tend to bind to graphene through non-covalent bonds, such as π-π stacking interaction, which is not customarily considered to induce a clear perturbation of the graphene electronic structure. In contrast to these expectations, we demonstrate that oxygen in nucleobases adsorbed on graphene with π-π stacking interaction, can clearly alter the electric current, even in water at room temperature. This property allows us to devise the strategies employing graphene as material of choice in bio-sensorics, bio-chips.

BP 14: Membranes and Vesicles

Time: Wednesday 9:30–13:00 Location: H 1028

Topical Talk BP 14.1 Wed 9:30 H 1028

Membrane transformations in vesicles enclosing aqueous two-phase polymer solutions — •Rumiana Dimova — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The interior of living cells is crowded with macromolecules. In such a concentrated environment, local phase separation may occur, involving local composition differences and microcompartmentation. Recently, giant vesicles loaded with polymer solutions were reported to exhibit spatial compartments formed by phase separation within the vesicle. We employed these artificial cell systems to study various phenomena related to molecular crowding and microcompartmentation in cells. We demonstrate that similarly to the wetting behavior of liquid droplets in contact with surfaces, different polymer aqueous phases in contact with membranes as a substrate can undergo complete to partial wetting transition (J Am Chem Soc, 2008, 130:12252). We find that the degree of wetting is characterized by a hidden material parameter - the intrinsic contact angle, which can be determined from effective contact angles observed by optical microscopy (Phys Rev Lett, 2009, 103:238103). Upon osmotic deflation of vesicles enclosing two aqueous phases that partially wet the membrane, one can observe vesicle budding and/or tube formation (Proc Natl Acad Sci USA, 2011, 108:4731) depending on the competition between the spontaneous curvature of the membrane and the wetting properties of the aqueous phases. Phase separation of aqueous polymer solutions in vesicles can lead to stable and retractable membrane nanotubes, which is relevant for membrane area storing and regulation in cells.

BP 14.2 Wed 10:00 H 1028

In vivo high pressure 1H NMR studies on oocytes of Xenopus laevis — •Joerg Koehler, Sebastian Dietz, Werner Kremer, and Hans Robert Kalbitzer — Institute of Biophysics and Physical Biochemistry, University of Regensburg, 93040 Regensburg, Germany

Oocytes of the African Clawed Frog Xenopus laevis are an excellent candidate for in vivo high pressure Nuclear Magnetic Resonance studies. This is due to their relative good resistance against mechanical stress compared to other living cells and on the other hand their quite large cell size.

We studied the oocytes in the pressure range from ambient pressure to 200 MPa by 1H NMR spectroscopy. The strongest signals come from the lipids contained in the oocytes. The signals of the lipids decrease with increasing pressure where the signals assigned to different groups behave differently. Signals due to protons in unsaturated fatty acids show a smaller pressure effect than signal arising from saturated fatty acids. The T2-values measured by a CPMG sequence are only weakly dependent on pressure. The data can be explained by a pressure dependent phase transition in the lipid droplets. The pressure induced effects observed by NMR spectroscopy are completely reversible up to a pressure of 120 MPa, which agrees well with the vitality measurements on pressure treated cells by patch-clamp experiments on the membrane.

BP 14.3 Wed 10:15 H 1028

Insights into the mechanics and uncoating of influenza virus from atomic force microscopy studies — •Frederic Eghiaian[1], Sai Li[1], Christian Sieben[2], Claudia Veigel[3], Andreas Herrmann[2], and Iwan Schaap[1] — [1]D.P.I, Georg-August-Universität Göttingen — [2]Institut für Biologie, Humboldt Universität, Berlin — [3]Lehrstuhl Zelluläre Physiologie and Centre for Nanosciences, Ludwig-Maximilians-Universität München

During the assembly and budding of the influenza virus, the viral genome is recruited in virions by the matrix proteins. This matrix forms a pseudo-continuous shell that coats the inner layer of the cellular membrane, following which capsule shaped viruses bud out of the cell. After infection this morphology, as well as the membrane-matrix-genome interaction is lost when the virus reaches the acidic endosomes, an essential step for fusion and the release of the viral genome. Using AFM we investigated the contribution of the different building blocks and the effect of pH on the mechanical properties of the virus. Contrary to protein-based capsids, Influenza virions proved highly flexible yet relatively hard to break open, a property that results from the selection of a lipid bilayer as a protective envelope. At the acidic pH of late-endosomes, the stiffness of the viruses decreased irreversibly to a value comparable to that of its lipid envelope alone. Interestingly, at the pH of early endosomes, the virus partially softened, which enhanced its fusion activity. Completed by fusion assays, our AFM study explains how low pH dismantles the flu virions, which has implications for both the viral budding and fusion mechanisms.

BP 14.4 Wed 10:30 H 1028

Local electric recordings of lipid bilayers supported on a microfabricated microporous device — •Theresa Kaufeld[1], Conrad Weichbrodt[2], Claudia Steinem[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut — [2]Fakultät für Chemie, Georg-August-Universität Göttingen, Germany

A powerful approach to study membrane proteins is the reconstitution in model membranes. Methods for artificial bilayer formation are e.g. membranes on a solid support, or the classical BLM. We have here focused on the formation of lipid bilayers on porous substrates combining the stability of solid supports and the accessibility of both sides of the bilayer of the classical BLM which is necessary for electrical recordings of membrane channels. Commercially available porous substrates however are typically not suitable for low-noise electrical experiments or for a combination with further manipulation techniques. We therefore designed a microporous substrate meeting several demands: (i) To

perform multiple experiments on one chip, we divided the device into arrays of pores with separate electrolyte compartments and integrated electrical connections. (ii) We designed a PDMS sample chamber in a way that allows us to perform electrical and fluorescence recordings at the same time and exchange solutions throughout the experiment. (iii) Large pores (1μm diameter) make it possible to address the bilayer with optically trapped particles. We probed bilayer formation by impedance spectroscopy and fluorescence microscopy. The electrical properties of the substrate and the pores as well as the function of inserted ion channels are measured by current recordings.

BP 14.5 Wed 10:45 H 1028

Rotational diffusion of micrometer-sized solid domains in lipid membranes — •Eugene P. Petrov, Rafayel Petrosyan, and Petra Schwille — Biophysics, BIOTEC, Technische Universität Dresden, Dresden, Germany

The Saffman–Delbrück approximation for translational and rotational diffusion of membrane inclusions [1] is widely used in biophysical studies to relate the inclusion size to the membrane viscosity, but is limited to small inclusion sizes, typically not exceeding 100 nanometers. Although an exact solution of the problem has been derived [2], its computational complexity precludes its practical applications. To overcome this difficulty, we recently developed a simple high-accuracy analytical approximation for the translational diffusion coefficient of a membrane inclusion [3]. Using a similar approach, here we develop a simple and accurate approximation for the rotational diffusion coefficient of a membrane inclusion valid for all combinations of the inclusion size and viscosities of the membrane and surrounding media. We demonstrate the utility of our approximation by using it to analyze our experimental data on rotational diffusion of gel-phase domains on giant unilamellar vesicles showing fluid–gel coexistence.

[1] P. G. Saffman and M. Delbrück, Proc. Natl. Acad. Sci. USA **72** (1975) 3111; P. G. Saffman, J. Fluid Mech. **73** (1976) 593
[2] B. D. Hughes, B. A. Pailthorpe, and L. R. White, J. Fluid Mech. **110** (1981) 349
[3] E. P. Petrov and P. Schwille, Biophys. J. **94** (2008) L41

BP 14.6 Wed 11:00 H 1028

Active membranes - photoswitching of azobenzene cholesterol in host lipid layers — Lars Jørgensen[1], Dordaneh Zargarani[2], Annika Elsen[3], Klaas Loger[3], Benjamin Runge[3], Christian Koops[3], Rainer Herges[2], Bridget Murphy[3], Olaf Magnussen[3], and •Beate Klösgen[1] — [1]University of Southern Denmark, Inst. f. Phys. Chem. and Pharm. - MEMPHYS, Odense, Denmark — [2]CAU Kiel, Otto Diels Inst.f. Org. Chem., Kiel, Germany — [3]CAU Kiel, Inst. for Exp. and Appl. Phys., Kiel, Germany

Phosphocholine (PC) lipid membranes exhibit a sequence of thermotropic lamellar states from solid to gel to liquid ordered (LO) to liquid disordered (LD). The LD membrane conformation is considered to be the biologically relevant phase. The inoculation of guest molecules into a host lipid layer may locally modify the initial state of the host; e.g., the incorporation of cholesterol passively induces the LO phase into a region that else how is in the LD state. The presence of a protein however may result in an active system fluctuating between the LO and the LD state, depending on the conformational changes of the protein as it conducts its functional work. We here present first results obtained from studies on an active membrane model system that consists of the photoswitchable variety of cholesterol, modified by an azobenzence group (azo-Ch), and a pure POPC host layer. Upon illumination, the azo-Ch can be reversibly switched (365nm * cis / 440 nm * trans). The functionalized cholesterol serves as a mesogen the conformation of which is coupled into the host system that in turn responds by acquiring an adjustment of its (local) structure upon switching.

15 min break

BP 14.7 Wed 11:30 H 1028

Critical and crossover phenomena in the phase separation of a two-component lipid membrane — Jens Ehrig[1], Eugene P. Petrov[1], Petra Schwille[1], and •Chiu Fan Lee[2] — [1]Biophysics, BIOTEC, Technische Universität Dresden, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Our recent lattice-based Monte Carlo simulations [1, 2] have shown that two-component lipid membranes are characterized by a non-trivial phase diagram and may show critical behaviour. To better understand our findings, we develop a theoretical description of the system by mapping the two-component membrane onto the Landau-Ginzburg model. This approach qualitatively reproduces the phase diagram obtained in our simulations and allows us to predict the values of the critical exponents. We compare these predictions with results of our simulations and find that, while very close to the critical temperature the system exhibits Ising universality, a crossover behaviour exhibiting non-Ising exponents takes place at higher temperatures. Experimental implications of these results will be discussed.

References: [1] J. Ehrig, E. P. Petrov, and P. Schwille, Biophys. J. **100**, 80 (2011). [2] J. Ehrig, E. P. Petrov, and P. Schwille, New J. Phys. **13**, 045019 (2011).

BP 14.8 Wed 11:45 H 1028

Dynamics of vesicle adhesion mediated by mobile lipid-anchored receptors and ligands — •Susanne F. Fenz[1], Ana-Suncana Smith[2], Rudolf Merkel[3], and Kheya Sengupta[4] — [1]LION, Leiden University, The Netherlands — [2]Institute of Theoretical Physics and Excellence Cluster, Engineering of advanced materials, University Erlangen-Nuernberg, Germany — [3]Institute of Complex Systems 7, Research Centre Juelich, Germany — [4]CNRS UPR 3118, Aix-Marseille Universite, France

Giant unilamellar vesicles (GUVs) adhering to supported lipid bilayers were used as a model system to mimic dynamics of receptor-ligand mediated cell-cell adhesion. We followed the adhesion process in real time by microinterferometry and determined the adhered area, as a function of time. The adhesion process exhibits three phases: nucleation, linear growth and saturation. We find that the onset of adhesion depends critically on the concentration of ligands in the GUV. The growth regime, on the other hand, is quite robust with respect to variations in receptor or ligand concentrations, but is conditioned by the tension in the GUV membrane. GUVs with a larger excess membrane area, exhibit higher fluctuations and form multiple nucleation centers while tense GUVs usually form only one nucleation center. Accordingly, the adhesion zone of tense GUVs grows slower. While the ligand concentration in the GUV membrane sets the timescale for the nucleation, the saturation time till a steady adhesion state is reached, depends on the receptor concentration on the bilayer. We give a qualitative discussion of these experimental results.

BP 14.9 Wed 12:00 H 1028

Effective Monte-Carlo simulations for the domain dynamics in membrane adhesion — •Markus Knoll[1], Timo Bihr[2], Udo Seifert[2], and Ana-Sunčana Smith[1] — [1]Institut für Theoretische Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg, Germany — [2]II. Institut für Theoretische Physik, Universität Stuttgart, Germany

The formation of domains in membrane adhesion arises from the competition of the nonspecific interactions with ligand-receptor binding. The latter deform the membrane and induce long-range effects between bonds. The dynamics of this process has been studied previously by Langevin simulations in which the membrane deformations and fluctuations, the diffusion of binders, and the specific ligand-receptor interactions have been treated explicitly as coupled stochastic processes (Reister et al. New J. Phys. 13, 025003, 2011). However, due to the limited system size, these simulations could not provide information on the domain morphology. By using the fact that the membrane shape and fluctuation profile can be calculated explicitly for an arbitrary distribution of bonds, we develop an effective Monte Carlo simulation scheme. Thereby, the membrane is not explicitly simulated but its influence is taken into account through a set of effective rates for the ligand-receptor (un)binding, the latter depending on the temporal local environment of the bond and the free binders. By using these rates we reproduce the equilibrium and the average domain growth dynamics observed in the Langevin simulations and at the same time, find several qualitatively different domain growth regimes.

BP 14.10 Wed 12:15 H 1028

Competing interactions for antimicrobial selectivity based on charge complementarity — Carola von Deuster and •Volker Knecht — Max Planck Institute of Colloids and Interfaces, 14424 Potsdam

An important property of antimicrobial peptides is their ability to discriminate bacterial from eucaryotic cells which is attributed to the difference in lipid composition of the outer leaflet of the plasma membrane between the two types of cells. Whereas eucaryotic cells usually expose zwitterionic lipids, procaryotic cells expose also anionic lipids

which bind the cationic antimicrobial peptides electrostatically. An example is the antimicrobial peptide NK-2 which is highly cationic and favors binding to anionic membranes. In the present study, the difference in binding affinity of NK-2 for palmitoyl-oleoyl-phosphatidyl-glycerol (POPG) and palmitoyl-oleoyl-phosphatidyl-choline (POPC) is studied using molecular dynamics simulations in conjunction with a coarse grained model and thermodynamic integration, by computing the change in free energy and its components upon the transfer of NK-2 from POPC to POPG. The transfer is indeed found to be highly favorable. Interestingly, the favorable contribution from the electrostatic interaction between the peptide and the anionic lipids is overcompensated by an unfavorable contribution from the change in lipid-cation interactions due to the release of counterions from the lipids. Overall the interaction between NK-2 and POPG is not determined by a single driving force but a subtle balance of competing interactions.

BP 14.11 Wed 12:30 H 1028

Two-component crystalline shells: invasion by a soft material — •Marc Emanuel, Andrey Cherstvy, and Gerhard Gompper — Institute of Complex Systems, ICS-2/IAS-2, Forschungszentrum Jülich, 52425 Jülich, Germany

We study the pattern formation of the ground state of two-component crystalline shells, with one component considerably softer than the other. Using approximate solutions of this nonlinear elasticity problem, we envisage the picture of invasion of the vesicle surface by the soft material. The energy minimum demands that the soft material occupies the regions of the surface with a maximal density of the elastic energy and stress. These are the 12 vertices and 30 ridges on the icosahedron that are preferred. Our theoretical results can be applicable to description of shape morphologies monitored for two-component elastic shells with very different bending and stretching moduli. From a biological perspective, the analysis can be relevant for formation of viral capsids from different protein capsomer subunits, in particular the shell of giant mimi viruses.

BP 14.12 Wed 12:45 H 1028

Dynamics of multiple vesicles under flow — •Badr Kaoui[1] and Jens Harting[1,2] — [1]Technische Universiteit Eindhoven, Postbus 513, 5600 MB Eindhoven, The Netherlands — [2]Institut für Computerphysik, Universität Stuttgart, Pfaffenwaldring 27, D-70569 Stuttgart, Germany

We study the dynamical behavior under flow of systems consisting of multiple vesicles. We are interested in suspensions of giant unilamellar vesicles (GUVs) and multilamellar vesicles (MLVs). To this purpose we developed a code combining the lattice Boltzmann method and the immersed boundary method. We present simulations of a single GUV under shear flow to validate our method and to investigate the effect of confinement on the GUV's dynamics [Kaoui, Harting and Misbah, PRE 83, 066319 (2011)]. Afterwards we demonstrate that our method is able to capture the physics of multiple vesicles. The effect of polydispersity, the size of the vesicles and the action of gravity on the dynamical response of multiple vesicles subjected to shear flow are investigated

BP 15: Proteins II

Time: Wednesday 15:00–17:30 Location: H 1058

Topical Talk BP 15.1 Wed 15:00 H 1058

Electron Paramagnetic Resonance in Protein Science — •Malte Drescher — Universität Konstanz, Konstanz, Germany

Electron paramagnetic resonance (EPR) spectroscopy has witnessed tremendous methodological and instrumental developments during the last two decades. These new methods have strong impact on various areas of chemistry, materials science, physics, and especially biophysics. With the advent of site-directed spin-labeling (SDSL) of proteins and DNA or RNA, EPR spectroscopy thus became a valuable technique for obtaining information on structure and dynamics of biomacromolecules.

Intrinsically disordered proteins (IDPs) form a unique protein category characterized by the absence of a well-defined structure and by remarkable conformational flexibility. SDSL EPR is amongst the most suitable methods to unravel their structure and dynamics.

This contribution summarizes methodological developments in the area of SDSL EPR and its applications in protein research. Recent results on the intrinsically disordered Parkinson's disease protein α-Synuclein illustrate that the method gains increasing attention in IDP research.

BP 15.2 Wed 15:30 H 1058

Probing the Ca2+ - switch of the neuronal Ca2+ sensor GCAP2 by time-resolved fluorescence spectroscopy — •Heiko Kollmann[1], Simon F. Becker[1], Javid Shirdel[1], Anna Osterndorp[2], Christoph Lienau[1], and Karl-Wilhelm Koch[2] — [1]Ultraschnelle Nano-Optik, Institut für Physik, Fakultät V, Universität Oldenburg, 26111 Oldenburg, Deutschland — [2]Biochemie, Institut für Biologie und Umweltwissenschaften, Fakultät V, Universität Oldenburg, 26111 Oldenburg, Deutschland

We report fluorescence lifetime and rotational anisotropy measurements of the fluorescence dye Alexa647 attached to the guanylate cyclase-activating protein 2 (GCAP2), an intracellular myristoylated calcium sensor protein operating in photoreceptor cells. By linking the dye to different protein regions critical for monitoring calcium-induced conformational changes, we could measure fluorescence lifetimes and rotational correlation times as a function of myristoylation, calcium and position of the attached dye, while keeping the GCAP2 protein operational. We observe distinct site-specific variations in the fluorescence dynamics when externally changing the protein conformation. A key feature of the dynamics of the protein-dye complex is the up- and down-movement of an α-helix that is situated between the two specific linking positions. Operation of this piston-like movement is triggered by the intracellular messenger calcium.

BP 15.3 Wed 15:45 H 1058

Photo-cycle dynamics of photo-activated adenylate cyclase (nPAC) from the amoeboflagellate *Naegleria gruberi* **NEG-M strain** — •Alfons Penzkofer[1], Manuela Stierl[2], Peter Hegemann[2], and Suneel Kateriya[3] — [1]Fakultät für Physik, Universität Regensburg, Universitätsstrasse 31, D-93053 Regensburg, Germany — [2]Institut für Biologie/Experimentelle Biophysik, Humboldt Universität zu Berlin, Invalidenstrasse 42, D-10115 Berlin, Germany — [3]Department of Biochemistry, University of Delhi South Campus, Benito Juarez Road, New Delhi 110021, India

nPAC comprises a BLUF domain (blue light sensor using flavin) and a cyclase homology domain (CHD). The nPAC gene was expressed heterologously in *E.coli* and the photo-dynamics of the nPAC protein was studied by optical absorption and fluorescence spectroscopy. Blue-light exposure of nPAC caused a typical BLUF-type photo-cycle behavior (spectral absorption red-shift, fluorescence quenching, absorption and fluorescence recovery in the dark). Additionally, time-delayed reversible photo-induced one-electron reduction of fully oxidized flavin (Fl_{ox}) to semi-reduced flavin ($FlH^{\cdot}$) occurred. Furthermore, photo-excitation of $FlH^{\cdot}$ caused irreversible electron transfer to fully reduced anionic flavin (FlH^{-}). A photo-induced electron transfer from Tyr to flavin ($Tyr^{\cdot +}$ - $Fl^{\cdot -}$ radical ion-pair formation) caused H-bond restructuring responsible for BLUF-type photo-cycling and permanent protein re-conformation enabling photo-induced flavin reduction by proton transfer. Some photo-degradation of Fl_{ox} to lumichrome was observed. A model of the photo-cycle dynamics of nPAC was developed.

BP 15.4 Wed 16:00 H 1058

A coarse-grained model for protein folding based on structural profiles — •Katrin Wolff[1], Michele Vendruscolo[2], and Markus Porto[3] — [1]SUPA, School of Physics & Astronomy, University of Edinburgh, UK — [2]Department of Chemistry, University of Cambridge, UK — [3]Institut für Theoretische Physik, Universität Köln

We present a coarse-grained protein model based on structural profiles and apply it to the study of protein free energy landscapes and folding trajectories. Our model's two main characteristics are a tube-like geometry to describe the self-avoidance effects of the polypeptide chain, and an energy function based on a one-dimensional structural representation [1]. The latter specifies the connectivity of a sequence in a given

conformation, so that the energy function, rather than favoring the formation of specific native pairwise contacts, promotes the establishment of a specific native connectivity for each amino acid. We illustrate our approach by applying the model to the folding of the villin headpiece domain to study its folding behavior and determine heat capacities, free energy landscapes and folding trajectories in various reaction coordinates [1,2]. The results closely resemble those found in extensive molecular dynamics studies and support the idea that coarse-grained models that solely rely on the self-avoidance and the connectivity of a polypeptide chain faithfully reproduce many aspects of the folding behaviour of proteins.

[1] K. Wolff, M. Vendruscolo, M. Porto, Phys. Rev. E **84**, 041934 (2011)
[2] K. Wolff, M. Vendruscolo, M. Porto, EPL **94**, 48005 (2011)

BP 15.5 Wed 16:15 H 1058

Dielectric Relaxation Spectroscopy of Ubiquitin by Poisson-Boltzmann-Monte Carlo Studies — •Stephan Kramer[1], Bartosz Kohnke[1], and Reiner Kree[2] — [1]Institut f. Numerische u. Angewandte Mathematik, Universität Göttingen, Lotzestrasse 16-18, D-37083 Göttingen — [2]Institut f. Theoretische Physik, Universität Göttingen, Friedrich-Hundt-Platz 1, D-37077 Göttingen

To reliably predict the function of ubiquitin it is necessary to know its conformational dynamics on all relevant time-scales. Due to its omnipresence in a multitude of key regulatory processes like molecular recognition or signal transduction these time-scales span from nano- to microseconds. Not all of them are accessible by NMR relaxation dispersion techniques which so far have been the standard way to measure conformational sampling. Only recently [1] dielectric relaxation spectroscopy (DRS) was introduced as further means to measure internal dynamics beyond the temporal resolution NMR is capable of. To get further insight into the measurement process we want to simulate DRS on a single molecule level using standard Monte Carlo techniques for the intramolecular motion. The properties of the ionic solvent and its interaction with the protein are assesed by solving the corresponding Poisson-Boltzmann equation by multigrid methods. For comparison with DRS experiments we compute dielectric loss spectra from the bulk dielectric moment to assess the the interconversion of different comformations of ubiquitin.

[1] David Ban et al. Kinetics of Conformational Sampling in Ubiquitin, Angew. Chem. Int. Ed. 2011, **50**, 11437-11440

BP 15.6 Wed 16:30 H 1058

Origin of decrease in potency against HIV-2 protease by HIV-1 protease inhibitors — •Parimal Kar and Volker Knecht — Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany

The acquired immune deficiency syndrome (AIDS) is caused by the human immunodeficiency virus (HIV) type 1 and 2 (HIV-1 and HIV-2). An important target for AIDS treatment is the use of HIV protease (PR) inhibitors preventing the replication of the virus. In this work, the popular molecular mechanics Poisson-Boltzmann surface area (MM-PBSA) method has been used to investigate the effectiveness of the HIV-1 PR inhibitors darunavir, GRL-06579A, and GRL-98065 against HIV-2 and HIV-1 protease. The affinity of the inhibitors for both HIV-1 and HIV-2 PR decreases in the order GRL-06579A < darunavir < GRL-98065, in accordance with experimental data. On the other hand, our results show that all these inhibitors bind less strongly to HIV-2 compared to HIV-1 protease, again in agreement with experimental findings. The decrease in binding affinity for HIV-2 relative to HIV-1 PR is found to arise from an increase in the energetic penalty from the desolvation of polar groups (DRV), or a decrease in the size of the electrostatic interactions between the inhibitor and the PR (GRL-06579A and GRL-98065). For GRL-98065, also a decrease in the magnitude of the van der Waals interactions contributes to the reduction in binding affinity. A detailed understanding of the molecular forces governing binding and drug resistance might assist in the design of efficient inhibitors against HIV-2 protease.

BP 15.7 Wed 16:45 H 1058

Dynamics of highly concentrated protein solutions around the denaturing transition — •Tilo Seydel[1], Marcus Hennig[1,2], Felix Roosen-Runge[2], Fajun Zhang[2], Stefan Zorn[2], Maximilian W.A. Skoda[3], Robert M.J. Jacobs[4], and Frank Schreiber[2] — [1]Institut Laue-Langevin, Grenoble, France — [2]Institut für Angewandte Physik, Universität Tübingen, Germany — [3]ISIS, RAL, Chilton, Didcot, UK — [4]CRL, University of Oxford, UK

We discuss the dynamics of highly concentrated aqueous protein solutions around the denaturing transition [1]. For the temperature range 280K $< T <$ 370K, the total apparent mean-squared displacement $\langle u^2 \rangle$ is recorded in solutions of bovine serum albumin by fixed-window neutron scattering. $\langle u^2 \rangle$ increases monotonically with T below and above denaturation, whereas it decreases strongly at the denaturing transition. This observation can be rationalized and modeled as a transition from a liquid protein solution to a gel-like state. Atomic vibrations as well as librations and diffusion of the entire protein contribute to $\langle u^2 \rangle$. The diffusion monitored by quasi-elastic neutron scattering [1,2] is consistent with a significant hindrance due to entanglement of the chains upon denaturing. The related pronounced decrease in $\langle u^2 \rangle$ is analytically separated. Thus, we extract the purely intramolecular dynamics around the denaturing transition of freely diffusing proteins. This analysis introduces a general concept, which is applicable to other colloid systems exhibiting both center-of-mass and internal dynamics [1].

[1] M. Hennig et al., Soft Matter, DOI:10.1039/c1sm06609a;
[2] F. Roosen-Runge et al., PNAS 2011, 108:11815

BP 15.8 Wed 17:00 H 1058

Correlates between Biophysical Dynamics and Sequence Evolution of Proteins — •Kay Hamacher — TU Darmstadt, 64287 Darmstadt, Germany

The evolution of proteins is shaped by two major evolutionary operators: mutation and selection. While entropy concepts from information theory reveal important patterns in the sequence space, the selective advantage of changes reveal themselves in the molecular phenotype. Therefore, to understand protein evolution in more detail, one needs to correlate the results of a sequence analysis with those from biophysical simulations of the expressed proteins. In this talk I will discuss several algorithmic improvements [1-3] and their applications to important proteins in medicinal physics/chemistry, namely the HIV1-protease and the acetylcholinesterase [4-6].

[1] K. Hamacher. Phys. Rev. E 84:016703, 2011
[2] K. Hamacher. J. Comp. Phys. 229:7309-7316, 2010
[3] M. Waechter, K. Hamacher, F. Hoffgaard, S. Widmer, M. Goesele. 9th Int. Conf. on Parallel Processing & Appl.Mathematics, 2011
[4] P. Boba, P. Weil, F. Hoffgaard, K. Hamacher. Springer Communications in Computer & Information Science 127:356-366, 2011
[5] S. Weißgraeber, F. Hoffgaard, K. Hamacher. Proteins 79(11):3144-3154, 2011
[6] K. Hamacher. Gene 422:30-36, 2008

BP 15.9 Wed 17:15 H 1058

Hierarchical Expansion of the Kinetic Energy Operator in Curvilinear Coordinates — Daniel Strobusch and •Christoph Scheurer — Lehrstuhl für Theoretische Chemie, TU München, Lichtenbergstr. 4, 85748 Garching, Germany

Multidimensional nonlinear IR experiments provide detailed dynamical information about peptides on short timescales. The interpretation of these spectra relies heavily on theoretical simulations of anharmonic vibrational systems. A powerful approach to calculate anharmonic vibrational spectra is the vibrational self-consistent field method (VSCF) and its configuration interaction extension (VCI).

Couplings and correlation between different modes can be reduced by employing curvilinear coordinates [1], which is of utmost importance for larger systems. However, these coordinates at the same time introduce a more complex form of the kinetic energy operator T, which has been known for a long time. Its evaluation is involved though, with coordinate dependent reduced masses and kinematic couplings.

A new systematic hierarchical expansion of T is presented, which allows us to judge the quality of simpler ad-hoc approximations [2]. VSCF and VCI calculations for small model systems were performed and the influence of different terms in the kinetic energy operator was studied in detail to allow for efficient approximations.

[1] M. Bounouar and Ch. Scheurer, *Chem. Phys.* 347 (2008), 194
[2] D. Strobusch and Ch. Scheurer, *J. Chem. Phys.* 135 (2011), 124102; *ibid.*, 144101

BP 16: Molecular Motors

Time: Wednesday 15:00–17:30 Location: H 1028

Invited Talk BP 16.1 Wed 15:00 H 1028

Molecular Crowding Creates Traffic Jams of Kinesin Motors On Microtubules — •Cecile Leduc[1,2], Kathrin Padberg-Gehle[3], Vladimír Varga[2], Dirk Helbing[4], Stefan Diez[2,5], and Jonathon Howard[2] — [1]LP2N-CNRS-U-Bordeaux 1 — [2]MPI-CBG, Dresden — [3]TU-Dresden — [4]ETH Zürich — [5]Technische Universität Dresden, B CUBE

Despite the crowdedness of the interior of cells, microtubule-based motor proteins are able to deliver cargoes rapidly and reliably throughout the cytoplasm. We hypothesize that motor proteins may be adapted to operate in crowded environments by having molecular properties that prevent them from forming traffic jams. To test this hypothesis, we reconstitute high-density traffic of purified kinesin-8 motor proteins along microtubules in a total-internal-reflection microscopy assay. We find that traffic jams, characterized by an abrupt increase in the density of motors with an associated abrupt decrease in motor speed, can even form in the absence of other obstructing proteins. To determine the molecular properties that lead to jamming, we altered the concentration of motors, their processivity and their rate of dissociation from microtubule ends. We find that traffic jams form when the motor density exceeds a critical value (density-induced jams) or when motor-dissociation from the microtubule ends is so slow that it results in a pile-up (bottleneck-induced jams). Through comparison of our experimental results with theoretical models and stochastic simulations, we characterize in detail under which conditions density- and bottleneck-induced traffic jams form or do not form.

Invited Talk BP 16.2 Wed 15:30 H 1028

Collective properties of molecular motors — •Jean-François Joanny — Institut Curie centre de recherche 26 rue d'Ulm 75248 Paris cedex 05

In many instances, in cells molecular motors such as myosins act in groups and show spectacular collective properties such as dynamic phase transitions, oscillations or bidirectional motion. We propose a "soft motor model" where the tail of the motors has a finite stiffness and is rigidly connected to the moving motor filament. The head of the motors is described by a classical two level system. The important parameter which governs the behavior of the motors is the pinning parameter which compares the maximum stiffness of the interaction potential to the stiffness of the motors.

At high enough activities, motor clusters can have two spontaneous velocities in opposite directions. If the number of motors in the cluster is not infinite, the motion reverses between the states corresponding to the two velocities over a finite reversal time. When the motors are rigidly bound to the motor filament, we calculate the reversal time as a first passage time between two non equilibrium states and show that it increases exponentially with the number of motors as found in simulations of Badoual et al.

Finally we discuss the case of molecular motors coupled via hydrodynamic interactions.

BP 16.3 Wed 16:00 H 1028

Forces and Fast Dynamics of Gliding Motors in Myxococcus Xanthus — •Fabian Czerwinski[1], Mingzhai Sun[1], Tam Mignot[2], and Joshua Shaevitz[1] — [1]Institute for Integrative Genomics, Princeton University, USA — [2]CNRS, Marseille, France

The gram-negative bacterium Myxococcus xanthus is an important model organism for studies of multicellular grouping as well as biofilm formation. Individual cells use a combination of twitching and gliding motility to form large, multicellular structures. We identified a new class of molecular motors that power gliding motility [1]. These motors, made of the AglQRS proteins, assemble within focal adhesion sites that link the bacterial cytoskeleton to the extracellular surroundings [2].

Our goal is to understand control and cooperativity of these motor complexes within single cells. For this purpose, we combined optical tweezers, fluorescence microscopy, and real-time tracking of attached marker beads. This allows us to assess the step-like activity of motors embedded in the adhesion complexes at high temporal and spacial resolution. We found motor function correlated to the helical pitch of the bacterial cytoskeleton. We further measured motor stalling forces and the time delay between single motor responses to various cell-motility regulators. Measurements of the gliding force of whole cells will complement our results. Our experiments quantitatively explain how the AglRQS motors drive cell gliding and the formation of multicellular structures.

[1] Sun et al., PNAS(108)7559, 2011. [2] Mignot et al., Science(315)853, 2007.

BP 16.4 Wed 16:15 H 1028

Altering the Native Neck-Linker Length Changes Processivity of Kinesin-5 Motor Proteins — •André Düselder[1], Christina Thiede[1], Stefanie Kramer[1], Stefan Lakämper[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]current address: Institute for Mechanical Systems, D-MAVT, ETH Zurich, Switzerland

Processivity for kinesins relies on communication between the two heads of a dimeric molecule, such that binding strictly alternates. The main communicating elements are believed to be the neck linkers (NL). One proposed mechanism for the coordination is the transmission of intra-molecular stress through the NL, a mechanism dubbed front- or rear-head gating. It is believed that the efficiency of gating should dependent on the length of the NL. Recent studies have presented support for a simple model in which the length of the NL directly controls the degree of processivity. Here, we have analyzed the motility of a set of six motor constructs, based on a previously published Kinesin-1/Kinesin-5 chimera, Eg5Kin, in which we have now varied the length of the NL, starting from 13 amino acids up to the native 18 amino acids of Eg5. We found, surprisingly, that neither velocity nor force generation depended on the NL length. We also found that even the construct with the shortest NL was highly processive, and that the longest NL (17 and 18 amino acids) allowed run lengths twice those of the other constructs. This finding challenges the simple model equating a short NL with tight communication, but suggests that different kinesins might be optimized for different NL lengths.

BP 16.5 Wed 16:30 H 1028

Distinct Transport Regimes for Two Elastically Coupled Molecular Motors — •Florian Berger, Corina Keller, Stefan Klumpp, and Reinhard Lipowsky — Theory & Bio-Systems, Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

Intracellular transport of cargos is mainly achieved by the cooperative action of molecular motors, which pull the cargos along cytoskeletal filaments. These motors are elastically coupled, which influences the motors' velocity and/or enhances their unbinding from the filament. We show theoretically that interference between two elastically coupled motors leads, in general, to four distinct transport regimes characterized by different effects on the mean velocity and/or the binding time. To gain an intuitive insight in the emergence of these transport regimes, we compare characteristic time scales for the strain force generation. These time scale arguments allow us to predict the transport regimes for different pairs of identical motors. In addition to a weak coupling regime, pairs of kinesin motors and pairs of dynein motors are found to exhibit a strong coupling and an enhanced unbinding regime, whereas pairs of myosin motors are predicted to attain a reduced velocity regime. All of the predicted regimes can be explored experimentally by varying the elastic coupling strength.

BP 16.6 Wed 16:45 H 1028

Direct observation of single dyneins diffusing and interacting with microtubules in vivo — •Nenad Pavin[1,2], Vaishnavi Ananthanarayanan[1], Martin Schattat[1], Sven Vogel[1], Alexander Krull[1], and Iva Tolic-Norrelykke[1] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia

Cytoplasmic dynein is a motor protein that exerts force on microtubules and in doing so, drives a myriad of intracellular activities from mitotic spindle positioning to chromosome movements in meiotic prophase. These forces require dynein to be anchored, where the anchoring sites are typically found at the cell cortex. The key question is which mechanism single dyneins use to accumulate at sites where they can generate large collective forces. Here we directly observe single dyneins in fission yeast, which allowed us to identify key steps of

the dynein binding process: (i) from the cytoplasm to the microtubule, and (ii) from the microtubule to the cortical anchors. We uncovered that dyneins on the microtubule move, surprisingly, either in a diffusive or a directed manner, where the switch from diffusion to directed movement occurs upon binding of dynein to the cortex. This dual behavior of dynein on the microtubule, together with the two steps of binding, constitute the mechanism how dynein finds cortical anchors in order to generate large-scale movements in the cell.

BP 16.7 Wed 17:00 H 1028

Transcriptional proofreading in dense RNA Polymerase traffic — •Mamata Sahoo and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

The correction of errors during transcription involves the diffusive backward translocation (backtracking) of RNA polymerases (RNAPs) on the DNA. A trailing RNAP on the same template can interfere with backtracking as it progressively restricts the space that is available for backward translocation and thereby ratchets the backtracked RNAP forward. We analyze the resulting negative impact on proofreading theoretically using a lattice model of transcription introduced earlier [1]. Our detail analysis indicates that the efficiency of error correction is essentially determined by the rate for the initial backtracking step, while a high transcript cleavage rate ensures that the correction mechanism remains efficient at high transcription rates [2]. Our analysis can also be applied to cases with transcription-translation coupling where the leading ribosome on the transcript assumes the role of the trailing RNAP.

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

[2] M. Sahoo and S. Klumpp, Euro. Phys. Lett. (in press) (2011).

BP 16.8 Wed 17:15 H 1028

Microtubules search for lost kinetochores by pivoting around the spindle pole — •Damien Ramunno-Johnson[1], Iana Kalinina[1], Amitabha Nandi[2], Alexander Krull[1], Benjamin Lindner[2], Nenad Pavin[1,3], and Iva Tolic-Norrelykke[1] — [1]MPI-CBG, Dresden, Germany — [2]MPI-PKS, Dresden, Germany — [3]University of Zagreb, Zagreb, Croatia

For a mother cell to divide its genetic material equally between the two daughter cells, the chromosomes have to attach to microtubules, which will pull them apart. The linkers between chromosomes and microtubules are kinetochores, protein complexes on the chromosome. The pioneering idea explaining how microtubules find kinetochores, termed "search-and-capture," states that microtubules grow radially from a centrosome in all directions and shrink back, thereby exploring the intracellular space and by chance hitting and capturing the kinetochores. In fission yeast, kinetochore capture by microtubules can be observed when kinetochores are lost in the nucleoplasm, which can be induced by spindle disassembly during metaphase. It is, however, unknown how microtubules find lost kinetochores. We observed that lost kinetochores are captured by microtubules pivoting around the spindle pole body, instead of extending towards the kinetochores. By introducing a theoretical model, we show that the observed random movement of microtubules is sufficient to explain the process of kinetochore capture. We thus reveal a mechanism where microtubules explore space by pivoting, as they search for intracellular targets.

BP 17: Posters: Physics of Cells

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

BP 17.1 Wed 17:30 Poster A

Complex flow patterns of microbial populations growing in constrained geometries — •Hedvika Toncrova and Oskar Hallatschek — Max Planck Research Group for Biophysics and Evolutionary Dynamics, MPI for Dynamics and Self-Organization, Göttingen, Germany

During biofilm development cells have to push away their surroundings to free space for their own growth and that of their offspring. Although a lot of interesting physics and biology is involved in this complex process, it remains poorly understood.

In an attempt to shed light on the mechanics of biofilm growth, we have measured the forces and flows that microbial populations generate when their growth is limited by space rather than nutrients. Using small populations of yeast cells confined in a microfluidic device we have measured pressures of approximately 0.5 MPa, generated purely by their growth and division. In addition, we have observed that imperfect caging of the cells leads to flows characteristic of granular media just above the jamming transition (succession of elastic and plastic events). We relate our measurements to a recently proposed theory of a homeostatic pressure arising in collective tissue dynamics.

BP 17.2 Wed 17:30 Poster A

Tracking and Simulation of Human T-Cells' Motility — •Marc Neef[1], Hélène Lyrmann[2], Carsten Kummerow[2], Markus Hoth[2], and Karsten Kruse[1] — [1]Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken — [2]Biophysik, Universität des Saarlandes, 66421 Homburg

As a part of cell-mediated immunity, killer T-cells detect infected or cancerous cells and trigger their programmed cell death. It has been shown, that T-cells perform an active, self-propelled random motion. However, the characteristics of this motion on large scales are unknown. Since the effectiveness of the immune response depends on how many defect cells can be eliminated within a certain period of time, we investigate the search mechanism of killer T-cells. To this end, we observe primary human T-cells under different conditions by light microscopy and analyse the motion using tracking algorithms and statistic methods. To analyse the data, we use a simple phenomenological stochastic model, where the motion of a single cell is caused by active forces of several pseudopodia. Comparing experimental and simulated data, we connect macroscopic parameters like motility and persistence of the cells' motion to microscopic variables like the (mean) number of active pseudopodia or the duration of their activity, and we determine how these values change under external signals.

BP 17.3 Wed 17:30 Poster A

The Mechanics of Cellular Compartmentalization and Its Impact on Tumor Spreading — •Steve Pawlizak, Anatol Fritsch, Mareike Zink, and Josef A. Käs — Institute for Experimental Physics I, Soft Matter Physics Division, University of Leipzig, Germany

Compartmentalization is a fundamental process of cellular organization that occurs in particular during embryonic development. A simple model system demonstrating compartmentalization involves mixing together two different populations of suspended cells. After a certain time, this mixture will eventually segregate into two phases, whereas mixtures of the same cell type will not. The *differential adhesion hypothesis* by Malcolm S. Steinberg (1960s) explains this organization behavior by differences in surface tension and adhesiveness of the interacting cells. To understand to which extent the same physical principles affect tumor growth and spreading between compartments [1], we investigate cellular mechanical properties and interactions of various cell types, such as healthy and cancerous breast cell lines of different malignancy as well as primary cells from human cervix carcinoma. To this end, a set of techniques is applied: The *Optical Stretcher* is used for whole cell rheology. Cell-cell-adhesion forces are directly measured with a modified *atomic force microscope*. 3D segregation experiments are employed with a newly developed setup for long-term observation of *droplet cultures*. The combination of these techniques will help to clarify the role of cellular adhesion for tumor spreading.

[1] A. Fritsch et al., Nature Physics **6** (10): 730–732 (2010)

BP 17.4 Wed 17:30 Poster A

Three-dimensional obstacles for bacterial surface motility — •Claudia Meel, Nadzeya Kouzel, Enno Oldewurtel, and Berenike Maier — Biozentrum, University of Cologne

Many bacterial species live at surfaces. On the one hand they must attach firmly to avoid clearance but on the other hand they must be motile to spread. Many species have solved this problem by using polymers called type IV pili. They use pili as grappling hooks for pulling themselves over surfaces. Here we addressed the question how moving bacteria behave when they encounter microscopic elevations at the surface. We used two different species with very different lifestyles and morphologies, namely both the round human pathogen Neisseria

gonorrhoeae and the rod-shaped soil-dweller Myxococcus xanthus. We showed microscopic elevations guide bacterial movement, i.e. bacteria preferentially move in groves whose dimensions are comparable to the size of the bacteria. Although both species sense the topology we propose that they derive different benefits from this ability in agreement with their different lifestyles.

BP 17.5 Wed 17:30 Poster A

Mechanical properties of filopodia quantified by photonic force microscopy — •Felix Kohler and Alexander Rohrbach — University of Freiburg, Germany

Filopodia are highly dynamic protrusions of the cell surface that are filled with tight bundles of actin. They can extend and retract on a timescale of seconds to minutes. We use photonic force microscopy (PFM) to investigate the mechanical concepts of the filopodial retraction. An optically trapped bead is attached to a tip of a filopodium. During retraction the motion of this bead is tracked interferometrically in 3D with nanometer precision at a microsecond timescale. We have measured F-actin dependent steps inside living cells during filopodial retraction likely belonging to actin-based molecular motors [1]. The high forces a filopodium can exceed as well as the retraction dynamics indicate that coordinated molecular motor movement controls filopodial mechanics. Experimental results are shown together with a Morkov chain model, which describes the cooperative behavior of molecular motors in biological systems like filopodia.

[1] Kress, H. et al.,"Filopodia act as phagocytic tentacles and pull with discrete steps and a load-dependent velocity", pnas ,Vol.104, 2007, 11633-11638

BP 17.6 Wed 17:30 Poster A

Different elasticity of left-ventricular and right-ventricular fibroblasts of DCM-patients — •Michael Glaubitz[1], Stephan Block[1], Jeannine Witte[2], Kay E. Gottschalk[3], Stephan B. Felix[2], Alexander Riad[2], and Christiane A. Helm[4] — [1]ZIK HIKE - Zentrum für Innovationskompetenz Humorale Immunreaktionen bei kardiovaskulären Erkrankungen, D-17487 Greifswald, Germany — [2]Universitätsmedizin Greifswald, Klinik und Poliklinik für Innere Medizin B, 17475 Greifswald — [3]Institut für Experimentelle Physik, Universität Ulm, D-89069 Ulm — [4]Institut für Physik, Ernst-Moritz-Arndt Universität, D-17487 Greifswald, Germany

Dilated cardiomyopathy (DCM) is a significant type of heart failure leading to increased morbidity and mortality. Left ventricular fibrosis and dilation are hallmarks of this disease. Cardiac fibroblasts (CF) are the main source for matrix regulating mediators in the heart, but their role in DCM is largely unknown. Using a colloidal particle as an AFM probe, we measure the cell elasticity of human cardiac fibroblasts derived from right and left ventricular endomyocardial biopsies. Spatially resolved measurements reveal that the elastic modulus is inhomogeneously distributed over a fibroblast, but shows less variation in the vicinity of the nucleus. By measuring at this position for several fibroblasts (of a certain patient) we observe a lognormal elastic modulus distribution. Interestingly, cells extracted from the left ventricle show generally a smaller average elastic modulus than the ones from the right side. Our findings indicate a contribution of the cellular mechanical properties to the etiology of DCM.

BP 17.7 Wed 17:30 Poster A

Microfluidic Shear Alters Network Dynamics in Living Cells — •Jens-Friedrich Nolting and Sarah Köster — Institute for X-Ray Physics and CRC Physics, University of Göttingen, Germany

Intermediate filaments are a major component of the eukaryotic cytoskeleton along with microtubules and microfilaments. They play a key role in cell mechanics, providing cells with compliance to small deformations and reinforcing them when large stresses are applied. Here, we present a study of fluorescent keratin intermediate filament networks in living cells with respect to their behavior in the presence of external forces. We expose the cells to controlled shear forces applied by microfluidic methods and investigate the response of the keratin network *in situ*. We track the nodes in the keratin network to deduce the dynamic behavior of the network as a function of the external shear forces. The time tracks show that the fluctuations dampen upon the application of flow. We then characterize the network dynamics by looking at the mean square displacements over time which grants access to effective diffusion constants. We find that the effective diffusion constant is reduced under shear flow conditions but seems to recover after a certain time. This may be a result of an adjustment of the cell as a response to the external shear forces.

BP 17.8 Wed 17:30 Poster A

Photo-switchable Cell Adhesion on Functionalized Nanostructures — •Laith Kadem[1], Michelle Holz[2], Saskia Viebig[1], Rainer Herges[2], and Christine Selhuber-Unkel[1] — [1]Institute for Materials Science, Technical Faculty, CAU Kiel — [2]Institute for Organic Chemistry, CAU Kiel

Cell adhesion is a crucial process, which plays an important role in a number of cell activities such as cell motility, differentiation and apoptosis. We aim at developing surfaces where light-induced switchable cell adhesion is feasible. On the one hand, we are preparing surfaces with photo-switchable hydrophobicity by using functionalized azobenzene molecules. On the other hand, we are using azobenzene molecules that are functionalized with RGD peptides in order to mediate specific cell adhesion to surfaces through integrins. Azobenzene molecules are reversible photo-induced isomerization units, so that the adhesion of cells can be photo-switched in a spatially and temporally defined fashion by UV and white light, respectively. The main adhesion platform for our adhesion experiments are nanostructured surfaces that have been fabricated using block-copolymer micelle nanolithography and that are functionalized with the azobenzene molecules. Here we show first results of cell adhesion on our photoswitchable surfaces.

BP 17.9 Wed 17:30 Poster A

Analysis of cell-substrate impedance fluctuations induced by motile cells — •Helmar Leonhardt[1], Carsten Beta[2], and Matthias Gerhardt[3] — [1]Universität Potsdam, Mathematisch-Naturwissenschaftliche Fakultät / Institut für Physik und Astronomie, Raum 2.28. 1.006 — [2]Raum 2.28 1.003 — [3]Raum 2.28 1.006

Electric cell-substrate impedance sensing (ECIS) measures the frequency dependent impedance of a small gold electrode to ac current flow. Cells on the electrode restrict the current path, forcing it to flow under the cells and out between neighboring cells or through the cell membranes. We have applied ECIS to the social amoebae Dictyostelium discoideum during starvation conditions, where chemotactic cells aggregate in streams to clusters. The chemotactic motility of Dictyostelium cells, requiring formation and retraction of lamellipodia, is connected with cyclic periodicities in changes of cell shape and size, which lead to distinct oscillations in the impedance signal due to waves of the chemoattractant cAMP, which are emitted from pacemaker centers and propagate through the population, thereby synchronizing the movement of neighboring cells. We investigated the role of actin disrupting drugs (Latrunculin A) on the fluctuations in the impedance signal and complemented our population data with systematic single cell recordings.

BP 17.10 Wed 17:30 Poster A

Cell migration on different substrates - An investigation with optical microscopy under homogeneous conditions — •Thorsten Robel[1], Daniele Martini[1], Michael Beil[2], and Othmar Marti[1] — [1]Institute for Experimental Physics, Ulm University, 89081 Ulm, Germany — [2]Internal Medicine I,Ulm University, 89081 Ulm, Germany

In this poster we discuss the influence of the substrate interaction of pancreatic carcinoma cells (line Panc-1).

The physical and chemical properties of different substrates can influence the cell motility. Over night time lapse video microscopy observations of cultivated cells were used to measure the Mean Square Displacement of the cells as well as their mean velocity. The set-up was based on an inverted Leica microscope (Leica Dmirb). An incubation chamber was used to regulate temperature, CO_2-concentration and humidity to assure identical environmental conditions for the cells. From time lapse images the trajectories of a subset of all cells were extracted with the program ImageJ.

First measurements to compare the motility of Panc-1 cells with different other cell lines were accomplished.

These observations revealed different motilities regarding cell type and substrate.

BP 17.11 Wed 17:30 Poster A

A real-time adaptive exposure system for studies of eukaryotic chemotaxis — •Alexander Anielski and Carsten Beta — Biological Physics, Universität Potsdam, Germany

The aim of our project is to quantify the chemotactic motion of eukaryotic cells. In particular, we developed a setup that allows us to separately address the dependencies of the chemotactic motion on the average background concentration and on the gradient steepness. Also,

the role of spatial versus temporal sensing can be analyzed with this setup. Our method is based on compensating the cell movement by automated motion of the microscope stage. To achieve this, a software grabs frames from a camera, recognize the cell position, and moves it to the center of the field of view by automatically adapting the position of the microscope stage. To generate a well definied gradient signal, caged compounds in a fluid flow are used in combination with a computer controlled switchable gradient mask (flow photolysis). We exemplify our method with chemotactic cells of the social amoeba Dictyostelium discodideum. The motion and fluorescence data will be used to test competing models of eukaryotic chemotaxis.

BP 17.12 Wed 17:30 Poster A

Ferromagnetic guidance of paramagnetic microspheres and magnetically marked cells — •Thorsten Grassmann[1], Yuri Koval[1], Ben Fabry[2], and Paul Müller[1] — [1]Dpt. of Physics and Interdisciplinary Center for Molecular Materials, Universität Erlangen-Nürnberg, Germany — [2]Dpt. of Physics and Center for Medical Physics and Technology, Universität Erlangen-Nürnberg, Germany

We investigated thin film stripes of a ferromagnetic Permendur alloy with a high saturation magnetization aligned in a zig-zag geometry. This setup shows highly localized and permanent magnetic field gradients, both attractive and repulsive, located at the stripes' kinks. External out-of-plane magnetic fields are used to simultaneously alter depth and height of the magnetic field gradients. An external in-plane magnetic field is used to create an asymmetry in the gradient, selecting a preferred direction. This device allows the controlled motion of paramagnetic microspheres and magnetically marked biological cells along the stripes in a liquid environment, floating from kink to kink. The force acting on the paramagnets shows an inverse square-law behavior. A hardware setup with a computer-controlled vector magnet for programmable control of the field gradients and a video camera for measuring the microspheres' positions and speed was developed. The forces acting on the microspheres were measured directly via Stokes' drag. The possibility to move single living biological entities has been verified using living mouse liver cells incorporating magnetic microspheres. It is shown that the acting forces are in a range useful for rheological studies of living cells.

BP 17.13 Wed 17:30 Poster A

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

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

To analyze the effect of substrate stiffness and correlate it with integrin expression, we performed experiments on cells growing on differently polydimethylsiloxane (PDMS). We then analyzed cell proliferation and morphology of the cells on the different substrates. We show that the substrate stiffness has an integrin subtype dependent influence on cell proliferation and cell shape.

BP 17.14 Wed 17:30 Poster A

Measuring local elasticity and membrane tension on differentiating cells — •Paula Sanchez[1], Kai Bodensiek[1], Schanila Nawaz[2], Mikael Simons[2], and Iwan Schaap[1] — [1]III Physikalisches Institut, Faculty of Physics, Georg-August Universität, Göttingen, Germany — [2]Max-Planck Institute for Experimental Medicine, Göttingen, Germany

The myelin sheet is a specialized membrane structure that allows rapid conduction of nerve impulses and it is essential for the integrity of the axon. In the central nervous system it is produced by differentiation of oligodendrocytes in a multistep process accompanied by dramatic changes in cell morphology. Because cell shape is controlled by cellular mechanics we want to study the mechanical properties of oligodendrocytes in order to better understand the mechanics of cell differentiation. We are using a combination of atomic force microscopy and vertical laser trapping to quantify the spatial distribution of elasticity and membrane tension over the whole cell. With our results we aim to provide links between the mechanical development of these cells and changes in their physiology and morphology.

BP 17.15 Wed 17:30 Poster A

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

Tissue cells communicate with their surroundings biochemically, but at the same time also sense the mechanics of their micro-environment. Cells can "feel" mechanical stress by generating contractile forces through their acto-myosin cytoskeleton and use these forces to actively probe the mechanical response of their extra-cellular matrix.

With a dual optical trap setup we have performed force measurements on cells suspended between two fibronectin-coated beads to ensure focal-contacts. We analyzed the correlated fluctuations of the beads with high spatial and temporal resolution by laser interferometry. Using a combination of active probing and passive recording of fluctuations (microrheology), we can simultaneously determine the (non-thermal) forces generated by the cells and quantitate their viscoelastic response properties.

The amount of contractile force transmitted to the outside varied with the trap stiffness. To elucidate the contributions of different mechanical elements to active and passive mechanical properties of the cell we employ biochemical perturbations and fluorescence microscopy allows us to visualize the distribution of cytoskeletal proteins in the cell.

BP 17.16 Wed 17:30 Poster A

Device for mechanical stretching of adherent cells and application to pancreatic carcinoma cells (type:PANC-1) — •Patrick Paul, Tobias Paust, and Othmar Marti — Institute for Experimental Physics, Ulm University, Ulm, Germany

The structural and mechanical properties of cells are determined in part by the properties of their cytoskeleton systems. Healthy cells and cancerous cells were found to differ in their viscoelastic behavior. Softer cells were found to migrate faster through narrow channels.

The quasi-static viscoelastic behavior of cells is investigated with a deformable substrate. The stress and stress rate of the substrate is controlled. The response of the adherent cells is monitored by optical microscopy. Our apparatus contains an opto-mechanical feedback loop which centers the cell under investigation at the optical axis of the microscope. We report on the performance of our stretching device and we show first measurements with PANC-1 cells.

BP 17.17 Wed 17:30 Poster A

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

Cytokinesis, the process of physically dividing the cell at the end of mitosis, is achieved through the regulated variations of forces within the cell. A key player in this process is the cell cortex, a thin layer of actin filaments and myosin molecular motors. Recently, Sedzinski *et al.* have introduced a mathematical model to describe the role of the cell cortex in cytokinesis [1]. The model has shown that one striking consequence of the contractile behavior of the cell cortex is the appearance of cell oscillations: because these oscillations can be seen as perturbations of the cellular shape, they give a window on important parameters controlling cell mechanics. Here we use this experimental assay to focus more particularly on the role of the lipid bilayer membrane in cytokinesis. The membrane is attached to the cell cortex and it has to mechanically balance the difference between extracellular and intracellular pressure. Under simple hypothesis on the membrane mechanical behavior and its area regulation by the cell, we investigate how its interaction with the cortex influences cell shape. Interestingly, preliminary results suggest that the membrane could play an important role in maintaining the cell shape stability.

[1] Sedzinski, J. *et al.* Polar actomyosin contractility destabilizes the position of the cytokinetic furrow. *Nature* **476**, 462-466 (2011).

BP 17.18 Wed 17:30 Poster A

Stochastic modeling of malaria parasite motility — •Thorsten Erdmann[1], Yin Cai[2], and Ulrich S. Schwarz[1,2] — [1]Institute of Theoretical Physics, Heidelberg University, Heidelberg, Germany — [2]BioQuant, Heidelberg University, Heidelberg, Germany

During its lifecycle, the unicellular malaria parasite from the *Plasmodium* family alternates between insect and vertebrate hosts. A critical step of its lifecycle is the entry of *Plasmodium* sporozoites into blood vessels after injection into the skin of a vertebrate host during a mosquito bite. *In vitro* experiments on two-dimensional substrates with microfabricated arrays of obstacles reveal complex motion patterns resembling the ones observed *in vivo* in the skin, with long stretches of circular or linear motion separated by abrupt changes of direction. We model the sporozoite motion using a stochastic glider model, in which the rod-like glider describes a circular path when unperturbed, but changes direction randomly upon collisions with an obstacle. This model leads to patterns of motion similar to those observed in experiment and describes well the average displacement as function of time. On the sub-second time-scale, sporozoites seem to move in a stick-slip-like fashion. In order to assess short time-scales, we introduce a model for the propulsion mechanism of sporozoites, in which the sporozoite body attaches to a substrate via specialized binding molecules, which are then displaced by small groups of non-processive motors.

BP 17.19 Wed 17:30 Poster A

Mechanics of cellular materials: Adhesion, disease and nonlinearities - a rheometric approach — •Mathias Sander and Albrecht Ott — Universität des Saarlandes

Biological cells are capable of sensing mechanical cues from their environment and they respond to them. The cell reactions range from cell adhesion, shape changes, motility, proliferation up to an adaption of mechanical properties (kinematic hardening, stress stiffening, fluidization) and even to gene expression modifications. All these abilities are essential for various biological processes among them tissue formation, wound healing or cancer metastasis. Investigation of cell mechanical properties has been driven for decades with various methods, however, it is still poorly understood, due to the complexity and the huge variety of cell behavior. In our experiments we investigate the nonlinearity of the cell mechanical response characterized by means of Fourier-Transform-Rheology. For this purpose we have developed a rheometric cell monolayer shear apparatus consisting of a commercial rheometer modified to accomodate the needs of biological cells. We also study cell adhesion, here on inorganic AL/Al2O3- nanowire-substrates, using the same technique. We also present data on tissue mechanics, namely the impact of atherosclerotic lesions on the mechanical properties of aortic tissue.

BP 17.20 Wed 17:30 Poster A

Influence of Extracellular Matrix Topography on Cell Motility — •Mari Gorelashvili and Doris Heinrich — Physics of Cell Dynamics Group, Physics Department and Center for Nanoscience CeNS, Ludwig-Maximilians Universität München, Geschwister-Scholl-Platz 1, 80539, Munich, Germany

Cell migration is governed by intracellular signaling in response to external stimuli. Recent advances have been made in investigating cell motility on flat 2D surfaces, but our understanding of basic cellular motility in 3D extracellular matrix (ECM) is less progressed.

Here, we investigate the influence of micro-scale surface topography on the amoeboid motility of D. discoideum. We aim at predicting and controlling cellular migration in well-defined pillar arrays by disturbing and eliminating key proteins in the cells. By using our home-made local mean-squared displacement algorithm we extract a time-resolved motility characterization.

Our results reveal that D. discoideum spontaneous migration consists of alternating phases of directed (dir) runs and random (rm) migration modes. Contrary to expectations, dir-runs are of lower frequency and of higher velocities in pillar array. Further, pillar network geometry is reflected in the migration angle distribution of wild type cells but not of cells lacking microtubules [1].

[1] D. Arcizet S. Capito, M. Gorelashvili, C. Leonhardt, M. Vollmer, S. Youssef, S. Rappl and D. Heinrich, Soft Matter, 2011, DOI: 10.1039/c1sm05615h

BP 17.21 Wed 17:30 Poster A

Three-dimensional templates produced by direct laser writing for dental implant surface optimization — •Judith Katharina Hohmann[1], Erik Waller[1], Rainer Wittig[2], Rudolf Steiner[2], and Georg von Freymann[1] — [1]Physics department and research center OPTIMAS, University of Kaiserslautern — [2]Institute for Laser Technologies in Medicine and Measurement Technology (ILM) at the University of Ulm

Dental implant failure occurs in up to eight percent, usually resulting from deficit osseointegration or insufficient adaptation of soft tissue. Many approaches to improve dental implant acceptance deal with chemical and/or physical surface treatments (e.g. acid-etching, sand blasting) leading to randomly shaped two-dimensional patterns. These patterns lack true three-dimensional motifs with defined sizes. In general, results generated in two-dimensional systems can hardly be transferred to natural, three-dimensional systems.

Our aim is to understand the relation between various three-dimensional candidate structures and differentiation of osteoblastic cells and to use these results to generate implant surfaces which promote osseointegration.

Structures are produced by direct laser writing and coated with titanium dioxide. Smallest feature sizes realized yet are 330 nm, allowing to design and generate structures on both nano- and micrometer scale. To observe cellular behavior, osteosarcoma cells are applied to the structures in order to test growth, morphology, adhesion and differentiation via fluorescence and staining techniques.

BP 17.22 Wed 17:30 Poster A

When Folding does not Imply Pullout: Different Modes of Growth Cone Collapse in NG 108-15 Cells — Philipp Rauch[1], •Paul Heine[1], Barbara Göttgens[2], and Josef Käs[1] — [1]Institute of Experimental Physics I, University of Leipzig, Germany — [2]Institute of Biology, University of Leipzig, Germany

Neuronal pathfinding is crucial for the proper wiring of the central and peripheral nervous system. A growth cone at the tip of every neurite detects and follows multiple guidance cues initiating directional changes, outgrowth, or neurite retraction. However, when focusing on cytoskeletal retraction mechanisms it is rarely considered that even partial retractions of the neurite appear excessive in cases where outgrowth is merely supposed to locally cease or stall.

We evaluated cytoskeletal dynamics of transiently transfected NG108-15 growth cones using fluorescence time lapse microscopy and could identify an alternative mode of growth cone collapse leading to a controlled halt of neurite extension without retraction. Our findings show that lateral movement and folding of actin bundles confine microtubule extension and limit their expansion. This process stands in stark contrast to neurite retraction where collapsing actin structures buckle microtubules. The flexure of these stiff polymers most likely generates considerable forces on the remaining adhesion sites, which inevitably leads to their disintegration and subsequent neurite retraction. Altogether the described mechanisms elucidate neuronal growth regulation by closing the gap between full retraction and small scale fluctuations.

BP 17.23 Wed 17:30 Poster A

Mitotic Spindle Positioning by Cortical Force Generators — •Rui Ma[1,2], Nenad Pavin[3], Liedewij Laan[4], Marileen Dogterom[4], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems (MPI-PKS), Dresden, Germany — [2]Institute for Advanced Study Tsinghua University, Beijing, China — [3]Department of Physics, Faculty of Science, University of Zagreb, Zagreb 10002, Croatia — [4]FOM Institute for Atomic and Molecular Physics (AMOLF), Science Park 104, 1098 XG Amsterdam, the Netherlands

In animal cells, the plane of cell division is determined by the position of the mitotic spindle. During asymmetric cell division of the C. elegans embryo the mitotic spindle is displaced away from the geometric cell center. This displacement results from the asymmetric activation of cortical force generators which pull on astral microtubules. We present a physical description of the interplay of pushing and pulling forces on astral microtubules in a three dimensional geometry. The Key element in this description is the fact that growing microtubules can slide along the cell cortex thus experiencing a pushing force. Once they are attached to a force generator, they would experience a pulling force before undergoing disassembly. We show that the net force acting on the pole depends on the angular distribution of astral microtubules which results from the combination of microtubule nucleation, growth, sliding and disassembly. Asymmetric activation of pulling force generators can lead to stable positioning of the the centrosome at positions displaced off the geometric center.

BP 17.24 Wed 17:30 Poster A

Static and dynamic adhesion of Staphylococci on model substrates, studied by AFM — •Nicolas Thewes, Christian Spengler, Peter Loskill, and Karin Jacobs — Saarland University,

Experimental Physics, D-66041 Saarbrücken, Germany

Bacterial adhesion to surfaces is a complicated process that depends on many factors such as the type of bacterium, the type of surface, the composition of the material and the time of contact. To distinguish effects due to the different factors, the relevant parameters have to be varied independently. A set of tailored silicon wafers allows for this variation. Using AFM-force spectroscopy, we studied the adhesion of bacteria of the Staphylococcus genus to these model substrates. Measurements on wafers with different oxid layer thicknesses show that the subsurface composition of the material influences the adhesion forces. Responsible for this fact are the different van der Waals interactions between the bacteria with wafers with thin and thick oxide layer. Furthermore, a variation of the time of contact between bacteria and substrate reveals differences in the dynamics of the adhesion forces for different species, viz. different call wall compositions.

BP 17.25 Wed 17:30 Poster A

Mechanical instabilities of tubular cellular protrusions — •Dominic Jourdain and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

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

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

BP 17.26 Wed 17:30 Poster A

Contact formation between pathogenic amoebae and target cells — •Julia Reverey[1], Saskia Viebig[1], Matthias Leippe[2], and Christine Selhuber-Unkel[1] — [1]Institute for Materials Science, Kaiserstr. 2, 24143 Kiel, Germany — [2]Zoological Institute, Am Botanischen Garten 1-9, 24118 Kiel, Germany

Acanthamoeba are parasitic amoebae, which can cause severe diseases, such as amoebic encephalitis and keratitis. They destroy certain target cells like nerve cells by an extracellular killing mechanism that is induced by the formation of a close contact between amoebae and nerve cells. In Acanthamoeba the target cell can be phagocytosed through membrane invaginations called food cups.

For a deeper understanding of this amoebic killing mechanism, Acanthamoeba are cocultured with nerve cells. Using high-speed live cell imaging, cocultures of amoebae and nerve cells are studied and the contact formation and related processes like phagocytosis are investigated. In order to mimic the contact formation, beads with different carbohydrate coatings are brought into contact with the amoebae. Also here live-cell imaging is used to achieve a better understanding of the interrelations between carbohydrate functionalization, contact formation and phagocytosis.

BP 17.27 Wed 17:30 Poster A

Cells & stress: integrin dependent mechanical properties of fibroblasts — •Fenneke KleinJan[1], Tobias Pusch[1], Thomas Kerst[1], Reinhard Fässler[2], and Kay Gottschalk[1] — [1]Ulm University, Institute of Experimental Physics, Ulm, Germany — [2]Max-Planck Institute of Biochemistry, Department of Molecular Medicine, Martinsried, Germany

Like humans, cells are often under stress. Blood flow influence endothelial cells, skin cells have to resist stretch and pressure. The protein-family of integrins is a key element in responding to this force, functioning as a bidirectional force signalling protein between the cytoskeleton and the extracellular matrix. Cells are able to respond to force by changing their internal structural elements (cytoskeletal filaments), thereby affecting their mechanical properties.

The 24 integrins in mammals form a dynamic and complex signalling network. In this study we use mouse fibroblasts with reduced complexity. They express or only one specific integrin ($\alpha\nu\beta3$ or $\alpha5\beta1$) or both ($\alpha\nu\beta3\alpha5\beta1$). So we can study the effect of different integrins individually and together on the mechanical properties of the cell.

Due to the structural heterogeneity of the cell we have to probe the mechanical response locally. Our main method is microrheology, where mechanical properties are extracted from moving micron-sized beads. We studied both living cells and isolated intermediate filament network, also as a function of force. Preliminary results show that cells expressing both integrins have a stiffness which is in between the $\alpha5\beta1$ (least stiff) and $\alpha\nu\beta3$ (most stiff).

BP 17.28 Wed 17:30 Poster A

Spontaneous actin waves in a deformable domain — •Alexander Dreher and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

The crawling of eukaryotic cells on substrates is driven by the cytoskeleton. How the cytoskeleton is organized in this process is still poorly understood. It has been suggested that spontaneous polymerization waves provide a possible answer to this question. We examine this possibility theoretically by analyzing a system of treadmilling filaments in a deformable domain. It is known that treadmilling filaments can spontaneously generate polymerization waves [1]. The domain boundary is characterized by a surface tension and a bending rigidity and evolves due to interactions with the filaments. We find spiral waves as well as states with a net directional motion of the system's geometric center of mass. In contrast to [2], we solve the full system of dynamic equations and consider a more realistic length regulation of the filaments.

[1] Doubrovinski and Kruse, *EPL* **83** (2008) 18003
[2] Doubrovinski and Kruse, *PRL* in press

BP 17.29 Wed 17:30 Poster A

Subsurface Imaging Using Atomic Force Acoustic Microscopy at GHz Frequencies — •Matthias Büchsenschütz-Göbeler[1], Yuansu Luo[1], Shuiqing Hu[2], Chanmin Su[2], Walter Arnold[1,3], and Konrad Samwer[1] — [1]1. Physikalisches Institut, Universität Göttingen — [2]Bruker-Nano Inc., Santa Barbara, CA, USA — [3]Department of Materials, Saarland University

We describe a technique to image subsurface structures using Atomic Force Acoustic Microscopy operated at 1 GHz. The devices or samples to be imaged are insonified with 1 GHz ultrasonic waves which are amplitude modulated at a fraction or multiple frequency of cantilever contact-resonance [1]. The transmitted signals are demodulated by the nonlinear tip-surface interaction, enabling one to image defects in the device based on their ultrasonic scattering power which is determined by the ultrasonic frequency, the acoustic mismatch between the elastic properties of the host material and the defects, by their geometry, and by diffraction effects. We investigated defect structures in specially prepared samples, in silicon wafers as well as the cytoskeleton in living cells. Concerning the living cells we are interested to understand the contrast mechanism for imaging and the response to different substrate morphologies. Especially the interplay of cellular elasticity, adhesion and motility are brought into focus.

Financial support by the DFG SFB 937 is thankfully acknowledged.

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

BP 17.30 Wed 17:30 Poster A

Live Cell Rheology — •Zhanna Santybayeva, Alexander Zielinski, Wolfgang Rubner, Johannes Fleischhauer, Bernd Hoffman, and Rudolf Merkel — Institute of Complex Systems 7, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Endothelial cells are responsive to mechanical stress. The objective of the current work is to observe immediate reaction of human umbilical vein endothelial cells upon single and cyclic stretch, and to analyze force exertion to an elastic substrate at adhesion sites. With the help of live cell imaging and fluorescence microscopy, whole cell reorientation and its inner reorganization can be detected, both during stretch and at extreme stretch amplitudes. The setup in development and specifically designed software allow observing cell immediate reaction to mechanical stress.

Precise alignment is achieved via programmable xy- and z-stages, enabling live acquisition. Devices are controlled individually or combined in a certain sequence, depending on the demands of an experiment, e.g. frequency and amplitude adjustable cyclic stretch, z-focus control with image processing on fly, multi-channel acquisition during stretch (movie), time-resolved z-stacks, etc. The substrate is a 350 um thick cross-linked silicone rubber (polydimethylsiloxane) with fluores-

cent beads embedded on the surface. When attaching to the substrate, cells exert point-like forces at adhesion sites, so called focal adhesions (FA). Displacements on the substrate give information on the force exercised at FA. Analyzing image sequences, we can reconstruct dynamics of force, focal adhesions and whole cell reorientation.

BP 17.31 Wed 17:30 Poster A

Cancer cell migration through narrow channels — •Caroline Gluth[1], Irina Harder[2], Amy C. Rowat[3], and Ben Fabry[1] — [1]LPMT, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]ODEM-Gruppe, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]SEAS, Harvard University, Cambridge, USA

Cancer cells have the ability to migrate through narrow pores and channels of the extracellular matrix. To study this process under defined conditions and to find a minimum pore size through which cancer cells can migrate, we used soft lithography to fabricate 3-dimensional polydimethylsiloxane (PDMS) substrates with rectangular channels of varying width (2 - 10 um) and height (3 - 7 um). The channels had a length of 20 um at constant width, or a length of 140 um with a tapered shape (opening angles of 4 - 16 deg) and a width of 2 um at the narrow end. MDA-MB-231 breast carcinoma cells were able to migrate through the narrowest openings (2 x 3 um). We found two dominating migration strategies which are not commonly observed in cells migrating on planar 2-dimensional substrates. The majority of cells protruded thin ($<$ 3 um) and long (order of 100 um) dendritic-like filopodia into the channel lumen, while some cells also showed extensive blebbing and amoeboid-like movements. Similar behavior can also be seen in mouse embryonic fibroblasts and in cancer cells migrating through a 3-dimensional collagen network. These results demonstrate that cancer cells are able to choose between multiple migration strategies for navigation through a highly confined environment.

BP 17.32 Wed 17:30 Poster A

Adhesion forces during immunological synapse formation — •Janosch Deeg[1,2], Anastasia Liapis[3], David Depoil[3], Catharina Cadmus[1,2], Michael Dustin[3], and Joachim Spatz[1,2] — [1]Max-Planck-Institute for Metals Research, Department of New Materials and Biosystems, Stuttgart, Germany — [2]University of Heidelberg, Institute for Physical Chemistry, Biophysical Chemistry Group, Heidelberg, Germany, — [3]Skirball Institute of Biomolecular Medicine, New York University School of Medicine, New York

A key element of the adaptive immune response is the interaction between T lymphozytes and antigen presenting cells (APC), which can lead to the so-called T cell activation. During interaction a complex molecular structure, the immune synapse (IS) at the T cell/APC-interface is formed. In order to quantify the interaction forces and kinetics during synapse formation we measured adhesion forces using an atomic force microscope. Our ongoing research focuses on mimicking the APC interface by a synthetic analogue allowing for the control of arrangement of involved proteins. Highly structured nanoparticles are employed as molecular anchor points for proteins of interest which in turn are then used to activate T cells and investigate the complex process of IS formation while having precise control over important parameters at the nanometer scale.

BP 17.33 Wed 17:30 Poster A

Insight into the cell-beam interaction in the Optical Stretcher — •Steffen Grosser, Anatol Fritsch, Tobias Kiessling, Roland Stange, and Josef Käs — Universität Leipzig, Leipzig, Germany

In the optical cell stretcher, force on cells is exerted by two counter-propagating beams. Usually, these forces are calculated using a ray-optics approach, assuming the same refractive index for all cells. The effect of the cells on the beam has so far been disregarded.

We use an extension of the optical stretcher setup that allows to partially track the laser beams after having passed the cell in the stretcher chamber. We report that the effect of the cells on the beam can, to first order, be described by a cell-lens analogy: The cells reduce the divergence of the laser beam or can even refocus the beams. Smaller cells have a higher radius of curvature and are thus stronger lenses; an expectation which we experimentally confirm.

Parameters such as cell size and ellipticity are used in a ray-transfer-matrix calculation to predict the expected focussing, making it possible to give an estimate of the refractive index of the individual cell by comparing the expected and the actual measured focussing. This in turn allows to readress the problem of determining the force exerted on the cell.

BP 17.34 Wed 17:30 Poster A

Filopodia-Lamellipodia Interaction Dynamics in Neuronal Growth Cones — Melanie Knorr and •Josef Käs — Universität Leipzig, Institut für Experimentelle Physik 1, Linnéstr. 5, 04103 Leipzig, Germany

Neurons are one of the most specialized cells in living organisms, capable of detecting weak signals in a very noisy environment. Explorations of its surrounding is guided by the so called growth cone, a thin veil-like structure at the tip of each neurite consisting of actin and microtubules. As these structures move on two-dimensional substrates, they exhibit vast fluctuations at their leading edge. These fluctuations are driven by the polymerization of the underlying actin network [1,2], switching stochastically between On and Off states. Previous studies investigated the dynamics of the growth cone lamellipodia, neglecting the contribution of filopodia to the dynamics. Therefore we focused on the interaction of filopodia and lamellipodia dynamics in primary neuronal growth cones and will show first results concerning correlations of speed, length and distances.

[1] T. Betz, D. Koch, D. Lim and J. A. Kas, Biophys. J., 2009, 96, 5130-5138.

[2] M. Knorr, D. Koch, T. Fuhs U. Behn and J. A. Kas, Soft Matter, 2011, 7, 3192-3203.

BP 17.35 Wed 17:30 Poster A

Random and directed modes of one-dimensional ameboid motion — •Oliver Nagel, Matthias Theves, and Carsten Beta — Institut für Physik und Astronomie, Universität Potsdam, Germany

We use narrow microfluidic channels to study the quasi one-dimensional motion of starvation developed Dictyostelium discoideum cells, a model organism for amoeboid movement. Confined in channels with a crosssection on the order of an average cell diameter (10 x 20 microns), two modes of movement were observed. On the one hand, cells may perform a one-dimensional random walk, frequently switching the direction of motion in the channel. On the other hand, we observed cells that moved persistently in one direction along the channel for more than half an hour without reversing their direction of motion. Surprisingly, these cells even continued their persistent movement in an unbounded area for several minutes after leaving the narrow confinement of the channel. Furthermore, we have performed fluorescence microscopy experiments that provide insight into the degree of cytoskeletal polarization of these persistently moving cells by imaging the intracellular distribution of actin and myosin II in the cell cortex.

BP 17.36 Wed 17:30 Poster A

Force Generation in Blood Platelets — •Sarah Schwarz G. Henriques[1], Hansjörg Schwertz[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics & CRC Physics, University of Göttingen, Germany — [2]Division of Vascular Surgery, University of Utah, USA

Cellular contraction is of vital importance to living organisms. Thus, for example, blood clotting is achieved by contracting blood platelets. To that effect, platelets activate at damaged blood vessel sites, aggregate and finally pull on intercellular fibrin links. Consequently, they solidify the clot mass, forming a plug to effectively seal the wound. Apart from being of great medical importance, blood platelets represent an ideal model system for studies of cellular contraction for two main reasons: They are simple, being anucleate, and their activation, which occurs within minutes, can be triggered and synchronized by the addition of thrombin. In our experiments we look at force generation at the level of single cells during platelet contraction. To this end, we use traction force microscopy, which provides access to the temporal evolution and spatial distribution of generated forces. Furthermore, we fix cells at different activation stages and stain actin in order to describe cytoskeletal reorganization steps. In combining both traction force microscopy and fluorescence imaging we can resolve traction force maps for single cells and simultaneously access information about force generating mechanisms in the cytoskeleton. We find that force transduction occurs predominantly at the periphery of the cell body and total forces are in the range of 30 nN, which is comparable to literature values.

BP 17.37 Wed 17:30 Poster A

Continuum Theory and Vertex Model Simulations of Self-organized Growth in Developing Epithelia — •Peer Mumcu[1], Ortrud Wartlick[2], Marcos González-Gaitán[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Biochemistry and Depart-

ment of Molecular Biology, Geneva University, Switzerland

Developing tissues possess intrinsic growth control mechanisms which determine the final size and shape. The basic principles of growth control are still poorly understood. However, there is a lot of evidence that certain morphogens act as growth factors and play a key role in this process. Morphogens are a special class of signaling molecules that are secreted from localized sources, spread throughout the tissue and form graded concentration profiles. We study growth control from a theoretical viewpoint using a two-dimensional vertex model that describes the organization of cells by a network of polygons, including the dynamics of morphogen distributions as additional variables. In this theoretical framework, we study the consequences of specific growth rules according to which cells divide when subject to relative temporal changes of the cellular morphogen levels. We discuss a scenario which is consistent with experimentally observed growth curves obtained in the fruit fly Drosophila. Furthermore we show that essential features of the vertex model simulations are captured by a simple dynamical system, which provides deeper insight into the dynamics and stability properties of the growing system.

BP 17.38 Wed 17:30 Poster A

Mechanics and morphology of the interface between two cell populations during tissue growth — •maryam aliee[1], Jens-Christian Röper[2], Christian Dahmann[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

During the development of tissues distinct cellular compartments are established. The interface between these compartments remains sharply defined and on average straight during growth and development. Using a vertex model to describe cell mechanics we discuss several physical mechanisms that contributes to interface morphology. We analyze the influence of cell bond tension, cell proliferation, oriented cell division, cell area pressure, and cell elongation, on the time dependence of interface morphology and mechanics. We show that a local increase in cell bond tension at the interface and a reduced cell proliferation rate in the vicinity of the interface produce effective interfacial tension and reduce the roughness of interfaces significantly. We also study the case in which orientation of cell division depends on cell shape and the case in which cell division rate is affected by cell area pressure. These two mechanisms have negligible contribution to the interfacial tension, however the interface roughness is significantly reduced when combined with a local increase of cell bond tension at the interface. In the case where cells are elongated by external shear stress, the interfacial tension is changed slightly, while there is a strong effect straightening the interface.

BP 17.39 Wed 17:30 Poster A

Critical behaviour and axis defining symmetry breaking in Hydra embryonic development — •Heike Dobicki[1], Andrea Gamba[2], Mario Nicodemi[3], Albrecht Ott[1], Aravind Pasula[1], Mathias Sander[1], and Jordi Soriano[4] — [1]Biol. Experimentalphysik, Univ. d. Saarlandes — [2]Politecnico di Torino and CNISM — [3]Dip.to di Science Fisiche, Universitá di Napoli "Federico II" — [4]Dept. d'ECM, Facultat de Física, Univ. de Barcelona

Axis-determination plays a pivotal role in embryogenesis, development and tissue regeneration. Before axis locking, animal embryos usually go through a phase, which features a fluid-filled cavity, surrounded by a sphere of cells, called a blastula. Hydra vulgaris, a fresh-water cnidarian, has a radial symmetry with a head-to-foot axis. It can reproduce either sexually or asexually by budding. The hydra regeneration process starts with a spherical shape similar to a blastula in embryonic development. The cell sphere actively oscillates until it establishes the head-to-foot axis and subsequently develops into a complete animal. We have observed a self-similar distribution of the ks1-gene on the cell sphere at the symmetry breaking moment. We suggest that the main features of hydra axis establishment can be inferred from the limited communication ability of the cells. A numerical simulation based on a fluctuating cell state, which spreads between neighboring cells only, reproduces all of the observed experimental data well. Besides the critical state that occurs at the axis locking moment, this also includes a bistable distribution of the axis orientation by a weak temperature gradient.

BP 17.40 Wed 17:30 Poster A

Impact of Temperature on Cell Nuclei Integrity in the Optical Stretcher — •Enrico Warmt, Tobias Kiessling, Anatol Fritsch, Roland Stange, and Josef Käs — University of Leipzig, Faculty of Physics and Earth Sciences, Institute of Experimental Physics I, Soft Matter Physics Division, Linnéstraße 5, 04103, Leipzig, Germany

The deformation of cells in Optical Stretcher experiments is considered to be caused exclusively by the deformation of the cellular cytoskeleton. However, the visual appearance of certain cell types during the stretching process implicates events taking place in the cell organelles, especially the cell nucleus. To obtain a more detailed view into the cell we dyed the nucleus in different cell lines and stretched many cells to examine the behavior of the nucleus. At a certain laser power, we observe an abrupt restructuring of the nucleus of MCF-7 cells. This restructuring is irreversible and does not occur during a second stretch of the same cell. Interestingly, the intensity of the restructuring differs between cell lines in a highly reproducible way: While MCF-7 and HMEC show a significant restructuring, less or even no restructuring is observed on MDA-MB-231, MDA-MB-436 and MCF-10A cells. By controlling the ambient temperature, we show that restructuring is triggered by a laser-induced increase in temperature during measurement. The underlying physical processes and the origin of the variations among cell lines has to be clarified.

BP 17.41 Wed 17:30 Poster A

Synchrotron-based functional imaging of prostate tissue samples — •Andrea Matschulat[1], Georgi Graschew[2], Anton Serdyukov[1], Arne Hoehl[1], Ralph Müller[1], and Gerhard Ulm[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]ECRC Campus Buch, Max-Delbrück-Centre of Molecular Medicine, Lindenberger Weg 80, 13125 Berlin, Germany

In our contribution we focus on the sensitive biochemical and functional imaging of human tissue samples with the help of synchrotron-based FTIR-microspectroscopy. FTIR-microspectroscopy is an optical non-invasive technique and has proven to be a fast diagnostic readout tool for multiplexed analysis of biomolecules, mainly in the biomedical field. Measurements were performed at the Metrology Light Source (MLS) of the PTB, an unique low-energy electron storage ring that provides broad-band synchrotron radiation. In our systematic approach we studied the MIR signatures of human benign and malign prostate tissue samples in the spectral range from 900 cm^{-1} to 3900 cm^{-1} under implementation of brilliant synchrotron radiation and globar source in the reflection mode. For a reliable clinical diagnosis with respect to distinct localization of benign and malign tissue areas, a sensitive detection of tissue samples with/without biomarkers is very important. Additionally, spectral quality, i.e., high S/N-ratios in spectral datasets and their correction by Mie scattering algorithms are needed. We will discuss the results of Mie-corrected MIR signatures of prostate tissues and evaluate their classification by multivariate statistics.

BP 17.42 Wed 17:30 Poster A

Biofilm Formation on Microstructured Components — •Jennifer Marx[1], Christine Müller[1], Christin Schlegel[3], Kai Muffler[3], Guido Schüler[2], Michael Walk[2], Jan C. Aurich[2], Roland Ulber[3] und Christiane Ziegler[1] — [1]Department of Physics and Research Center OPTIMAS — [2]Institute of Manufacturing Technology and Production Systems — [3]Institute of Bioprocess Engineering

As soon as a biological molecule, for example bacteria, gets in contact with a surface, they adsorb to the surface. As result a biofilm is established. Especially in bioreactors the bacteria are used to gain for example pharmaceutical products. In this work micro milled titanium compared to native titanium is used as substrate for the biofilms. The biofilm establishment, the morphology of the bacteria and the adhesion of the cells is investigated by a combination of fluorescence microscopy and scanning force as well as scanning electron microscopy (SFM, SEM) as a reference method. The fluorescence dyes show the genetic material in the bacteria in combination with the extracellular matrix and in addition the discrimination between live and dead cells in the biofilm. An almost living biofilm can be observed on natural titanium. The calibration of optical microscopy and SFM allows the detailed imaging of the cells. On natural titanium a multi-layered biofilm with a fusion of colloidal cells to chains is observed. The SEM approves this observation. and provides an insight into detailed structures of the biofilm. On microstructured titanium a biofilm in the microstructures was observed.

BP 18: Posters: Statistical Physics in Biological Systems

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

BP 18.1 Wed 17:30 Poster A

Adaptive walks and extreme value theory — •Johannes Neidhart and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Deutschland

We study biological evolution in a high-dimensional genotype space in the regime of rare mutations and strong selection. The population performs an uphill walk which terminates at local fitness maxima. Assigning fitness randomly to genotypes, we show that the mean walk length is logarithmic in the number of initially available beneficial mutations, with a prefactor determined by the tail of the fitness distribution. This result is derived analytically in a simplified setting where the mutational neighborhood is fixed during the adaptive process, and confirmed by numerical simulations.

BP 18.2 Wed 17:30 Poster A

Emergence of stable epidemic oscillations due to a small weather-based parametric excitation — •Eugene Postnikov and Dmitry Tatarenkov — Staatliche Universität Kursk, Kursk, Russland

The problem of mathematical description of seasonal epidemics of common diseases, e.g. flu, is one of hot topics joining mathematical epidemiology and theory of dynamical systems. The known results of stochastic simulations [Dushoff et al., 2004] demonstrate an evidence of 1:1 dynamical resonance between periods of parameter and solution variations. At the same time a deterministic model revealing this property is still an open problem.

We present the model based on SIRS (Susceptible-Infected-Recovered-Susceptible) approach: $\dot{S} = -kIS + \theta^{-1}R, \dot{I}dt = kIS - \tau^{-1}I$, $\dot{R} = \tau^{-1}I - \theta^{-1}R$ $(S + I + R = 1)$ with the variable parameter $k = k_0\,[1 + \delta\sin(\omega t)]$. It has been shown that that this system can be transformed into the second-order non-autonomous ODE with free the term $R_s\theta^{-1}\tau^{-1}\sin(\omega t)$, where R_s is a fixed point for R in the case $k = k_0 = \text{const}$. In other words, the proposed coordinate transformation reveals the used parametrical excitation as a kind of outer one that allow us to clarify 1:1 character of the resonance.

To prove the obtained model, we analyze data on flu dynamics obtained from `Google Flu Trends` and corresponding weather conditions (mean temperature and humidity) from `European Climate Assessment & Dataset`. The processing of these curves confirms the proposed mathematical model.

BP 18.3 Wed 17:30 Poster A

Correlated mutations in protein sequences due to stability constraints — •Jonas Minning[1], Ugo Bastolla[2], and Markus Porto[3] — [1]Technische Universität, Darmstadt, Germany — [2]Centro di Biología Molecular, 'Severo Ochoa', CSIC-UAM, Madrid, Spain — [3]Universität zu Köln, Germany

Correlations between amino acids at different sites in protein sequences of the same protein family may yield important information on the protein three-dimensional structure and its evolution. We recently proposed an analytical approach which allows to quantitatively predict correlations that arise from selective constraints on unfolding and misfolding stabilities. Our approach is based on a cluster expansion of sequence entropy up to pairwise terms, with stability constraints represented through Lagrange multipliers. These Lagrange multipliers can be obtained either directly from data of correlated mutations or via the constraints on the cumulants of the partition function of the native and the misfolded ensemble, yielding very similar values. We show that in the latter case, the constraints can be written in good approximation as linear functions of the Lagrange multipliers, and that the coefficients quantify the strength of selective constraints on unfolding and misfolding stabilities on the correlation.

BP 18.4 Wed 17:30 Poster A

Emergence of robustness against noise: A structural phase transition in evolved models of gene regulatory networks — •Tiago P. Peixoto — Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany

We investigate the evolution of Boolean networks subject to a selective pressure which favors robustness against noise, as a model of evolved genetic regulatory systems. By mapping the evolutionary process into a statistical ensemble, and minimizing its associated free energy, we find the structural properties which emerge as the selective pressure is increased, and identify a phase transition from a random topology to a "segregated core" structure, where a smaller and more densely connected subset of the nodes is responsible for most of the regulation in the network. This segregated structure is identical to what is found in gene regulatory networks, where only a much smaller subset of genes — those responsible for transcription factors — is responsible for global regulation. We obtain the full phase diagram of the evolutionary process as a function of selective pressure and the average number of inputs per node. We compare the theoretical predictions with Monte-Carlo simulations of evolved networks, and with empirical data for *Saccharomyces cerevisiae* and *Escherichia coli*.

References:

[1] Tiago P. Peixoto, "Emergence of robustness against noise: A structural phase transition in evolved models of gene regulatory networks", arXiv:1108.4341

BP 18.5 Wed 17:30 Poster A

Evolution of drug resistance in a spatially structured environment — •Bartlomiej Waclaw, Philip Greulich, and Rosalind Allen — School of Physics, University of Edinburgh

Evolution of drug-resistant cells is an increasingly important problem in our quest to combat diseases such as bacterial infections or cancer. Many methods have been proposed to circumvent this problem, ranging from switching the drug periodically on and off, using a combination of drugs, or alternating drugs belonging to different classes. However, the majority of these studies (experimental and theoretical) have been carried out for well-mixed populations with spatially uniform distribution of the drug. Here we theoretically analyse the effect of a non-uniform distribution of a drug (e.g. an antibiotic) on the emergence of resistance to it, in a spatially structured population of malignant cells. Motivated by recent experiments on bacteria, we propose a simple stochastic model in which pathogenic microbes replicate, mutate, die and migrate in a box in which the antibiotic concentration changes in space from sub-lethal to overkill levels. We assume that resistance occurs by a sequence of consecutive mutations. Depending on the resistance levels of intermediate mutants (the "pathway to resistance"), we show that heterogeneous drug distribution can either dramatically speed up or slow down the evolution of resistance compared to the case of uniform distribution. We also discuss practical implications of our results for various modes of disease treatment.

BP 18.6 Wed 17:30 Poster A

Fluctuations in meta-population transport models — •Tobias Galla — Complex Systems and Statistical Physics Group, School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom

We introduce meta-population models of transport processes. Particles move along a chain of cells, each of which can hold a number of particles up to a maximum carrying capacity. Particles can only advance along the chain if the patch ahead is not fully occupied. Viewing each patch as a separate population of particles this effectively generates a 'population of interacting populations', hence the term meta-population. Based on a master equation approach and a subsequent system-size expansion we compute the spectral properties of fluctuations in such models about their naive deterministic limit. This naive limit corresponds to models with an infinite patch size. The other extreme, a carrying capacity of one, on the other hand reproduces commonly used single-occupancy models. Our approach allows one to interpolate between the two limits. Specific applications we will discuss include asymmetric exclusion processes with single or multiple types of particles, frequently used as stylized models of biological transport.

BP 18.7 Wed 17:30 Poster A

Thin Films of chiral Fluids — •Sebastian Fürthauer[1,2], Maria Strempel[1,2], Stephan W. Grill[1,2], and Frank Jülicher[1] — [1]Max Planck Institut für die Physik komplexer Systeme, Dresden — [2]Max Planck Institut für Molekulare Zellbiologie und Genetik, Dresden

Hydrodynamic flows in biological systems are often generated by active chiral processes near or on surfaces. Important examples are beating cilia, force generation in actomyosin networks, and motile bacteria in-

teracting with surfaces. We develop a coarse grained description of active chiral films that captures generic features of flow and rotation patterns driven by chiral motors. We discuss force and torque balances within the film and on the surface and highlight the role of the intrinsic rotation field. We arrive at a two dimensional effective theory and discuss our results in the context of ciliary carpets and thin films of bacterial suspensions.

BP 18.8 Wed 17:30 Poster A

Nucleation of ligand-receptor-domains in membrane adhesion — •Timo Bihr[1], Udo Seifert[1], and Ana-Sunčana Smith[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart — [2]Institut für Theoretische Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg

We investigate the nucleation of adhesion domains consisting of ligand-receptor bonds forming between membranes that also interact by a nonspecific potential. We first determine the critical size of the nucleus within the capillary approximation. The time evolution of the nucleation process is considered to take place in a number of rate-dependent coupled stochastic events, each denoting the association or dissociation of a bond. The effective rates for each of these events are calculated by taking into account the membrane deformation and fluctuations. Based on these rates, we construct a discrete master equation from which the characteristic nucleation time is obtained numerically or as an analytic estimate. We validate our model by performing extensive Langevin simulations of an adherent fluctuating membrane, including the ligand-receptor unbinding. We find excellent agreement between the different approaches, particularly in the regime of strong intra-bond correlations.

We show that for experimentally relevant parameters a stable nuclei consists typically of only a few bonds. Furthermore, we find a strong dependence of the characteristic nucleation time on the distance between the receptors which could explain some of the recurrent threshold length-scales in cell adhesion assays.

BP 18.9 Wed 17:30 Poster A

The effect of metabolic theory on life histories — •Yixian Song[1], Stefan Scheu[3], and Barbara Drossel[2] — [1]Max Planck Institute for Evolutionary Biology, Plön, Germany — [2]Institute for Condensed Matter Physics at Darmstadt University of Technology, Darmstadt, Germany — [3]J.F. Blumenbach Institute of Zoology and Anthropology at Georg-August University of Göttingen, Göttingen, Germany

We explore the consequences of metabolic theory on life histories and life history evolution. We use a mathematical model for an iteroparous species and its resources, taking into account the allometric scaling of consumption, metabolism and mortality with consumer body mass. Mortality is assumed to be density-dependent, and the dynamics of resources are explicitly modeled. We find that populations that have more or faster growing resources have a shorter life span and a higher mortality, and that populations with a larger adult biomass have a larger number of offspring per female and a larger biomass density. When we allow the adult body mass to evolve, it increases with time without limits. When we allow the offspring body mass to evolve, it becomes smaller. Both trends result from the allometric scaling of mortality and are kept in limits by trade-offs other than those included in our model.

BP 18.10 Wed 17:30 Poster A

Nonequilibrium clustering of self-propelled particles — •Fernando Peruani[1] and Markus Bär[2] — [1]Universite de Nice - Sophia Antipolis, France — [2]Physikalisch-Technische Bundesanstalt, Braunschweig und Berlin, Germany

It is known from simulations and experiments that many systems of interacting self-propelled particles (SPP) exhibit two phases: i) a monodisperse phase where the cluster size distribution (CSD) is dominated by an exponential tail, and ii) an aggregated phase characterized by the presence of non-monotonic cluster size distributions with a peak at large cluster sizes. At the transition between these two phases, the CSD has a power-law shape with a critical exponent. This qualitative change in the functional form of the CSD can be used as a criterion to define the onset of collective motion in SPP systems as this change in the cluster-size distribution is connected with a strong increase of average cluster sizes. This criterion is particularly useful for application in experimental SPP system where other quantities indicating collective motion like a global orientational order parameter are often not observed. We show that a simple kinetic theory is sufficient to reproduce this transition and allows prediction of the exponent of the power-law of the CSD.

BP 18.11 Wed 17:30 Poster A

Directed Transport of Confined Brownian Particles with Torque — •Paul Radtke and Lutz Schimansky-Geier — Institute of Physics, Humboldt University at Berlin, Newtonstr. 15, D-12489 Berlin, Germany

We consider the motion of Brownian particles who are confined in tunnel with differently shaped walls. The particles are driven by random fluctuations modeled by the Ornstein-Uhlenbeck process with given correlation time τ_c. It is implemented as both a thermal and nonthermal process. Furthermore, the particles' trajectories possess a nonzero mean curvature.

We investigate numerically whether the particles diffuse symmetrically in both directions, or a net transport into one direction emerges. In this case our setup realizes a ratchet mechanism; random fluctuations in the thermodynamic nonequilibrium are rectified. For the nonthermal noise we find the emergence of transport. It is investigated with respect to the correlation time, the mean curvature and the tunnel's geometry. Eventually, the mechanism of the symmetry breaking is elucidated.

BP 18.12 Wed 17:30 Poster A

Single-molecule FRET experiments analyzed by likelihood-based methods — •Bettina G. Keller and Frank Noé — Freie Universität Berlin, Arnimallee 6, 14195 Berlin

The conformational equilibrium of single molecules can be probed by a variety of experimental techniques, such as fluorescence resonance energy transfer (FRET) spectroscopy, fluorescence quenching or atomic force experiments. However, constructing a consistent kinetic model from the measured data is difficult because (i) the conformational states of the molecule are typically related to overlapping value ranges of the observable, (ii) single-molecule experiments suffer from a low-signal to noise ratio, and (iii) the influence of measurement errors, as for example spectral cross-talk, on the signal is sizable. Likelihood-based analysis methods, such as hidden Markov models, are much more apt in dealing with overlapping states than conventional histogram analyses. However, due to problems ii and iii, their application to experimental data has remained challenging. Using a novel likelihood function, which explicitly accounts for the background noise in the experimental signal, we have constructed hidden Markov models of single-molecule FRET data of two experimental systems: the presumed two-state folder rRNA three-helix junction and the ribozyme Diels-Alderase, known to show a complex folding behavior. The analyses reveal multi-state kinetic networks including transition rates, state life times, and associated FRET efficiencies. The networks are hierarchically organized, such that at low state resolution the results of conventional histogram analyses are largely recovered.

BP 18.13 Wed 17:30 Poster A

Heterogeneous short-term plasticity enables spectral separation of information in the neural spike train — •Felix Droste, Tilo Schwalger, and Benjamin Lindner — Bernstein Center for Computational Neuroscience, Haus 2, Philippstrasse 13, 10115 Berlin, Germany

In order to understand how information is processed in the brain, i.e. how signals are encoded, transmitted, and gated, it is vital to investigate how a single neuron responds to inputs that encode multiple signals. Here, we study a scenario in which a neuron receives two stimuli through populations of facilitating and depressing synapses, respectively. We show that this leads to a spectral separation of information into high and low frequency bands. This spectral separation is based on the respective other signal acting as a kind of noise in the disfavored frequency band. We also show that the total information transfer about one signal can still benefit from the presence of the other signal through a form of stochastic resonance.

BP 18.14 Wed 17:30 Poster A

Dynamics of resting brain fluctuations — •Vesna Vuksanovic[1,2] and Philipp Hövel[1,2] — [1]Technische Universität Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Germany

Despite important progress over the last few years, brain functional connectivity at rest "i.e." under no stimulation and in the absence of any overt-directed behaviour, is still not well understood. In stud-

ies on goal-directed mental activity, spontaneous brain activity at rest has been considered as random enough to be averaged out across many trials. However, well organized spatio-temporal low-frequency fluctuations (<0.1 Hz) have been observed in blood-oxygen-level-dependent (BOLD) fMRI signal of human subjects during rest. These well organized patterns of activity, suggest the existence of underlying dynamics that governs intrinsic brain processes. Here, we address resting brain fluctuations in fMRI data proposing some possible routes of studying the underlying dynamics.

BP 18.15 Wed 17:30 Poster A

Understanding electrical currents in DNA translocation experiments — •Stefan Kesselheim and Christian Holm — Institut für Computerphysik, Universtät Stuttgart

DNA translocation through synthetic nanopores is considered a technologically promising candidate for rapid DNA sequencing and is physically interesting because the experiments allow to probe single DNA molecules. The most important observable, the electrolyte-based conduction is only partly understood. We analyze this situation from different perspectives and show many different effects are important: We discuss an complex interplay of attraction of counterions, steric exclusion of ions, hydrodynamic interactions, ion correlations and electrofriction. Our analysis tool is molecular dynamics simulation including hydrodynamic interaction by means of the Lattice-Boltzmann method.

BP 18.16 Wed 17:30 Poster A

Influence of dielectric background on biophysical simulations — •Florian Fahrenberger and Christian Holm — Institut für Computerphysik, Universität Stuttgart, Deutschland

In today's computer simulations, especially in but not limited to biophysics, electrostatic interactions play a crucial role in the behaviour of experimentally relevant systems. They also take up a major amount of the computation time and are very complicated to parallelize.

We present an electrostatics algorithm that is intrinsically local and therefore straight forward to parallelize. One of the main advantages of the algorithm's locality is that one can apply spatially varying dielectric properties to the simulation background. For many coarse-grained simulations of biophysical systems this is of high interest, since the dielectric permittivity is directly dependent on the salt concentration in water, which can vary significantly in inhomogeneously distributed systems.

We present the theory behind this algorithm and show the influence of variations in salt concentration in some typical simulation setups.

BP 18.17 Wed 17:30 Poster A

A facilitated diffusion model with two conformational states — •Maximilian Bauer[1] and Ralf Metzler[2,3] — [1]Physics Department, Technical University of Munich, Germany — [2]Institute for Physics and Astronomy, Potsdam University, Germany — [3]Physics Department, Tampere University of Technology, Finland

Transcription factors (TFs) such as the lac repressor find their target sequence on DNA at remarkably high rates. In the established facilitated diffusion model for this search process the TF alternates between three-dimensional diffusion in the bulk solution and one-dimensional sliding along the DNA chain. In similar models the TF was considered as being present in two conformations (search state and recognition state) between which it switches stochastically. Combining both approaches we obtain a generalised model, that comprises the previous models as special cases. We treat the bulk excursions explicitly for rod-like chains arranged in parallel and consider a simplified model for coiled DNA.

BP 18.18 Wed 17:30 Poster A

Reduction of Scattered Light by Müller Cells in the Human Retina — •Oliver Bendix, Ragnar Fleischmann, and Theo Geisel — Max Planck Institute for Dynamics und Self-Organization, Göttingen, Germany

It is a long standing question why in the mammalian eye photoreceptors are positioned at the back of the retina, forcing photons to travel through various neuronal layers of the retina before the light-sensitive rods and cones can detect them. Recent studies suggest that certain retinal glial cells – called Müller cells (MCs) – play an important role in answering that question. Recent experiments have suggested that MCs extracted from the retina can act as optical fibers [1].
To understand the light guiding properties of the MC in the natural fluctuating optical environment, we developed a model to analyze the light reflection and transmission of MCs embedded in a random medium neuronal tissue. With these quantities and a simplified geometrical eye model we study how light is scattered in the eye. We found that MCs can lead to a substantial increase of the signal-to-noise ratio (SNR), the ratio of the intensity of direct incident light at a photoreceptor to the intensity of back-scattered light from other areas of the retina. The SNR is most pronounced in the vicinity of the fovea and can be more than an order of magnitude.

References

[1] Franze et. al., Müller cells are living optical fibers in the vertebrate retina. Proc. Natl. Acad. Sci. U.S.A. **104**, 2007.

BP 18.19 Wed 17:30 Poster A

Short Range Interaction Dynamics of Colloidal Particles in a Single Optical Potential — •Benjamin Tränkle and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Germany

In many biological systems, binding and unbinding events are of vital importance. Here, the accomplishment of initial contacts not only depend on a time independent association probability, but also on time dependent conformational changes of the interaction partners and therefore on a interaction duration τ_{on}. Furthermore, interaction dynamics are affected by long and short ranging forces, such as hydrodynamic, entropic and steric forces. Colloidal particles can serve as a model system for the investigation of such interaction events. We measure the 3D trajectories of two particles in a single potential, which is generated by an oscillating optical line trap. In this geometry, the reaction rate is increased due to the confined space, while rotational and translational degrees are preserved. With our setup, we can trap multiple beads and analyse particle motions at a spatial precision in the nanometer range and scanning frequencies up to 10 kHz. We show how various controls, i.e. the reaction volume or inter-particle potentials affect the interaction duration τ_{on}.

BP 18.20 Wed 17:30 Poster A

Neural dynamics during sleep: state switching and oscillations — •Jens Christian Claussen — Institut für Neuro- und Bioinformatik, Universität zu Lübeck

The mammalian brain during sleep exhibits various interesting dynamical phenomena including switching processes from the neural microscale [1] to collective phase transitions, which, including regulatory mechanisms, give rise to the sleep-wake cycle. In addition, sleep state switching shows stochasticity [2,3]. On the time scale, the processes are separated from spikes (1ms) to spindle and burst lengths (1s) [4,5] via sleep states (100-10000s) to the ultradian (1.5h) and circadian rhythm. Sleep-associated oscillations are also separated in the frequency domain, and show rich complexity [3] including entrainment of spindles (12-15 Hz) by slow oscillations (0.8 Hz) [6]. In some cases, these oscillations can be influenced by electrical stimulation, observing a significant phase-dependence [4].
[1] J. Mayer et al, PRE 73, 0131908 (2006), [2] Lo et al. EPL 57, 625 (2002), [3] E. Olbrich, J.C. Claussen, P. Achermann, Phil. Trans. Roy. Soc. A 369, 3884 (2011), [4] A. Weigenand, T. Martinetz and J.C. Claussen (subm.), [5] H.-V. Ngo et al, EPL 89, 68002 (2010), [6] J. Mayer et al, PRL 99, 068102 (2007)

BP 18.21 Wed 17:30 Poster A

Effects of interactions between ion channels on neuronal dynamics — •Ekaterina Zhuchkova, Dmitry Zarubin, and Susanne Schreiber — Institute for Theoretical Biology, Humboldt-Universität zu Berlin and BCCN Berlin, Germany

Electrical signaling in our brain and heart relies on the opening or closing of individual stochastic units, so-called ion channels. Since Hodgkin and Huxley's model of action potential (AP) initiation, the prevailing assumption is that ion channels act independently; they change their open probability in response to a common signal such as the membrane voltage, but do not directly influence each other. However, evidence for additional interactions between channels accumulates.

Consequences of such enhancing or hindering interactions between ion channels for neuronal spiking dynamics can be expected. Nevertheless, they have so far received relatively little attention in the analysis of excitable membranes. Here, we use bifurcation analysis and stochastic simulations of an extended Morris-Lecar model to understand how cooperative and anticooperative gating between ion channels changes basic sub- and suprathreshold voltage dynamics. The effects of chan-

nel interactions include the modification of the range of sustained firing and cell-intrinsic noise, the prolongation of AP duration, the occurrence of multistability and type-3-like firing. We hypothesize that channel interactions could be an efficient mechanism to regulate neuronal activity.

Acknowledgments.—Funded by BMBF (01GQ0901, 01GQ1001A, 01GQ0972).

BP 18.22 Wed 17:30 Poster A

Modeling the swimming African Trypanosome using mulit-particle collision dynamics — •Sujin Babu and Holger Stark — Institute for Theoretical Physics, Technische University Berlin, D-10623 Berlin, Germany

The African Trypanosome is a unicellular organism which attacks the central nervous system of humans, causing the deadly disease called the sleeping sickness. The spindle-shaped flexible cell body of the African Trypanosome possesses some bending rigidity due to its cytoskeleton. A single flagellum runs from the posterior end to the anterior end of the cell body and is firmly attached to it. By propagating a wave along the flagellum from the anterior to the posterior end, the Trypanosome propels itself. However, the details of how the flagellum is attached to the cell body and its propulsion mechanism is still under debate. Our goal is to study a model Trypanosome in its viscous environment. We model the cell body and the flagellum (attached either straight or helical to the cell body) as a mesh of vertices connected by springs with some resistance to bending. A bending wave passing through the flagellum propels the organism in the direction opposite to the propagating wave. We simulate the flow field around the model Trypanosome using the method of multi-particle collision dynamics, which is an effective solver for the Navier-Stokes equations. We will demonstrate that our model is able to reproduce the experimental results both qualitatively and quantitatively. We will also show that the so called sperm number used in resistive force theory reveals a characteristic scaling in the dynamics of such a self-propelled elastic body.

BP 18.23 Wed 17:30 Poster A

Identification of Metastable States through dynamical clustering of Free Energy Landscape of Biomolecules — •Abhinav Jain and Gerhard Stock — Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, 79104 Freiburg.

Recent simulation of peptides, proteins and RNA have shown that in many cases the free energy landscape can be well characterized in terms of metastable conformational states. They can be employed to construct transition networks of the system, reveal relevant pathways, and influence the average folding times by means of kinetic traps. We introduce a new approach that consists of (i) initial preprocessing to reduce the dimensionality of the data via principal components analysis, followed by k-means clustering to generate microstates [1], (ii) the *most probable path* algorithm to identify the metastable states of the system, and (iii) boundary corrections of these states to obtain the correct dynamics. The potential of the method is demonstrated with application to the villin headpiece subdomain.

[1] Jain; Hegger; Stock. J. Phys. Chem. Lett. 2010, 1, 2769 - 2773

BP 18.24 Wed 17:30 Poster A

Poisson ratio and local stress in the phospholipid membrane — •tayebeh jadidi[1], Alireza Mashaghi[2,3], Hamid Seyyed-Allaei[4], Philipp Maass[1], and Mohammad Reza Rahimi Tabar[1,4] — [1]university of osnabrueck, osnabrueck, Germany — [2]FOM Institute AMOLF, Science Park 104, 1098XG Amsterdam, The Netherlands — [3]ETH Zürich, Department of Materials, Wolfgang-Pauli-Strasse 10, CH-8093 Zürich, Switzerland — [4]Department of Physics, Sharif University of Technology, 11365-9161, Tehran, Iran

We calculate the poisson's ratio and local stress tensor of the lipid bilayer membrane at gel-, fluid-, interdigitated- and ripple phases. We propose a general algorithm for calculating Poisson's ratio for membranes with periodic boundary conditions; we show that gel-phase lipid membranes has a positive Poisson's ratio and therefore do not behave like crystalline (polymerized) membranes. The distribution of locally stored energy is calculated from the stress tensor for membrane at different phases and the stability of the ripple phase is studied by determining the ripple-gel transition energy barrier. Finally we report on the thermal expansivity of the lipid membrane.

BP 18.25 Wed 17:30 Poster A

Stochastic bifurcations in biological systems — •Anna Zakharova[1], Aneta Koseska[1], Juergen Kurths[2,3], and Tatyana Vadivasova[4] — [1]Center for Dynamics of Complex Systems, University of Potsdam, Potsdam, Germany — [2]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [3]Institute of Physiscs, Humboldt University Berlin, Berlin, Germany — [4]Saratov State University, Saratov, Russia

The influence of noise on nonlinear dynamical systems is one of the most relevant and intensively developing research directions of nonlinear dynamics. The investigation of stochasticity is very important for understanding the dynamical features of real systems, since they are inevitably affected by noise. In the present work we define a concept of stochastic bifurcations as an approach to the analysis of noisy systems. First, we apply this method to a Duffing-Van der Pol oscillator and further extend it to biological systems. On the example of gene relaxation oscillator we demonstrate that a concept of stochastic bifurcations is suitable to investigate the dynamical structure of cellular networks. Furthermore, we show that under stochastic influence the expression of given proteins is defined via the probability distribution of the phase variable, representing one of the genes consisting the system. Moreover, for the isochronous case we found out the presence of coherence resonance-like (CR-like) effect. We also show that under changing stochastic conditions the probabilities of expressing certain concentration values are different, leading to different functionality of the cells, and thus to differentiation of the cells in the various types.

BP 18.26 Wed 17:30 Poster A

Non-Equilibrium Phase Transition in a Biofilm Growth Model — •Florentine Mayer and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Germany

Biofilms show remarkable resistance to environmental stress as, for example, introduced by antibiotics. This is because biofilms promote growth by diversifying cells: faster growing, more sensitive phenotypes are protected by resistant phenotypes. As environmental conditions change, the fitness of phenotypes may change, which increases the benefit of heterogeneous populations. While models for well-mixed systems reproduce the advantage of heterogeneity in changing environments, the situation for spatial settings has received less attention so far. To analyze biofilm growth we set up a two-species automaton model in which growth and death rates depend on the environmental conditions. These fluctuate, resulting in periodically interchanged growth and death rates of the two phenotypes. Depending on the rates we find either fast extinction or thriving biofilms with intriguing spatio-temporal patterns. Close to the region of extinction patterns become self-affine, which is the hallmark of a phase transition to an absorbing state (i.e. an empty lattice). Employing extensive stochastic simulations we measure critical exponents of our non-equilibrium phase transition and find universal scaling behavior, which characterises the universality class of our model.

BP 18.27 Wed 17:30 Poster A

Physical description of centrosome assembly using a phase separation process — •David Zwicker[1], Markus Decker[2], Steffen Jaensch[2], Anthony Hyman[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

The size of many cell organelles is strongly correlated with cell size. Achieving this requires a robust mechanism for organizing and scaling subcellular structures. Here, we propose a theoretical description of the growth phase of the centrosome, an organelle involved in mitosis. We identify a possible mechanism based on phase separation by which the centrosome volume may be controlled. Specifically, a chemical reaction driving the phase separation process accounts for the temporal and spatial evolution observed in experiments. We also take surface tension effects into account.

Our theory explains the growth dynamics of centrosomes for all cell sizes down to the sixteen cell stage of the C. elegans embryo, and it also accounts for data acquired in experiments with aberrant numbers of centrosomes and altered cell volumes. Furthermore, the model can describe the dissolution phase occurring during cell division and unequal centrosome sizes observed in cells with disturbed centrioles.

BP 18.28 Wed 17:30 Poster A

Cell-Cell-Desynchronization in Yeast Cell Populations — •André Weber[1,2], Werner Zuschratter[2] und Marcus Hauser[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität

Magdeburg, Germany — [2]Leibniz-Institut für Neurobiologie Magdeburg, Germany

Colonies of the yeasts *Saccharomyces carlsbergensis* and *Saccharomyces cerevisiae* have been used as stable model organisms to investigate glycolytic oscillations over years. The dynamics of the cell population depend on the cell density: At high cell densities all cells of the population show synchronous and coherent oscillations, which can be detected as global oscillations. The collective behaviour ceases at a critical, low cell density, but the nature of the dynamics at single cell level remained an open question. Recent reports predicted a 'quorum sensing' mechanism, where all cells stop oscillating synchronously below the quorum. Using single photon counting fluorescence microscopy, we study the dynamics of individual yeast cells at low cell densities for both yeast strains. Our focus lies in elucidating the mechanism of the transition between individual and collective dynamics. At very low cell densities, the individual cells still perform metabolic oscillations, the frequencies of which show a very broad distribution. Thus the cells oscillate in a desynchronous fashion. As the cell density increases, we observe that the frequency distribution narrows and synchronized collective behaviour sets in. We can preclude a dynamical quorum sensing phenomenon for glycolytic oscillations in yeast strains *S. carlsbergensis* and *S. cerevisiae*.

BP 18.29 Wed 17:30 Poster A

Dynamics of a spherical microswimmer in Poiseuille flow — •Andreas Zöttl and Holger Stark — Institut für Theoretische Physik, TU Berlin

Microorganisms in the human body have to respond to confining boundaries and fluid flow, like sperm cells in the Fallopian tube or pathogens in blood vessels. Also, artificial microswimmers would have to swim in narrow channels like arteries if one day they may be used as drug deliverers in the human body. Due to vorticities in the flow field and hydrodynamic interactions with bounding surfaces, microswimmers change their swimming speeds and orientations.

To capture both effects of fluid flow and confinement, we analyze the dynamics of a spherical microswimmer in Poiseuille flow, moving in a cylindrical microchannel. Neglecting the finite extent of the swimmer and its hydrodynamic interaction with the bounding wall, the dynamic equation for a swimmer in 2D is given by a simple pendulum equation. Swimmers swing around the centerline of the channel while oriented upstream, or tumble when the flow is strong enough. In 3D the swimmer can perform helical and helical-like trajectories while its angular momentum is conserved. Accounting also for hydrodynamic interactions between the swimmer and the wall, we show that *pushers* such as sperm cells or bacteria and *pullers* like the algae *Chlamydomonas* show different behavior. We find that upstream motion in the center of the channel is stabilized for pullers but becomes unstable for pushers which move on a stable limit cycle.

BP 18.30 Wed 17:30 Poster A

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

Principal component analysis is widely used to obtain coordinates that monitor essential dynamics of high-dimensional biomolecular systems. Applying this technique to MD simulations of various peptides allows a separation of slow large-amplitude motions and high-frequency fluctuations [1]. A Langevin simulation on the first few principal components using local estimates of drift and diffusion fields is shown to reproduce the conformational dynamics of those peptides [2]. Particularly, a set of short trajectories can be used instead of one continuous trajectory as input. We demonstrate thermodynamical characteristics of the studied peptide systems revealed by this method. Furthermore, we present first attempts to construct an analytical model to characterize the free energy landscape.

[1] A. Altis, M. Otten, P.H. Nguyen, R. Hegger and G. Stock, J. Chem. Phys. 128, 245102 (2008)
[2] R. Hegger and G. Stock, J. Chem. Phys. 130, 034106 (2009)

BP 18.31 Wed 17:30 Poster A

The dynamics of stochastic slowdown in evolutionary processes — •Philipp M. Altrock[1], Tobias Galla[2], and Arne Traulsen[1] — [1]Max-Planck-Institute Evolutionary Biology, Plön — [2]School of Physics & Astronomy, University of Manchester

We study the stochastic dynamics of evolutionary games, and focus on the so-called 'stochastic slowdown' effect, previously observed in (Altrock et al. 2010, PRE 82, 011925) for simple evolutionary dynamics. Slowdown here refers to the observation that a neutral mutation may fixate quicker than a beneficial one under certain forms of frequency dependent selection. More precisely the fixation time, conditioned on paths in which the mutant takes over, has a maximum value at intermediate selection strength. This phenomenon is present in the prisoners dilemma game. Additional analysis of a co-existence game reveals even more intricate behavior of the fixation times. In small populations, the conditional average fixation time shows multiple extrema as a function of the selection strength. We establish the microscopic origins of these phenomena and calculate the mean conditional sojourn times, identifying those transient states which contribute most to the slowdown effect.

BP 18.32 Wed 17:30 Poster A

Predictability of evolution depends nonmonotonically on population size — •Ivan G. Szendro[1], Jasper Franke[1], J. Arjan G.M. de Visser[2], and Joachim Krug Krug[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Laboratory of Genetics, Wageningen University, The Netherlands

We study Wright-Fisher dynamics on an empirical 8-locus fitness landscape (FL) obtained experimentally for the filamentous fungus *Aspergillus Niger*. In order to measure predictability, we define entropy measures on the observed paths. We find a non monotonic dependance of the entropy on population sizes, N, for fixed mutation rates, μ. The initial decrease of entropy and the subsequent increase, for ever larger N, are governed by the scales $N\mu$ and $N\mu^2$, respectively, and the amplitude of this pattern is determined by the magnitude of μ. We also study the departure from the strong selection weak mutation regime, when increasing N, for the probability of the largest subpopulation to end up on the wild type genotype. To show that our observations are generic, we compare our findings for the experimental FL with data obtained on a simple model landscape.

BP 18.33 Wed 17:30 Poster A

Fast GPU-based Hologram Generation for Real-Time Optical Neurostimulation — •Johannes Hagemann[1], Hecke Schrobsdorff[2], and Stephan Kramer[3] — [1]Institut f. Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]MPI f. Dynamik und Selbstorganisation, Institute for Nonlinear Dynamics, Am Fassberg 17, 37077 Göttingen — [3]Institut f. Numerische und Angewandte Mathematik, Lotzestr. 16-18, 37083 Göttingen

For optical neurostimulation, holograms have proven to be particularly efficient. Fast and flexible stimulation is crucial for e.g. controlled synaptic learning experiments. Since a spatial light modulator used for hologram generation can only shift phases, hologram computation is a complex process. Up to now, no direct method to determine a corresponding phase mask exists. Current algorithms consist of a series of iterative fourier transforms and projections, with sometimes very slow convergence speeds. Fortunately, the matrix formulation of existing algorithms is data-parallel and thus can directly be implemented on a GPU. We present a CUDA-based implementation for computing phase-only holograms which are used for a selective excitation of individual light-sensitive neurons. We focussed on a modular structure to be flexible for changing experimental hardware or for incorporating advancements in parallel computing or new algorithms. We compare the performance of the well-known GS algorithm [1] with the recently introduced Relaxed Averaged Alternating Reflections [2].

[1] R. W. Gerchberg and W. O. Saxton, Optik **35**, 237 (1972)
[2] D. R. Luke, Inverse Problems **21**,37 (2005)

BP 18.34 Wed 17:30 Poster A

Describing non-linear attentional modulation patterns through ring-architecture neural circuits — •Markus Helmer[1,4], Vladislav Kozyrev[2,3], Stefan Treue[2,4], Theo Geisel[1,4], and Demian Battaglia[1,4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen — [2]Deutsches Primatenzentrum, Göttingen — [3]Institute of Neuroinformatics, Ruhr-University Bochum — [4]BCCN, Göttingen

We analyzed recordings in area MT from macaque monkeys performing a transparent motion task. They were presented random-dot-patterns (RDP) at two distinct locations within the receptive field of the recorded cell. Attention was directed to a fixation spot or to only one of the two RDPs. The angle between the two RDPs was kept fixed at 120 degrees so that covarying the motion directions pro-

vided tuning curves with two peaks. We found that the positions of the response peaks were different from what the single-motion orientation-preferences of the cell predicted. Furthermore they depended on the attentional condition, showing strong signatures of non-linear interactions during the integration of the two stimuli by MT neurons, including peak repulsion or attraction. By using a mean-field ring model, we could reproduce all the observed response non-linearities independently in broad regions of the parameter space. However, to find the specific combination of non-linearities observed across attentional conditions a fine tuning of the parameters was required. We explored therefore multi-areal network models with multiple coupled rings to achieve a more robust description of non-linear attentional modulation patterns.

BP 18.35 Wed 17:30 Poster A

Modeling of the theta rhythm patterns in septo-hippocampal area — •Sebastian Milster, Anastasia Lavrova, and Lutz Schimansky-Geier — HU Berlin, Institut für Physik

Theta (3 - 12 Hz) and gamma (30 - 70 Hz) oscillations in rodent's hippocampal and septal areas have been throuroughly studied in vivo as well as in vitro. They occur during distinct cognitive states. It has been shown that theta and gamma oscillations in hippocampus are modulated by inhibitory inputs from the septum.

The focus of this work is to study the influence of the connection between the septum and the hippocampus CA3 area. We use the Hodgkin-Huxley equations to construct a minimal septo-hippocampal circuit. By changing the coupling strengths between the cells we define the parameter range at which different oscillatory regimes emerge. We analyze how the main characteristics of self-sustained oscillations as phase shift and frequency change at the switching between different rhythms. The model is to examine the mechanism of disinhibition and its contribution to the modulation of these rhythms.

BP 18.36 Wed 17:30 Poster A

Biocompatibility of Parylene-coated GaAs Substrates and Microtubes — •Cornelius Bausch, Eric Stava, and Robert Blick — Institute for Applied Physics, University of Hamburg

The strain caused by the mismatch of the lattice constants of two epitaxially grown semiconductor layers can be exploited to roll up microtubes. Recently, arrays of such semiconductor tubes have been fabricated as a method to create three-dimensional spatial confinement for in vitro neurite outgrowth. Thereby, the tube walls resemble the myelin sheath, which accelerates signal propagation through the axon.

Our rolled-up microtubes are fabricated from gallium arsenide, which is known to be toxic. Parylene C, a biocompatible, chemical vapor deposited poly(p-xylylene) polymer, can be used as a coating to prevent the poisonous effects of As. We test the biocompatibility of GaAs substrates coated with parylene by means of cell culture. Additionally, we test the layer quality of the parylene coating on the outside and inside of GaAs-semiconductor tubes.

[1] Yu, M. R. et al., Semiconductor Nanomembrane Tubes: Three-Dimensional Confinement for Controlled Neurite Outgrowth. Acs Nano **5**, 2447-2457 (2011)

BP 18.37 Wed 17:30 Poster A

Virtual Networks of In Vitro Neurons by Patterned Photostimulation — •Kai Bröking[1,3,6], Ahmed ElHady[1,2,5,6], Ragnar Fleischmann[1], Theo Geisel[1,3,5,6], Walter Stühmer[2,5,6], Fred Wolf[1,3,5,6], and Gert Rapp[4] — [1]MPI für Dynamik und Selbstorganisation, Göttingen — [2]MPI für experimentelle Medizin, Göttingen — [3]Fakultät für Physik, Georg-August-Univ. Göttingen — [4]Rapp OptoElectronic GmbH, Hamburg/Wedel — [5]Bernstein Center for Computational Neuroscience, Göttingen — [6]Bernstein Focus for Neurotechnology. Göttingen

Transfecting neurons with light-gated ion channels and -pumps, e.g. Channelrhodopsin2 [1], makes it possible to precisely control their activity noninvasively, by means of photostimulation.

Here, we present an experimental setup for the patterned photostimulation with continuous signals which can be modulated on the millisecond-scale. It allows to artificially link biological neurons into virtual networks of arbitrary topology. The setup consists of an LED-based multi-spot illumination device, a data aquisition and processing unit, and a software system for input-driven stimulus generation. Local neural activity measured from neurons living on a grid of electrodes in a Multi-Electrode Array (MEA) is used to induce activity elsewhere in the culture by means of generating dynamic photostimulation signals as live feedback. We characterize the performance and limitations of our closed-loop feedback system with respect to latency, long-term stability, and photoelectric articfacts. [1] Boyden, E., et.al., Nat Neurosci 8, 1236-1268(2005), doi:10.1038/nn1525

BP 18.38 Wed 17:30 Poster A

Modeling of rhythmic patterns in hippocampus — •Anastasia Lavrova[1], Michael Zaks[2], and Lutz Schimansky-Geier[1] — [1]Institut für Physik, HU — [2]Institut für Mathematik

The hippocampal circuit can exhibit network oscillations in different frequency ranges (*gamma* - 30-80 Hz; *theta* - 4-12 Hz; as well as *theta/gamma* or a bursting regime) both in vivo and in vitro and switch between them. . The hippocampal neuronal network consists of various types of connected cells, which allows them to provide oscillations with different periods, amplitudes, and phase shifts.

We propose the minimalistic model for the description of generation of such polyrhythmic signals in the hippocampal area CA3. The network includes two fast- and two slowly-spiking cells which are described by the FitzHugh-Nagumo equations and coupled by means of synaptic connections. We analyze the influence of synaptic strengths on the synchronization in the network. Mechanisms of switching between different rhythms are discussed.

BP 18.39 Wed 17:30 Poster A

Artificial Neuron — •Matthias Garten[1], Gilman Toombes[2], Sophie Aimon[1], and Patricia Bassereau[1] — [1]Institut Curie, Paris, France — [2]NIST Center for Neutron Research , Gaithersburg, USA

Signal processing in the brain builds up on biophysical principles that are the bases for essential features like protein targeting, voltage sensing and signal propagation amongst many others. Many open questions remain that are difficult to attack as the cellular environment is inherently complex.

In this study, an ex-vivo, bottom-up approach was pursued by reconstituting the purified voltage sensitive potassium channel of Aeropyrum pernix (KvAP) into cell-sized artificial lipid vesicles (giant unilamellar vesicles - GUVs). The next step is to gain electrical control over the system to investigate the function of voltage-gated ion channels (here KvAP), but also pumps and porins in the controlled ex-vivo environment. The prospect is then to create a model system for action potential propagation in a biomimetic axon that can be formed by pulling a lipid nano-tube from the giant vesicle thus providing a biomimetic neuronal geometry in which membrane curvature, lipid composition and protein concentration can be controlled in contrary to an in-vivo Neuron.

This work will contribute to our understanding of the effect of membrane morphology on ion channels distribution and provide experimental data for the theory of signal propagation with respect to axon diameter, morphology and stochastic noise.

BP 19: Symposium SYND: Control of Network Dynamics (with DY and SOE)

Time: Thursday 9:30–12:00 Location: H 0105

Invited Talk BP 19.1 Thu 9:30 H 0105

Controlling Complex Networks with Compensatory Perturbations — •Adilson E. Motter — Department of Physics & Astronomy and NICO, Northwestern University, USA

A fundamental property of networks is that the perturbation of one node can affect other nodes, in a process that may cause the entire or a substantial part of the system to change behavior and possibly collapse. Recent research in metabolic and ecological networks has demonstrated that network damage caused by external perturbations can often be mitigated or reversed by the application of compensatory perturbations. Compensatory perturbations are constrained to be physically admissible and amenable to implementation on the network. However, the systematic identification of compensatory perturbations that conform to these constraints remains an open problem. Here, I will

present a method to construct compensatory perturbations that can control the fate of general networks under such constraints. Our approach accounts for the full nonlinear behavior of real complex networks and can bring the system to a desired target state even when this state is not directly accessible. Applications to genetic networks show that compensatory perturbations are effective even when limited to a small fraction of all nodes and that they are far more effective when these are the highest-degree nodes in the network. The versatility of our methodology is illustrated through applications to associative-memory, power-grid, and food-web networks. The approach is conceptually simple and computationally efficient, making it suitable for the rescue, control, and reprogramming of large complex networks in various domains.

Invited Talk BP 19.2 Thu 10:00 H 0105

Toward control, prediction, and optimization of biological and engineering complex networks — •Kazuyuki Aihara — Institute of Industrial Science, University of Tokyo, Tokyo, Japan

In this talk, I will review our recent works on control, prediction, and optimization of biological and engineering complex networks. The topics include bifurcation and control of information representation in a complex neural network in the prefrontal cortex, stability analysis of biomolecular networks as well as a possibility of control and optimization in engineering complex networks such as power grids.

Invited Talk BP 19.3 Thu 10:30 H 0105

Design of robust functional networks as complex combinatorial optimization problem — •Alexander S. Mikhailov — Abteilung Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

Robustness against local damage and distributed noise is a fundamental property of biological systems. Their level of robustness by far exceeds what is typical for modern industrial and transportation networks. As manufacturing and transportation systems become more complex and should be often built from individual units subject to failure and variations, requirements of robustness and resilience start to play a decisive role in technological applications too. Ideally, a functional system should acquire high robustness capacity without a significant increase of its size and of the frequency of regulatory interactions. Thus, various - and often conflicting - constraints need to be satisfied in system's design, leading to situations characterized by frustration. The natural solution provided by biological organisms to such problems is that they are treated through the process of evolution. The question is whether evolutionary optimization methods can also be applied to design artificial functional systems with high robustness. In this talk, we show that artificial network-based systems with high levels of functional robustness, comparable to those of actual biological organisms, can indeed be obtained through the optimization of network architecture based on simulated annealing. As two examples, synthetic oscillatory genetic networks and flow distribution networks, representing prototypes of industrial or logistic networks, are chosen.

Invited Talk BP 19.4 Thu 11:00 H 0105

Braess Paradox, (In-)Stability and Optimal Design: Nonlinear Dynamics of Modern Power Grids — •Marc Timme[1,2], Dirk Witthaut[1], Martin Rohden[1], and Andreas Sorge[1,2] — [1]Network Dynamics Group, MPI for Dynamics and Self-Organization, Goettingen — [2]Faculty of Physics, University of Goettingen

Distributed, renewable energy sources will dominate the dynamics of future electric power grids. Upgrading grids for decentralized sources poses an enormous challenge for its design and stable operation and constitutes a multi-billion Euro business.

Bridging the gap between abstract statistical physics and detailed engineering device modeling, we are aiming to understand nonlinear power grid dynamics at an intermediate level using simple but dynamic coarse-scale oscillator models. Substantial results so far include: 1) The addition of new transmission lines may *destabilize* power grid operation (via Braess paradox that we identified in oscillator networks). 2) More and smaller, but distributed power sources may *stabilize* grid operation. Our results indicate that coarse-scale modeling of power grids by oscillator networks seems feasible for the study of their self-organized synchronization dynamics.

References:

Dirk Witthaut and Marc Timme, Braess Paradox in Oscillator Networks and Power Outage, under review (2012)

Martin Rohden, Andreas Sorge, Marc Timme, and Dirk Witthaut, Self-Organized Synchronization of Decentralized Power Grids, in prep. (2012)

Invited Talk BP 19.5 Thu 11:30 H 0105

Delay-Coupled Laser Networks: Complex Behavior, Synchronization and Applications — •Ingo Fischer — IFISC (Instituto de Física Interdisciplinar y Sistemas Complejos), Campus UIB, 07122 Palma de Mallorca, Spain

Semiconductor lasers are known to be very sensitive to external feedback, as well as to input from other lasers. This sensitivity, due to the nonlinear interaction of lasing field and semiconductor medium and the unavoidable delays in feedback and coupling, often results in emerging complex behavior. At the same time the nonlinear interactions lead to synchronization phenomena. For a long time such behavior has been considered undesired and difficult to treat experimentally and theoretically. Recently, tools to treat these systems have been developed, coupled lasers are serving as testbed systems for delay-coupled networks and suggestions for applications have been proposed. In this presentation we provide examples of the advances and discuss the perspectives of such systems.

BP 20: Regulation

Time: Thursday 9:30–13:00 Location: H 1058

Invited Talk BP 20.1 Thu 9:30 H 1058

Precision of sensing, memory, and fluctuating environments — •Robert Endres[1,2] and Gerardo Aquino[1,2] — [1]Division of Molecular Biosciences, Imperial College, London, UK — [2]Centre for Integrative Systems Biology and Bioinformatics, Imperial College, London, UK

Biological cells are known to sense their chemical environment with astonishing accuracy, crucial for nutrient scavenging, mating, immune response, and development. It is unknown if this sensing near the single-molecule detection limit is due to highly precise single measurements or due to learning over time. In this work, we analyze if cell memory can allow cells to sense beyond current estimates of the fundamental physical limit. By merging Bayesian inference with information theory, we derive analytical formulas which show that memory helps for sensing of correlated fluctuating environments, but not for sensing of strongly uncorrelated fluctuating environments. Despite many analogies with problem-solving strategies in engineering, our theory shows fundamental differences in interpreting noisy stimuli in the microscopic and macroscopic world.

BP 20.2 Thu 10:00 H 1058

Precision and synchronization of coupled genetic oscillators — •David J. Jörg[1], Luis G. Morelli[1,2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany

Biological systems rely on oscillatory processes serving as pacemakers to control important functions during development and life. Within cells, periodic patterns of activity can be generated by oscillations of protein concentrations. Intracellular fluctuations in protein numbers impair the precision of oscillations and thus limit their viability as pacemakers. In multicellular systems, communication between cells can couple their dynamics, give rise to synchronization, and affect the precision of oscillations. To study the effects of coupling on cell-autonomous oscillators in small cell clusters, we have devised a generic stochastic model that comprises negative feedback oscillators coupled through mutual regulation of protein production. We found that average coupling delays determine whether coupling improves or impairs the precision of oscillations and the ability to synchronize.

BP 20.3 Thu 10:15 H 1058

Rare switching in non-stationary gene regulation networks —

•Nils Becker and Pieter Rein ten Wolde — AMOLF Institut, Amsterdam

Rare barrier-crossing events act as dynamical bottlenecks in a broad variety of physical and biological systems. Examples include crystal nucleation, earthquakes, population genetics, protein folding and genetic switches. In biological systems, the switch-like response to a time-dependent signal can be central to their function. For in- stance, metastable biochemical networks switch in response to time- dependent stimuli in a switch-like manner, and sensory cells react stochastically to weak transient signals. Here the system response depends on the temporal characteristics of the input and cannot be characterized by a single rate constant. We present a novel enhanced sampling method, Non-Stationary Forward Flux Sampling, that al- lows efficient simulation of rare events in these systems. Using the method, we investigate the time-dependent response of a model system based on the phage-lambda genetic switch.

BP 20.4 Thu 10:30 H 1058

Sources of Stochasticity in Protein Synthesis — •David Gomez[1,2], Rahul Marathe[1], and Stefan Klumpp[1] — [1]Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam, Germany. — [2]Freie Universität Berlin, Arnimalle 14, 14195 Berlin, Germany

All living organisms are unique, even isogenic one in the same environmental conditions or have the same history. An explanation of such behavior is given by the fluctuations of the biochemical reactions within them. These fluctuations are become important when the number of the molecules involved in the biochemical reactions is low. Because the number of proteins, DNA, RNA are often small in the cell, one can expect large variation in the biochemical reactions.

The objective of this work is to model the variations of the protein synthesis in the by cell birth-death processes. To do that, we considered protein synthesis in cells, that after a cell division time, T , divide into two daughter cell. This process is done either in a deterministic or a stochastic way. In a first approximation the volume of the cells was not considered, but to describe protein concentrations, the growth and division of the cell volume was also incorporated into the model.

The consideration of the volume in our model, leaves us the opportunity to study regulatory cell processes, which are concentration-dependent, such as the negative feedback regulation model.

BP 20.5 Thu 10:45 H 1058

Consequences of degradation and aging of messenger RNA — •Carlus Deneke, Angelo Valleriani, and Reinhard Lipowsky — MPI für Kolloid- und Grenzflächenforschung, Department of Theory and Bio-Systems, Potsdam, Germany

In gene expression, the transcription and degradation of mRNA plays a central role. Various degradation mechanisms exist that actively regulate the stability of mRNA. The stability not only determines the steady state amount of mRNA in each cell, it sets also important time scales when transcription is either turned on or off.

In this contribution, we present a theoretical framework that describes various transient phenomena in gene expression. It extends previous studies as it is capable of considering various biochemical mechanisms of degradation. Furthermore, it also fully accounts for the stochasticity of both, transcription and degradation of mRNA. This framework will allow to describe the response of the cell to external stimuli which modulate the transcription of certain genes.

BP 20.6 Thu 11:00 H 1058

Maximising positional information of morphogen gradients in the Drosophila embryo — •Tiago Ramalho and Ulrich Gerland — Arnold Sommerfeld Center, Dept. of Physics, Ludwig Maximilians Universität München, Theresienstr. 37 80333 München, Germany

Information about position along the antero-posterior axis in Drosophila can be encoded in morphogen spatial distribution profiles. To decode this position, a parameter estimation procedure must be implicitly used by the biological system. Fisher information, an abstract measure of the precision with which a parameter can be estimated is applied to this context and resulting optimal profiles are calculated. The information theoretical results are compared to a model which optimizes morphogen profiles for biological function.

15 min break

BP 20.7 Thu 11:30 H 1058

On the role of intrinsic noise on the response of the p53-Mdm2 module — Lidice Cruz[1], Nuris Figueroa[1], and •Roberto Mulet[1,2] — [1]Group of Complex Systems. Physics Faculty. University of Havana — [2]Quantum optics and statistics Institute of Physics Albert Ludwigs University of Freiburg

The protein p53 has a well established role in protecting genomic integrity in human cells. In particular, the p53-Mdm2 feedback loop seems to be the key circuit in the response of cells to damage. Recent measurements in individual human cells have shown that p53 and its regulator Mdm2 develop sustained oscillations over long periods of time, with essentially fixed frequency but variable amplitudes. Here, we propose that the noise that stabilizes the fluctuations is the intrinsic noise due to the finite nature of the populations of p53 and Mdm2 in a single cell.

We study three stochastic models of the p53-Mdm2 circuit. The models intend to capture the response of the p53-Mdm2 circuit in its basal state, in the presence of DNA damage, and under oncogenic signals.

We show that the in all the cases the noise induced by the finite size of the populations is responsible for the existence of sustained oscillations in the response of the p53-Mdm2 circuit. This noise alone can explain most of the experimental results obtained studying the dynamics of the p53-Mdm2 circuit in individual cells.

BP 20.8 Thu 11:45 H 1058

A kinetic model for RNA interference of focal adhesions — •Max Hoffmann[1,2] and Ulrich Schwarz[1,2] — [1]Bioquant, Heidelberg University, Heidelberg, Germany — [2]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

Focal adhesions are integrin-based cell-matrix contacts and transduce and integrate mechanical and biochemical cues from the environment. More than 150 different proteins localize to focal adhesions and have been systematically classified in the adhesome project (www.adhesome.org). First RNAi-screens have been performed for focal adhesions and corroborated the hierarchical structure suggested by the adhesome project. We have developed a kinetic model for RNA interference of the focal adhesion hierarchy with explicit representation of siRNA-concentration and implicit effects of mechanical force. For the first time a link is made between the dynamics of RNA interference and the assembly dynamics of focal adhesions. Our kinetic model shows a variety of features for focal adhesions under the influence of RNA interference. Two basic time scales of the dynamics of RNAi-influenced focal adhesions are verified: a short one for the adaptation of the focal adhesions to changes in the environment, and a much longer one that controls the siRNA-mediated knockdown. A sensitivity analysis provides insight into the response of the focal adhesions to rate or parameter changes. This knowledge can be used to optimize the effect of RNA interference on focal adhesions. We show that different force models can lead to largely differing results.

BP 20.9 Thu 12:00 H 1058

Modeling MARCKS and Protein Kinase C binding at cellular membranes — •Sergio Alonso and Markus Bär — Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, 10587 Berlin, Germany

Phosphorylation and dephosphorylation of proteins are mechanisms of activation and deactivation which regulate many cell processes. MARCKS is a protein which binds to the membrane by electrostatic interaction. It is phosphorylated by Protein Kinase C and translocated from the membrane. In the cytoplasm phosphorylated MARCKS is dephosphorylated by phosphatases and can bind again at the membrane. The three processes give rise to a cyclic dynamics known as myristoyl-electrostatic switch. We propose a reaction-diffusion model obeying mass conservation for the binding, phosphorylation and dephosphorylation of MARCKS proteins. Furthermore, we add to the model the dynamics of binding and unbinding of PKC enzymes, which are activated by spikes of calcium.

BP 20.10 Thu 12:15 H 1058

Emergence of Information Transmission in a Prebiotic RNA Reactor — •Benedikt Obermayer[1], Hubert Krammer[2], Dieter Braun[2], and Ulrich Gerland[2] — [1]Department of Physics, Harvard University, Cambridge, USA — [2]Physics Department, Ludwig-Maximilians-Universität München

A poorly understood step in the transition from a chemical to a biological world is the emergence of self-replicating molecular systems. We

study how a precursor for such a replicator might arise in a hydrothermal RNA reactor, which accumulates longer sequences from unbiased monomer influx and random ligation [1]. In the reactor, intra- and intermolecular base pairing locally protects from random cleavage. Analyzing stochastic simulations, we observe a strong bias towards long sequences with complex secondary structures, which would facilitate the emergence of ribozymes. Further, we find temporal sequence correlations that constitute a signature of information transmission, weaker but of the same form as in a true replicator.

[1] B. Obermayer, H. Krammer, D. Braun, U. Gerland, Phys. Rev. Lett. **107**:018101 (2011)

BP 20.11 Thu 12:30 H 1058

Physical limits of replication accuracy under nonequilibrium prebiotic conditions — Benedikt Obermayer[1] and •Ulrich Gerland[2] — [1]Department of Physics, Harvard University, USA — [2]Department of Physics, LMU München, Germany

Without the help of kinetic proofreading enzymes that can employ chemical energy to improve the accuracy of template-directed replication processes, the mutation rate of these processes is limited from below by fundamental principles of statistical physics. This limit is particularly relevant for prebiotic copying processes of a polynucleotide such as RNA, before the advent of kinetic proofreading enzymes. Under equilibrium conditions, the limit is directly related to a free energy of discrimination related to the difference in the thermodynamic stability of the correct and the incorrect products. However, when the system in which the copying process takes place is not in equilibrium, the lower physical limit on the mutation rate can be changed. We discuss a situation where physical nonequilibrium can improve the replication accuracy, optimize the conditions of the system, and relate our scenario to recent experiments on non-enzymatic template-directed copying processes.

BP 20.12 Thu 12:45 H 1058

One Dimensional Evolution of DNA-Fragment Replication — •Emanuel Worst[1], Eva Wollrab[1], Philipp Zimmer[2], Karsten Kruse[2], and Albrecht Ott[1] — [1]Universität des Saarlandes, Biologische Experimentalphysik, Postfach 151150, 66041 Saarbrücken — [2]Universität des Saarlandes, Theoretische Biologische Physik, Postfach 151150, 66041 Saarbrücken

We study the dynamics of an enzyme-based, self-replicating system consisting of DNA fragments and Taq DNA ligase. The aim is to achieve a dynamic equilibrium of self-reproducing DNA strands that evolve towards longer strands in a stepwise manner, through the occurrence of rare events. In the present realization, the ligation of DNA molecules A and B by Taq DNA ligase creates a DNA molecule T with a low probability. Hybridization of A and B on the template T brings the reactive 3‘-end (hydroxyl group) of A and 5‘-end (phosphate group) of B very close to each other. This increases the ligation probability by the Taq DNA-ligase and leads to strongly increased replication of T. Presently the autocatalytic reproduction of even longer strands is insufficient, it is prevented by strong side reactions. This is a problem, which needs to be addressed in the future.

BP 21: Focus: Stress Relaxation in Polymers - From single molecules to biological cells (with CPP)

The session provides a synopsis of stress relaxation in polymeric materials, ranging from synthetic to biological polymers and from single molecule studies to network properties and their relevance for live cells and tissues. (Organizers: R. Magerle, K. Kroy)

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

Invited Talk BP 21.1 Thu 9:30 C 243

Stress relaxation and chain dynamics in entangled polymer melts — •Ralf Everaers — Laboratoire de Physique, ENS Lyon, 46 allee d'Italie, F-69364 Lyon, France

High molecular weight polymeric liquids display remarkable viscoelastic properties. Contrary to glassy systems, their macroscopic relaxation times are not due to slow dynamics on the monomer scale, but arise from the chain connectivity and the restriction that the chain backbones cannot cross. We use a combination of analytical theory and computer simulations to arrive at a quantitative description of the complex relaxation scenario expected from current versions of the tube model. Our data for the stress relaxation in equilibrium and step-strained bead-spring polymer melts allow us to explore the chain dynamics and the shear relaxation modulus, $G(t)$, into the plateau regime for chains with $Z = 40$ entanglements and into the terminal relaxation regime for $Z = 10$. We have performed parameter-free tests of several different tube models using the known (Rouse) mobility of unentangled chains and the melt entanglement length determined via the primitive path analysis of the microscopic topological state of our systems. We find excellent agreement for the Likhtman-McLeish theory using the double reptation approximation for constraint release, if we remove the contribution of high-frequency modes to contour length fluctuations of the primitive chain. In particular, we rationalize the onset of entanglement constraints in polymeric liquids via an analysis of the short-time dynamics of (primitive) chains.

BP 21.2 Thu 10:00 C 243

Direct stress measurements in nonequilibrium thin polymer films. — •Katherine Thomas[1] and Ullrich Steiner[2] — [1]Max Planck Insitute for Dynamics and Self-Organisation, Goettingen, Germany — [2]Department of Physics, University of Cambridge, UK

Residual stresses in polymer films often arise from the solution deposition protocol. The origin of stresses in polymer films is easily justified: film formation by solvent evaporation steadily increases the polymer concentration, raising the glass transition temperature of the solution. When Tg reaches the ambient temperature the polymer vitrifies, suppressing further equilibration of the chains. Due to the entangled nature of the polymer network, evaporation of the remaining solvent induces substantial biaxial tensile stresses. Stresses in thin films are not, however, easy to measure and can often only be deduced indirectly.

Here stresses were quantitatively determined by measuring the deflection of cantilevers cut from film-covered SiN membranes using a focused ion beam. Spin-cast films showed notably high residual stresses, far greater than the bulk polymer tensile strength. Stress relaxation via thermal annealing suggests two relaxation mechanisms, both much faster than the reptation time. The fast relaxation indicates that the stress arises from segmental deformations of the chains, rather than entropic effects. Comparison of these data with EHD film stability experiments, suggests the same relaxation mechanisms, providing further evidence for the existence of a thin, highly stressed layer at the surface of the film. These experiments show the utility of our method for the systematic examination of non-equilibrium thin film properties.

BP 21.3 Thu 10:15 C 243

Mechanical stress relaxation in polymers followed by low-field NMR — Ute Böhme and •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Low-field NMR provides information on molecular mobility over a wide range of rates of motion. In-situ low-field NMR has been applied on polymers under uniaxial stress [1]. Strongest stress-induced effects have been observed in T2 (indicative for slow motion) and T1rho (indicative for mtion of rates of kilohertz) both indicating restictions in the motion of polymer segments. In elastomers the changes a reversible after release of the external stress. Time-dependent experiments at constant extension on semicrystalline polymers show a return of both relaxation times to the values of the non-stressed sample. However, the time constant of that return is significantly longer than that observed in mechanical stress-relaxation experiments.

[1]Böhme, U.; Gelfert, K.; Scheler, U. Solid-state NMR of polymers under mechanical stress AIP conference proceedings 1330 (2011) 109

BP 21.4 Thu 10:30 C 243

Stress Induced Single Molecule Reorientation Motion in Elas-

tomeric Polypropylene — •Stefan Krause, Martin Neumann, Melanie Bibrach, Robert Magerle und Christian von Borczyskowski — Fakultät für Naturwissenschaften, TU Chemnitz, D-09107 Chemnitz

The fluorescence of a single molecule (SM) is a very sensitive probe for its environment and changes of the fluorescence lifetime, emission wavelength, and polarization can report spatial and temporal variations in the surrounding structure of the fluorescent dye. Here we report on SM microscopy and spectroscopy studies of stress relaxation in thin films of elastomeric polypropylene (ePP), a semicrystalline polymer with a complex microstructure of crystalline and amorphous regions on the nanometer scale. The films are stretched using a micro tensile testing setup. Simultaneously, perylenediimide dyes functionalized with hexadecane were embedded in the ePP film and report via their molecular dynamics changes within their local environment. Orientation fluctuations were investigated via SM polarization dependent microscopy. This experiment allows for insights into dynamical processes within the amorphous regions of ePP which are not accessible using other microscopy techniques.

Invited Talk BP 21.5 Thu 10:45 C 243

Slow stress relaxation in recoiling polymers — •Ulrich F. Keyser — Cavendish Lab, University of Cambridge, JJ Thomson Ave, Cambridge, CB3 0HE, UK

The internal dynamics of semi-flexible chains in response to external forces is an important problem in soft matter, polymer and biological physics. Here, we describe a novel method to experimentally determine the relaxation of a single DNA molecule with one free end. The electric field in a nanopore[1] or nanocapillary[2] is used to apply a controlled force to one end of a DNA molecule while the other end is held in an optical trap[3,4]. High-speed video tracking of the colloidal particle[5] allows for a direct measurement of the relaxation in the recoiling DNA upon release from the nanopore. We show and discuss our single-molecule experiments for a range of forces and find that stress relaxation and recoiling is much slower than expected from the simple worm-like chain model. Our results pave the way towards investigating the nonlinear dynamics of semiflexible polymer relaxation and test recent theories[6] on propagation and relaxation of backbone tension in DNA.

[1] Keyser et al., Nature Physics 2, 473 (2006) [2] Steinbock et al., Nano Letters 10, 2493 (2010) [3] Steinbock et al., J. Phys. Cond. Mat. 23, 184114 (2010) [4] Otto et al., Rev. Sci. Instr. 82, 086102 (2011) [5] Otto et al., Optics Express 18, 22722 (2010) [6] Hallatschek et al., Phys. Rev. E 75, 031906 (2007)

BP 21.6 Thu 11:15 C 243

Non-Equilibrium Relaxation in Polymer Solutions — •Chien-Cheng Huang, Gerhard Gompper, and Roland G. Winkler — Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

Individual DNA molecules in shear flow exhibit large conformational changes due to tumbling motion. A polymer continuously undergoes stretching and compression cycles with a characteristic frequency, which depends on the shear rate. To characterize the tumbling behavior, we perform large-scale non-equilibrium mesoscale hydrodynamic simulations of semidilute polymer solutions, which combine molecular dynamics simulations and the multiparticle collision dynamics approach. The non-equilibrium polymer end-to-end vector relaxation times in the stationary state exhibit the shear rate dependence $\dot{\gamma}^{-2/3}$. In the dilute limit, the relaxation times for the various spatial directions are identical. For semidilute solutions, screening of hydrodynamic interactions leads to a slower and faster relaxation in the vorticity and gradient directions, respectively. The relaxation times are equal to the tumbling times extracted from cross-correlation functions of fluctuations of radius-of-gyration components. Furthermore, we find a memory effect in the tumbling dynamics, which causes an oscillatory relaxation along the flow and gradient directions. This memory effect decreases with increasing polymer length and is believed to be less pronounced or even absent for long polymers.

BP 21.7 Thu 11:30 C 243

Stress relaxation through crosslink unbinding in biopolymer assemblies — •Claus Heussinger — Institute for theoretical physics, University Göttingen

The cytoskeleton is a complex meshwork of long elastic filaments coupled together with the help of numerous, rather compact crosslinking proteins. An important aspect of a cytoskeletal polymer network is its dynamic nature, which allows it to react to external stimuli and adapt its internal structure and mechanical properties according to the needs of the cell. The reversible nature of crosslink binding is an important mechanism that underlies these dynamical processes.

In this contribution we devise a simple model polymer network to study the effect of network deformation on the crosslink binding processes. We evidence a discontinuous and sudden rupture transition after which the network is no longer able to resist the external load. By combining MC simulation with a necklace-type model (M. Fisher, J. Stat. Phys. (1984)) we discuss the role of the mechanical stiffness of the crosslinks and the fluctuation properties of the filaments. This allows to address the interplay of strain stiffening inherent in the entropic response of individual polymers, and strain softening due to crosslink unbinding.

BP 21.8 Thu 11:45 C 243

Thermorheology of single living cells — •Tobias R. Kiessling, Anatol W. Fritsch, Roland Stange und Josef Käs — Universität Leipzig, Institut für Experimentelle Physik I, Physik der weichen Materie, Linnéstr. 5, 04103 Leipzig

Within reasonable temperature ranges, many biological functions are known to undergo modulations, like myosin motor activity, CO2 uptake of cultured cells or sex determination of several species. As mechanical properties of living cells are considered to play a key role for plenty of cell functions ranging from stem cell differentiation to cancer progression, it is surprising that only little is known on how their rheology is affected by temperature. Using an Optical Stretcher, thousands of single cell experiments were performed to systematically assess the effect of temperature on cell deformability. The impact of slow temperature changes occurring on a scale of about 30 minutes is compared to the influence of defined heat shocks in a range of milliseconds. Differences of thereby revealed temperature dependencies are discussed and compared to findings from in vitro rheological studies on polymer solutions.

Invited Talk BP 21.9 Thu 12:00 C 243

Cytoskeletal stress in collective cell migration — •Xavier Trepat — Institute for Bioengineering of Catalonia, Barcelona, Spain

For a group a living cells to migrate cohesively, it has long been suspected that each constituent cell must exert physical forces not only upon its extracellular matrix but also upon neighboring cells. I will present the first comprehensive maps of these distinct force components. These maps reveal an unexpectedly rich physical picture in which the distribution of physical forces is dominated by heterogeneity, both in space and in time, which emerges spontaneously propagates over great distances, and cooperates over the span of many cell bodies. Both in epithelial and endothelial cell sheets, these heterogeneous forces are mechanically linked to cell velocities through a newly discovered emergent mechanism of innately collective cell guidance: plithotaxis.

BP 22: Statistical Physics of Biological Systems III (with DY)

Time: Thursday 15:00–17:30 Location: H 1058

BP 22.1 Thu 15:00 H 1058

Predicting the evolution of the transport network of *Physarum polycephalum* — •Werner Baumgarten and Marcus Hauser — Abteilung Biophysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Germany

The plasmodium of the unicellular slime mould *Physarum polycephalum* forms a characteristic two-dimensional vein network, which extends in search of food. Protoplasm is transported periodically back and forth through the tubular network. With time, the network coarsens by deletion of the least efficient pathways.

The vein network of *P. polycephalum* is a weighted, undirected, regular graph where the veins form the edges and the branching points the nodes [1,2]. The weight is given by the local drag through each vein segment and the efficiency of the transport pathways is calculated using Dijkstra's algorithm [3] and the edge betweenness. This provides for a predictive tool to identify the least effective veins, and to predict the evolution of the network.

[1] W. Baumgarten, M.J.B. Hauser, Phys. Rev. E 82, 046113 (2010).
[2] W. Baumgarten, M.J.B. Hauser, J. Comp. Interdisc. Sci. 1, 241 (2010).
[3] E.W. Dijkstra, Num. Math. 1, 269 (1959).

BP 22.2 Thu 15:15 H 1058

Universal Network Percolation in the Slime Mold *Physarum polycephalum* — •Adrian Fessel[1,2], Christina Oettmeier[1,2], Erik Bernitt[1,2], and Hans-Günther Döbereiner[1,2] — [1]Institut für Biophysik, Universität Bremen, 28334 Bremen, Germany — [2]Mechanobiology Institute, National University of Singapore, 117411 Singapore, Singapore

The tubular vein network formed by the true slime mold *Physarum polycephalum* during its plasmodial phase has been subject to various recent studies. However, only the late stages of network growth have been thoroughly investigated. We analyze fusion-driven early morphogenesis of the plasmodial network via advanced digital image processing, revealing a prominent percolation transition universally present in biological networks. Physarum networks are grown from scattered microplasmodia on an agar-covered petri dish. Images are taken every minute over multiple days using a high-resolution digital camera. We found an exact solution to the percolation transition for small link degree which predicts the percentage of nodes observed in the largest component without an adjustable parameter.

BP 22.3 Thu 15:30 H 1058

Mutual Repression enhances Gene Boundary Precision by Steepening — •Thomas R. Sokolowski[1], Thorsten Erdmann[2], and Pieter Rein ten Wolde[1] — [1]FOM Institute AMOLF, Science Park 104, 1098XG Amsterdam, The Netherlands — [2]University of Heidelberg, Institute for Theoretical Physics, Philosophenweg 19, 69120 Heidelberg, Germany

Embryonic development is driven by spatial patterns of gene expression that determine the fate of each cell in the embryo. While gene expression is often highly erratic, embryo development is usually exceedingly precise. How development is robust against intra- and inter-embryonic variations is not understood. To assess the role of mutual repression in the robust formation of gene expression patterns, we have performed spatially resolved large-scale stochastic simulations of two gap genes in Drosophila melanogaster, hunchback (hb) and knirps (kni), which are activated by their morphogens Bicoid (Bcd) and Caudal (Cad), respectively, and mutually repress each other. Our analysis shows that mutual repression can markedly increase the steepness and precision of the gap gene expression boundaries. Moreover, it dramatically enhances their robustness against embryo-to-embryo variations in the morphogen levels. Finally, our simulations reveal that diffusion of the gap proteins plays a critical role not only in reducing the width of the gap gene expression boundaries via the mechanism of spatial averaging, but also in repairing patterning errors that could arise because of the bistability induced by mutual repression.

BP 22.4 Thu 15:45 H 1058

Buffering of the intracellular ribosome pool and protein production by ribosomal queues — •Philip Greulich[1], Luca Ciandrini[2], Mamen C. Romano[2], and Rosalind J. Allen[1] — [1]ICMCS, School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom — [2]Institute for Complex Systems and Mathematical Biology, King's College, University of Aberdeen, Aberdeen, United Kingdom

In cells, mRNAs compete for a finite number of ribosomes when producing proteins. Thus, high production of one protein can lower the expression of others, since many ribosomes are bound on mRNAs of the former one and are not available for others. This effect is also known as "protein burden".

mRNA sequences can contain "slow" codons where ribosomes proceed much slower than on other parts of mRNA. These slow codons act as bottlenecks to protein synthesis, which can lead to ribosome queues on the mRNA molecules. We present a stochastic model for the traffic of ribosomes on many mRNAs competing for a finite pool of particles. Using realistic sequences of fast and slow codons, we show that ribosomal queues can effectively buffer the free ribosome pool, making it independent of fluctuations in mRNA-number and total amount of ribosomes. The effect can reduce the protein burden due to high expressions of a single gene. This mechanism works instantaneously and does not require explicit regulation of the ribosome pool.

Our results may have significant implications for cells' ability to respond independently to multiple demands on the ribosome pool.

BP 22.5 Thu 16:00 H 1058

Modeling a Circadian Clock's Slave Oscillator in *Arabidopsis thaliana* — •Christoph Schmal[1,2], Dorothee Staiger[1], and Peter Reimann[2] — [1]Molecular Cell Physiology, Faculty of Biology — [2]Condensed Matter Theory, Faculty of Physics, Bielefeld University

Circadian clocks, generating self-sustained or slowly damped oscillations with a period of approximately 24 hours are usually described as transcriptional-translational feedback loops and can be found in nearly all eukaryotes and some prokaryotes. Entrainment by environmental signals, e.g., light, synchronizes the clock to the period of the Earth's rotation.

It still remains unclear how the rhythmicity of the clock is transmitted to its output pathways. Slave oscillators could be candidates. The RNA binding proteins *At*GRP7 and *At*GRP8 may represent such a slave oscillator. The transcription of both genes is rhythmically repressed by the partially redundant core oscillator genes LHY/CCA1 and they further shape their oscillatory profile via auto- and cross-regulating each other using an alternative splicing mechanism.

We model the system in terms of ordinary differential equations and estimate the barely known parameters with a cost function that quantifies the overlap between our model and key experimental features. Properties such as the waveform, the period and the phase of the oscillations, the mRNA and protein half-life and the response to varying photoperiods found in our simulations are compared with experimental findings. We make also suggestions and predictions for further experiments.

BP 22.6 Thu 16:15 H 1058

Investigating intrinsic fluctuations in biochemical systems — •Joseph Challenger[1], Jürgen Pahle[2], Alan McKane[1], and Pedro Mendes[2] — [1]School of Physics and Astronomy, The University of Manchester, Manchester, UK — [2]Manchester Interdisciplinary Biocentre, The University of Manchester, Manchester, UK

In many biochemical reaction systems it is important to be able to quantify the stochastic fluctuations that are present. Deterministic rate equations, which are often used to describe these systems mathematically, do not allow for these fluctuations. An alternative, probabilistic, formalism is available, using the master equation. An approximate solution to this equation can be found using the van Kampen expansion, which provides leading order corrections to the rate equations. The terms in the expansion relate to objects in the rate equations in a very general way. We show how this approach can be generalised to biochemical systems which involve many neighbouring compartments.

We have incorporated this technique into COPASI, a software package designed to study biochemical reaction systems. This allows the procedure to be automated. Given a particular reaction system, COPASI calculates the fluctuations around the system's steady state. This analysis can be performed in tandem with the other tasks available in COPASI e.g. parameter scanning or optimisation. This is useful if there is uncertainty associated with numerical values of some of the reaction parameters. If the fluctuations are calculated via numerical simulation, these tasks can be computationally expensive. In contrast, these calculations can be done quickly using our approach.

BP 22.7 Thu 16:30 H 1058

Brownian dynamics simulation with hydrodynamic interactions of crowded protein solutions — •Paolo Mereghetti[1,2] and Rebecca Wade[1] — [1]Heidelberg Institute for Theoretical Studies (HITS) gGmbH, Schloß-Wolfsbrunnenweg 35, 69118 Heidelberg, Germany — [2]Interdisciplinary Center for Scientific Computing (IWR), University of Heidelberg, Im Neuenheimer Feld 368, 69120 Heidelberg, Germany

The study of solutions of biomacromolecules provides an important basis for understanding the behavior of many fundamental cellular processes, such as protein folding, self-assembly, and signal transduction. We have developed the SDAMM Brownian dynamics simulation software to investigate the dynamic and structural properties of dilute protein solutions. In the model used, the proteins are treated as

atomically detailed rigid bodies moving in a continuum solvent. The method showed good agreement with experimental data for proteins of concentrations up to 60 g/L even though hydrodynamic interactions were neglected. We here describe new developments of the simulation model to extend the range of applicability to protein solutions as concentrated as cell-like environments where the effect of hydrodynamic interactions cannot be neglected. To take hydrodynamic interactions into account, we use a mean field model and we apply the method to investigate the behaviour of concentrated solutions (up to 40% volume fraction) of normal and sickle cell hemoglobin, and of myoglobin. From these simulations, we assessed the effects of hydrodynamic interactions, short-range interactions and excluded volume effects on diffusion.

BP 22.8 Thu 16:45 H 1058

Implicit Electrohydrodynamics of Polyelectrolytes Using Lattice-Boltzmann — •Owen A. Hickey and Christian Holm — Institut für Computerphysik, Universität Stuttgart, Deutschland

We make use of an implicit method to simulate the electrohydrodynamics of a polyelectrolyte to an external electric field. The method uses a new coupling of Lennard-Jones beads to a lattice-Boltzmann fluid which forces the difference between the velocity of a bead and the local fluid velocity to be the Smoluchowski slip velocity. The method is validated by first simulating the free solution electrophoresis of polymers. The technique is then used to verify the surprising result that the force necessary to hold a charged polymer at rest in an electric field is proportional to the hydrodynamic radius, and not the total charge on the polymer. Further results show other surprising effects, like how heterogeneously charged objects with no net charge can have non-zero mobilities and that they can even move perpendicular to the applied electric field.

BP 22.9 Thu 17:00 H 1058

Using Branching Processes to Model Critical Neuronal Networks — •Anna Levina[1,2], J. Michael Herrmann[3], and Theo Geisel[1,4] — [1]BCCN Göttingen, Germany — [2]MPI MIS, Leipzig, Germany — [3]University of Edinburgh, UK — [4]MPI DS, Göttingen, Germany

Many authors use branching processes (BPs) formalism to model critical neuronal networks. It is indeed very tempting, because BP are a well studied mathematical concept, where it is easy to define what is critical and what is not. Additionally, for BPs it is proved, that a distribution of avalanche sizes follows a power-law with an exponent -3/2. However, only in very few cases does the approximation of activity propagation in a neuronal network by BPs have a rigorous basis. Moreover, a straightforward BPs approximation fails in the presence of delays in the network. Nevertheless, this approach is still used unrestricted to argue about a critical network even for the small system sizes, where the discrepancies are very large.

Here we present analytical and numerical results illustrating reservations in using BPs approximation and ways to overcome them. We show analytically that in the case of a simple neuronal network with a probabilistic synaptic transmission BPs can be used as a valid model in the large network limit. However, for small networks the finite-size corrections are required. We derive these corrections and also discuss how to modify them in the presence of delays. This topic is especially interesting for a growing field of self-organized critical neuronal networks, where branching approximation is used ubiquitously.

BP 22.10 Thu 17:15 H 1058

Solution of the Fokker-Planck equation for neurons with adaptation — •Tilo Schwalger and Benjamin Lindner — Institute of Physics, Humboldt-University at Berlin; Bernstein Center of Computational Neuroscience, Berlin, Philippstr. 13,10115 Berlin

Firing rate adaptation is an ubiquitous features of neurons throughout the nervous system. Slow adaptation currents that act as a negative feedback give rise to an intricate neuron dynamics leading to a characteristic spiking statistics already in the spontaneous firing activity. A prominent example are negative correlations between interspike intervals, which have been frequently measured in experiments. We have recently derived an analytical expression of the correlation coefficient of a perfect integrate-and-fire neuron with an adaptation current [1]. This result holds in the deterministic limit, where the white-noise driving is infinitesimally small. To extend the result to stronger noise driving, it is necessary to determine self-consistently the stationary distribution of the adaptation current sampled at the spike times. To this end, we solve the associated two-dimensional Fokker-Planck equation about the deterministic limit distribution: this amounts to a WKB approximation for weak noise. Our approximations of the solution are compared with extensive simulations of the adapting neuron model.

[1] Schwalger T, Fisch K, Benda J, Lindner B, Plos Comp Biol., 2010

BP 23: Cytoskeletal Filaments

Time: Thursday 15:00–17:00 Location: H 1028

Invited Talk BP 23.1 Thu 15:00 H 1028

Actin network architecture determines myosin motor activity — •Laurent Blanchoin — CNRS & UJF, Grenoble, France

The organization of actin filaments into higher-ordered structures governs overall eukaryotic cell shape, mechanical integrity and directed movement. Global actin network size and architecture is maintained in a dynamic steady-state through regulated assembly and disassembly. We use geometrically controlled and polarized in vitro actin structures to evaluate how myosin motors, that play a critical role in this process, influences network architecture. Direct visualization of filaments demonstrates the spectacular myosin-induced actin network deformation. We determine that during this reorganization myosins selectively contract and disassemble anti-parallel actin structures while parallel actin bundles remain unaffected. This orientation selection reveals how the spatial organization and dynamics of the cellular actin cytoskeleton is locally controlled by actomyosin contractility.

BP 23.2 Thu 15:30 H 1028

Mechanical properties of actin bundles — •Florian Rückerl, Timo Betz, and Cécile Sykes — Institut Curie, Laboratoire P.C.C. (UMR168), Paris

Actin bundles can be used as simple models to understand the mechanical properties of filopodia. In our experiments the actin filaments and actin bundles are produced by polymerization by the formin mDia1(FH1FH2). To probe their dynamics and mechanics, we use a state of the art optical tweezers setup and create multiple traps with acousto-optical deflectors (AODs). Digitally controlled AODs in time sharing mode allow to position and move several traps simultaneously. Employing a four quadrant diode as a position detector results in high temporal and spatial resolution, 10μs and <1nm, respectively.

By attaching several beads to individual bundles we can create picoNewton forces in arbitrary directions. This allows the manipulation of individual bundles and, thereby, the investigation of their mechanical properties. These properties, mainly bending rigidity and viscoelasticity, are then probed by bending, pushing and pulling on the bundle.

Effects of different bundling mechanisms, e.g. by depletion forces induced by methyl cellulose (MC) or by crosslinkers like Fascin, as well as the influence of increased Mg^{2+} concentration are being investigated. Preliminary results show, that only low forces (≈8pN) are needed to bend the actin bundles formed by MC, while the elongation of these bundle requires much higher forces (>30pN). Elevated Mg^{2+} concentration (10mM) increases the force in both cases.

BP 23.3 Thu 15:45 H 1028

Direct mechanical evidence of a far reaching soft actin network around reconstituted bead motility systems — •Matthias Bussonnier, Kevin Carvalho, Cécile Sykes, and Timo Betz — Institut Curie, UMR 168, 11 rue Pierre et Marie Curie, 75005 Paris, France

Many fundamental biophysical and biochemical question have been resolved thanks to the bead motility system that mimics *Listeria* motility, where a reconstituted protein mix polymerizes an actin network around the surface of a polystyrene bead. The newly formed actin layer creates mechanical tension by pushing the previously formed actin shell. To gain insight into the mechanical properties of this actin shell we measure the gel mechanics by optical tweezers in a probe-indentation experiment. Approaching a naked probe bead to an actin

coated bead, we directly measure the elastic properties of the gel and find clear evidence of an elastic network extending far away from the bead. A detailed analysis of the data shows that besides the dense and stiff actin gel around the bead, a yet unseen second actin cloud extends around the bead. We measure a distance dependent Youngs modulus that is inversely proportional to the bead distance. This measurement can be explained by a small number of actin filaments, polymerizing away from the bead. To test this model we use different concentration of capping proteins and find a clear influence on the size of the actin cloud. These results further increase the understanding of the *Listeria* motility, and set clear experimental limitations for the analysis of motion in the bead motility system.

BP 23.4 Thu 16:00 H 1028

Formation of regular actin networks as general feature of entropic forces — •Florian Huber, Dan Strehle, Jörg Schnauss, and Josef Käs — Division of Soft Matter Physics, Institute of Experimental Physics I, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Biopolymer networks contribute mechanical integrity as well as functional organization to living cells. The protein actin is one of the major constituents of those structures and was found to be present in a large variety of different network architectures ranging from extensive networks to densely packed bundles or fibers.

We developed a reduced experimental bottom-up system to study the formation of confined actin networks by entropic forces. Experiments based on molecular crowding and counterion condensation allow separating mixing effects from cross-linking effects. This reveals a very general tendency of homogeneous filament solutions to aggregate into regular actin bundle networks connected by aster-like centers. Drastic changes in network architecture directly follow from filament ordering or from flow-induced perturbations of the system.

Complemented by coarse-grained modeling the experiments suggest that regular bundle networks might be a rather general feature of isotropic, homogeneous filament solutions subject to uniform attractive interactions. Due to the fundamental nature of the interactions considered, we further expect severe consequences or restrictions to cytoskeletal network formation on the more complex level of living cells.

BP 23.5 Thu 16:15 H 1028

Evolution of actin networks and bundles in cell-sized confinements — •Siddharth Deshpande and Thomas Pfohl — Department of Chemistry, University of Basel, Switzerland

Actin microfilaments, intermediate filaments and microtubules form the cytoskeleton of a cell along with hundreds of associated proteins. A bottom up *in vitro* approach suits very well to address such a complex system. We study the spatiotemporal evolution of actin network in quasi-2D cell-sized compartments, termed microchambers using a microfluidic system. The solution composition inside the microchambers can be tuned in a controlled manner by changing the composition of the controlling channel to which they are attached. Thus it is a diffusion limited open system.

Atto488 labeled actin monomers along with time-lapse fluorescence microscopy allow us to visualize the formation and evolution of actin networks and actin bundles under different geometric constraints. At higher concentrations of actin (> 1mg/mL) and divalent counterions (Mg^{2+}), stable networks of actin bundles without any cross-linking proteins are obtained and are further analyzed for distribution of link lengths and orientations, connectivity distribution of nodes, etc. The effect of different concentrations of divalent cations (Ca^{2+} and Mg^{2+}) on the network formation is studied and further compared with networks obtained using actin associated proteins like α-actinin.

BP 23.6 Thu 16:30 H 1028

Cooperative dynamics of microtubule ensembles under force — •Björn Zelinski and Jan Kierfeld — TU Dortmund University, Physics Department, Dortmund, Germany

We investigate the cooperative dynamics of an ensemble of microtubules growing against an external elastic force. Stochastic simulations show that the interplay between force sharing and dynamic instability gives rise to complex dynamics with collective catastrophe and collective rescue events. We quantify the dynamic behaviour by a mean field theory, which allows us to estimate the average number of cooperatively pushing microtubules and to calculate the generated ensemble polymerization force and its dependence on microtubule number. We also investigate the dependence on switching rates of the dynamic instability, which can be involved in cellular regulation mechanisms.

BP 23.7 Thu 16:45 H 1028

Structure and dynamics of in vitro cytokeratin networks — •Paul Pawelzyk[1], Harald Herrmann[2], and Norbert Willenbacher[1] — [1]Karlsruhe Institute of Technology (KIT), Institute for Mechanical Process Engineering and Mechanics, Gotthard-Franz-Str. 3, 76131 Karlsruhe, Germany — [2]German Cancer Research Center, Division of Molecular Genetics, Im Neuenheimer Feld 280, 69120 Heidelberg, Germany

Intermediate filament (IF) networks in epithelia cells consist of basic and acidic cytokeratin proteins, which join to heterodimers that assemble into filaments with a diameter of 10 nm. We have investigated networks of keratin 8 and 18 (K8/18) *in vitro* at different protein and $MgCl_2$ concentrations using a combined approach including linear and non-linear rheology, scanning electron microscopy (SEM) and classical biochemical methods. The plateau modulus exhibits only a weak dependency on concentration ($G_0 \sim c^{0.5\pm0.1}$) which is attributed to filament bundling at higher keratin concentrations as confirmed by SEM. The onset of the non-linear stress response σ_{crit} depends only weakly on these parameters. In contrast, the stress σ_{max} at which the network ruptures and the corresponding differential modulus K'_{max} strongly increase with increasing K8/18 or $MgCl_2$ concentration. All data collapse onto a single master curve if K'/G_0 is plotted versus σ/σ_{crit}. Two scaling regimes with different exponents $K' \sim c^{\alpha_i}$ are observed as already predicted by a composite network model including stiff rods connected by flexible linkers, but the experimentally obtained α-values ($\alpha_1 = 1$, $\alpha_2 = 0.6$) are clearly lower than those predicted theoretically.

BP 24: Posters: DNA/RNA and Related Enzymes

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

BP 24.1 Thu 17:30 Poster A

Information transfer and readout in complex DNA mixtures — Harish Bokkasam[1] and •Christian Trapp[2] — [1]Institute for Biological Experimental Physics, University of Saarland, Saarbruecken, Germany — [2]Institute for Biological Experimental Physics, University of Saarland, Saarbruecken, Germany

Project: Development of an enzyme based method for the copy of oligos with predetermined length from biological template, given knowledge of the therein contained oligonucleotide sequence. In this project, we modify the conventional PCR technique by to generate linearly amplified copies of single stranded oligos. To recover the ssDNA transcripts from the linear PCR reaction, various techniques like gel extraction, column filtration, magnetic beads are used. These purified transcripts are fluorescently labelled in different ways like in-strand labelling and 5/3 end labelling for microarray analysis. To visualize ssDNA fragments of very short length and low concentration here denatured polyacrylamide gel electrophoresis with silver staining is used. From this gel electrophoreses we can approximate the length of the product.

Conclusion: Our method has given very promising results so far. An improvement would be to narrow the length distribution of the transcribed sequences further. Currently we are validating our technique by using a DNA microarray.

BP 24.2 Thu 17:30 Poster A

Stable conformations of a single stranded deprotonated DNA i-motif — •Jens Smiatek[1], Dongsheng Liu[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, WWU Münster, D-48149 Münster, Germany — [2]Department of Chemistry, Tsinghua University, Beijing 100190, P. R. China

We present Molecular Dynamics simulations of a single stranded de-

protonated DNA i-motif in explicit solvent. Our results indicate that hairpin structures are stable equilibrium conformations at 300 K. The entropic preference of these configurations is explained by strong water ordering effects due to the present number of hydrogen bonds. We observe a full unfolding at higher temperatures in good agreement to experimental results.

BP 24.3 Thu 17:30 Poster A

Models of Base Excision Repair — •Laurin Lengert — TU Darmstadt, Hessen

Our goal is to study simple models of DNA repair networks. One such network is the base excision repair network which is involved in the repair of single strand breaks. We will discuss the minimal set of repair proteins needed for a model that is able to reproduce the time course of protein recruitment data revealed by experiments. Furthermore, we will analyze how the properties of these simple models affect the data produced in computer simulations. This in turn enables us to interpret various features of the experimental curves in terms of the underlying processes.

BP 24.4 Thu 17:30 Poster A

DNA in an infinite nanochannel — •Wojciech Müller, Stefan Kesselheim, and Christian Holm — ICP, Stuttgart, Deutschland

We perform full atomistic molecular dynamics simulations, where an infinite b-DNA helix is enclosed in an infinite channel. The DNA is solvated in an explicit SPC water model, enriched with ions of various concentrations. The ion distribution and the flow is then compared to results from coarse grained models. The goal is to find the limits of these coarse grained models and identify effects which are not captured by them.

BP 24.5 Thu 17:30 Poster A

mechanical properties of DNA through numerical method and monte carlo simulation — •hassan chatrsahar[1] and mohammad hossein yamani[2] — [1]Islamic Azad University of Takestan, Takestan, Iran — [2]Johannes Gutenberg University, Mainz, Germany

DNA as an anisotropic flexible polymer contains bioinformation of all living cells. Interactions between DNA and proteins that cause deformations in the structure of DNA are essentially ubiquitous during many life processes inside cells. We study the persistence length of DNA in two and three dimensions, considering the elastic bending anisotropy and twist-bend coupling through Worm-Like Chain model (WLC) and Metropolis Monte Carlo simulation. We compare the persistence length of DNA in two and three dimensions. We show although twist-bend coupling does not affect the persistence length in three dimensions, it increases the persistence length in two dimensions by a few percents. Also, through Elastic Rod model we derive the energy equation of a deformed DNA and by minimizing the conformation energy and solving the equations through numerical method, the spatial conformation of a DNA under various boundary conditions and integral constrains is studied. After that, effects of the twist-bend coupling and anisotropy in DNA conformation and its energy are probed.

BP 24.6 Thu 17:30 Poster A

Ab Initio Study of The Electric Hyperfine Interactions: DNA Bases With Metal Cations (Cd and In). — •Philippe Alexandre Divina Petersen, Marcos Brown Gonçalves, and Helena Maria Petrilli — Instituto de Física, DFMT, Universidade de São Paulo, São Paulo, SP, Brazil

The hyperfine interactions provide information around the probe atom. This information is given in nanometer scale and through interactions between the nuclear quadrupole moment of the atom and the charges in its surroundings. Nuclear quadrupole coupling constants (vQ) in molecules depends on the nuclear quadrupole moment and the Electric Field Gradient (EFG) at the nucleus. Thus, the theoretical analysis of EFG is interesting because it can help both interpreting experimental results and estimate the adequacy of structural models. Metal cations bound to DNA bases can change many aspects of the base pairing [1]. They also facilitate or difficult the breakdown of this bases, depending on the location where the Cd and In are linked to DNA. The methodology used for the electronic structure calculations is based on the Kohn-Sham [2] scheme of the Density-Functional Theory (DFT). The computational code used is the Projector Augmented-Wave Method [3] combined with the Car-Parrinello [4] scheme(CP-PAW).

[1] J. V. Burda, J. Sponer, J. Leszczynski, P. Hobza,J.Phys. Chem.B., 101, 9670 (1997). [2] W. Kohn, L. J. Sham, Phys. Rev. B., 140,1133 (1965). [3] P. E. Blöchl, Phys. Rev. B., 50, 17953 (1994). [4] R. Car e M. Parrinello, Phys. Rev. Lett. 55, 2493 (1985). [5] A. S. Silva,A. W. Carbonari (Private Communication).

BP 24.7 Thu 17:30 Poster A

Imaging of DNA overwinding and splitting — •Hua Liang, Nikolai Severin, and Jürgen Rabe — Department of Physics, Humboldt University Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Unwinding and melting a DNA double helical structure at a specific region is the initiation step for DNA replication, the precise mechanism of which remaining still ambiguous (1). Experimental and theoretical studies on stretching and twisting of double-stranded (ds-) DNA reveal its chirality by mechanical twist-stretch coupling: small stretching along the DNA backbone induced torsional stress along the molecular backbone and vice versa (2). It has been theoretically shown that ds-DNA may release its torsional stress inhomogeneously along the backbone with localized, sequence-dependent structural failure to preserve its B-form, when supercoiling is not allowed (3). However, the pulling experiments were carried out in solution, where it is difficult to access the direct conformational changes during stretching. Here we report the experimental observation of plasmid DNA (pUC19 and pBR 322) overwinding with local splitting of the double helix into two single strands when stretched on a surface. Only one split is observed for different lengths of DNA, with the splitting length proportional to the total length. We discuss a possible unwinding and splitting mechanism analogue to many biological processes which involve DNA in vivo such as replication, transcription initiation, and DNA repair. [1]M. L. Mott, J. M. Berger, Nature Reviews Microbiology 5, 343 (2007. [2]J. Gore et al., Nature 442, 836 (2006). [3]G. L. Randall, L. Zechiedrich, B. M. Pettitt, Nucleic Acids Research 37, 5568 (2009).

BP 24.8 Thu 17:30 Poster A

Thermal and photothermal dissociation of DNA-gold nanoparticle networks of different sizes — •Malte Linn[1], Anne Buchkremer[2], Ulrich Simon[2], and Gero von Plessen[1] — [1]Inst. of Physics (IA), RWTH Aachen University, Germany — [2]Inst. of Inorganic Chemistry, RWTH Aachen University, Germany

The functionalization of gold nanoparticles (AuNPs) with DNA allows the construction of DNA-AuNP networks, which have the ability to act as both optical sensors and actuators. By using optical extinction spectroscopy (OES), it is possible to monitor the state of the networks, since the mutual electromagnetic coupling of individual particles inside each network leads to a red shift of the plasmon peak position with respect to single particles. Since DNA dehybridization is temperature-sensitive, network dissociation can be triggered either by mere conventional heating or by introducing additional photothermal heating via irradiation with cw laser light. In this work, we tailor the size of the DNA-AuNP networks by varying the ratio of complementarily functionalized AuNPs. The size dependence of the optical and chemical properties of the networks is investigated and quantified by means of OES and dynamic light scattering. These properties depend on the network size, because larger networks involve a greater number of AuNPs and DNA bonds. The influence of additional photothermal heating on the dissociation temperature associated with each network size is also investigated.

BP 24.9 Thu 17:30 Poster A

Kinetics of DNA hairpin-loops in crowded and non-crowded fluids — •Olivia Stiehl, Maria Hanulova, Gernot Guigas, and Matthias Weiss — University of Bayreuth, Bayreuth, Germany

Single-stranded DNA hairpin-loops are involved in many biological processes, e.g. in the regulation of gene expression and DNA recombination. Investigating the kinetics of hairpin loops yields a better quantitative understanding of such processes and therefore may help to improve, for instance, the efficiency of antisense drugs. Using a combination of fluorescence correlation spectroscopy and fluorescence energy transfer, we have investigated the kinetics of thermally induced DNA hairpin-loop fluctuations. In particular, we were interested in the influence of macromolecular crowding on the time constant of opening/closing of the DNA loop and on the fraction of open DNA loops. Our measurements were performed with the crowding agent dextran at different concentrations and molecular weights. We found that both, a purely viscous as well as a crowded environment lead to a slower kinetics. Furthermore, our measurements indicate that a viscous surrounding does not affect the fraction of open DNA loops, whereas an increased crowding enhanced the fraction of closed DNA loops.

BP 24.10 Thu 17:30 Poster A

AFM imaging of conformational changes in DNA after hydroxyl radical attack — Janine Wilken[1] and •Stephan Block[2] — [1]Institut für Physik, Ernst-Moritz-Arndt Universität, Felix-Hausdorff-Str. 6, D-17487 Greifswald, Germany — [2]ZIK HIKE - Zentrum für Innovationskompetenz Humorale Immunreaktionen bei kardiovaskulären Erkrankungen, Fleischmannstr. 42 - 44, D-17487 Greifswald, Germany

AFM is used to directly visualise changes in the conformation of DNA after attack of reactive oxygen species (ROS). In detail, the plasmid pBR322 is mixed with Fentons reagent, whereby the ratio R of hydroxyl radical molecules to DNA base pairs is varied. After the radical attack the negatively charged plasmid is immobilized onto mica surfaces that are functionalized with positively charged poly(allylamine hydrochloride) (PAH). At R = 2.5 most of the plasmid adopts the supercoiled (double-stranded) conformation and only few chains are split up by the radical attack. An increase in hydroxyl radical concentration also increases the power of the radical attack, leading to a rising number of shorter (single-stranded) fragments of plasmids. Interestingly, these fragments are often surrounded by plateaus (0.2 nm in height) which might be attributed to the aggregation of base pairs, which are chemically modified after the radical attack.

BP 24.11 Thu 17:30 Poster A

Optical Tweezers Force Spectroscopy on Protein Nanopores in Lipid Bilayers — •Andy Sischka[1], Lorena Redondo-Morata[2], Helene Schellenberg[1], Andre Spiering[1], Sebastian Knust[1], Katja Tönsing[1], Fausto Sanz[2], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanosciences, Faculty of Physics, Bielefeld University — [2]Physical Chemistry Department, University of Barcelona

We are aiming to investigate the controlled translocation of individual DNA molecules through protein nanopores with our quantitative 3D optical tweezes system, similarly to recent single molecule threading experiments through solid-state nanopores (nanopore force spectroscopy) [1, 2]. There, quantitative translocation forces and ionic current signals of individual DNA molecules and DNA-protein complexes were identified and related to the respective protein type and charge.

Since we want to improve our understanding of the molecular translocation dynamics and increase the sensitivity of the translocation force and the ionic current, we extend these experiments towards biological nanopores and membranes by measuring both current and forces acting on a single-stranded DNA molecule that will be threaded through a protein nanopore inside a lipid bilayer. This bilayer is immobilized on a Si_3N_4 membrane support by vesicle spreading or Langmuir-Blodgett transfer. We will discuss first results with single-pore forming proteins like alpha-hemolysin.

[1] A. Sischka et al.: J. Phys.: Condens. Matt. **22**: 454121 (2010)
[2] A. Spiering et al.: Nano Letters **11**: 2978 (2011)

BP 24.12 Thu 17:30 Poster A

Video-based axial force analysis for 3D quantitative optical tweezers — •Sebastian Knust, Andy Sischka, Andre Spiering, and Dario Anselmetti — Experimental Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld Institute for Biophysics and NanoScience (BINAS), Bielefeld University, 33615 Bielefeld, Germany

We developed and included video-based axial force analysis into our previously described optical tweezers setup [1]. By measuring the radius of a trapped microbead we achieve an overall force resolution along the z-axis in the range of 0.2pN with a bandwidth of 120Hz, only limited by our CCD camera. With this video-based method we overcome the remaining weak interference effects in backscattered light based force analysis when operating a microsphere in the vicinity of an interface.

We tested our setup by investigating the controlled threading and translocation of individual lambda-DNA molecules with and without attached DNA-binding ligands through solid-state nanopores and comparing these results with previous measurements realized with photodiode intensity detection [2, 3].

[1] A. Sischka et. al., Rev. Sci. Instrum. **79**, 063702 (2008)
[2] A. Sischka et. al., J. Phys.: Condens. Matter **22**, 454121 (2010)
[3] A. Spiering et. al., Nano Lett. **11**, 2978 (2011)

BP 24.13 Thu 17:30 Poster A

Nanopore Translocation Dynamics of a Single DNA-Bound Protein — •Andre Spiering[1], Sebastian Getfert[2], Andy Sischka[1], Katja Tönsing[1], Karsten Rott[3], Peter Reimann[2], and Dario Anselmetti[1] — [1]Experimental Biophysics and Applied Nanoscience, Bielefeld University, 33615 Bielefeld, Germany — [2]Soft Matter Theory, Bielefeld University — [3]Thin Films and Physics of Nanostructures, Bielefeld University

The single molecule translocation dynamics of various dsDNA-protein complexes upon threading through a solid-state NP was investigated by quantitative 3D-optical tweezers (OT) in the presence of an electric field (NP force spectroscopy). In our single molecule translocation experiments, we find distinct asymmetric force signals that depend on the protein type and charge, the DNA elasticity and its counterionic screening in the buffer **[1,2]**. In order to increase the resolution of these force signals even further we drastically decreased the thickness of the membrane containing the nanopore. We prepared graphene monolayers by exfoliation from graphite, transferred them to Si/Si_3N_4-support chips and milled the freestanding graphene membrane (with a focused ion beam or a TEM) to produce graphene nanopores of diverse size and shape. Comparing the results for different membranes and nanopores is the basis to further understand the exact physical properties of such translocation dynamics and may lead to the development of novel nanopore sensing and sequencing devices.

[1] A. Sischka et al.: *J. Phys.: Condens. Matter* **22**: 454121 (2010)
[2] A. Spiering et al.; *Nano Letters* **11**: 2978-2982 (2011)

BP 25: Posters: Molecular Motors

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

BP 25.1 Thu 17:30 Poster A

Cargo-regulated directionality switching of *S. cerevisiae* Kinesin-5 Cin8 — •Christina Thiede[1], Alice Wiesbaum[1], Adina Gerson-Gurwitz[2], Natalia Movshovich[2], Vladimir Fridman[2], Maria Podolskaya[2], Tsafi Danieli[2], Stefan Lakämper[1], Larisa Gheber[2], Dieter R. Klopfenstein[1], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Department of Chemistry, Ben-Gurion University of the Negev, Israel

In mitotic spindle morphogenesis and dynamics kinesin-5 motors fulfil essential roles as slow, processive microtubule (MT) plus-end directed sliding motors. Eg5, the kinesin-5 from *X. leavis*, switches from a diffusive to a directional mode upon cross-linking a pair of microtubules. The mechanism may be related to kinesin-1 cargo regulation effected by a back-folding of the tail. Recently Cin8, a kinesin-5 from S. *cerevisiae*, was surprisingly found to be able to switch from processive plus-end to processive minus-end motility. Here we have studied the *in vivo* and *in vitro* properties and regulation of Cin8 using single-molecule fluorescence assays. In high salt, Cin8 moved rapidly and processively towards the MT minus-end. In low salt, Cin8 was 10x slower and moved towards the MT plus-end. Phosphorylation sites located in the unique 99 amino acids insert in Cin8's loop 8 influence the switching. The most striking effect was, however, that Cin8 switched from minus- to plus-end directed motility as soon as it was located between two microtubules. This finding suggests that in Cin8 not only the mode of motility is regulated by cargo binding, but also its directionality.

BP 25.2 Thu 17:30 Poster A

The highly-processive kinesin-8, Kip3p, derails from microtubule protofilaments — •Aniruddha Mitra[1,2], Bert Nitzsche[1,2], Volker Bormuth[1,3], Felix Ruhnow[1,2], Marko Stroch[1], Burkhard Rammner[4], Jonathon Howard[1], and Stefan Diez[1,2] — [1]MPI-CBG, Dresden, Germany — [2]B CUBE, Dresden, Germany — [3]Institut Curie, Paris, France — [4]Scimotion, Hamburg, Germany

Kinesin-8 controls microtubule length based on its depolymerization activity at microtubule plus-ends preceded by highly processive motility. However, the mechanism confering high motor processivity even on crowded microtubules in the cytoplasm is not known. We therefore asked if kinesin-8 is capable of switching protofilaments during

its plus-end directed motility along the microtubule lattice. We performed in vitro gliding motility assays on surfaces coated with the budding yeast kinesin-8, Kip3p, and measured the rotations of the microtubules around their longitudinal axis using quantum dots in combination with fluorescence-interference contrast microscopy and 2D nanometer tracking. We observed counterclockwise rotations with periodictities unrelated to the microtubule supertwist. Such rotations indicate that the motors do not follow the axes of individual protofilaments but rather switch between them perpetually. We hypothesize that this behaviour, which distinguishes kinesin-8 from the processive protofilament tracker kinesin-1, (i) results from a comparetively long neck linker, non-centrally attached to the motor domain and (ii) is essential for high processivity.

BP 25.3 Thu 17:30 Poster A

Studying collective motor effects by fast optical tracking of gold nanoparticles — •Wiebke Jahr, Rene Schneider, and Stefan Diez — B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden

This study focuses on the usage of gold nanoparticles (GNPs) for the fast optical tracking of microtubules gliding on motor-coated surfaces. GNPs are strong light scatterers and can be functionalized to bind to microtubules via biotin-streptavidin or antibody interactions. In contrast to conventional fluorophores, GNPs show neither photobleaching, photon blinking nor emission saturation. Thus, GNPs are ideal probes to study the motion of filaments on short time scales with high precision. Their signal only depends on their radii and the incoming light intensity so that data acquisition rates are not limited by saturation effects.

In combination with the software package FIESTA [1] (Fluorescence Image Evaluation Software for Tracking and Analysis) stepping events of single and multiple kinesin-1 molecules are investigated at full ATP concentration. Moreover, the effects of roadblocks on the movement of motor proteins is studied. The insights gained from these experiments are applicable to the design of early diagnosis mechanisms for diseases, such as Alzheimer's, which is initiated by overexpression of microtubule-associated proteins, leading to blockages on the motor paths.

[1] F. Ruhnow, D. Zwicker, S. Diez, "Filament localization with nanometer accuracy", Biophys J 98, 363a-363a, (2011).

BP 25.4 Thu 17:30 Poster A

Nanometer precision in filament localization allows for precise off-axis tracking of molecular motors — •Felix Ruhnow[1,2], David Zwicker[3], and Stefan Diez[1,2] — [1]B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Measuring the exact path of molecular motors, such as cytoskeletal motor proteins, on their tracks has proven to be difficult without knowing the precise location of the filaments. Up to now, off-axis stepping has therefore mostly been inferred from the tracked positions of the motors with respect to the fitted path of the motors instead of determining the filament centerline. Obviously, this limits the precision of the measurements and may lead to errors due to the sometimes complex three-dimensional structure of the filaments. We developed a filament tracking algorithm to determine the centerline position of fluorescently labeled filaments with nanometer precision. This allowed us to observe the non-parallel movement of kinesin-1 motors with respect to the microtubule centerline, which is consistent with kinesin-1 following a protofilament of a supertwisted microtubule. Combined with methods to measure nanometer heights above substrate surfaces, such as fluorescence interference contrast or parallax, our algorithm presents a promising tool for optical 3D-nanometry.

BP 25.5 Thu 17:30 Poster A

Efficiency of a tightly coupled molecular motor — •Eva Zimmermann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

Most molecular motors gain energy for their mechanical motion from the hydrolysis of ATP. We use a simple one-state-model for such a motor protein that performs a one-dimensional (discrete) stepwise motion within an aqueous solution containing non-equilibrium nucleotide concentrations. In our model, the motor protein hydrolyzes one ATP molecule per step which represents tight mechanochemical coupling.

Based on this model we numerically and within an approximation also analytically investigate dynamics and efficiency of the motor protein in the presence of an attached cargo. We are especially interested in the dependence of the motor protein's behavior on different nucleotide concentrations as well as on several internal parameters of the model. Compared with recent experiments, the model seems to capture the basic properties of such a motor protein quite well.

BP 25.6 Thu 17:30 Poster A

Coarse-grained simulations of active protein machines in biological membranes with a solvent — •mu-jie huang[1], raymond kapral[2], alexander s. mikhailov[3], and hsuan-yi chen[1] — [1]Department of Physics and Institute of Biophysics, National Central University, Jhongli 32001, Taiwan — [2]Chemical Physics Theory Group, Department of Chemistry, University of Toronto, Ontario, Canada — [3]Abteilung Physikalische Chemie, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany.

Protein machines, cyclically changing their conformations, play a fundamental role in the living cells; many of them are found in cellular membranes. Since the cycles of the machines are in the millisecond range, approximate coarse-grained descriptions are needed. Recently, entire operation cycles of some protein machines could already be reproduced by using coarse-grained models, with solvent included. Here, we proceed further and demonstrate that dynamical cycle simulations of machines immersed into a membrane are possible. Our approach combines the elastic-network description for a machine with the multiparticle-collision modeling for the solvent and a reduced description for the lipids. Membrane-mediated synchronization of machine cycles has been found in our simulations.

BP 25.7 Thu 17:30 Poster A

Spatio-temporal guiding of gliding microtubules by local heating on micro-structured surfaces — •Viktor Schroeder[1,2], Ivan Maximov[3], Till Korten[1,2], Heiner Linke[3], and Stefan Diez[1,2] — [1]MPI-CBG, Dresden, Germany — [2]B CUBE, Dresden, Germany — [3]nmC@LU, Lund University, Sweden

To use gliding microtubules as carriers in molecular sorting devices, methods for spatio-temporal control of transport need to be developed. Our approach is based on composite surfaces where functional kinesin motor proteins are adsorbed onto planar substrates between surface-grafted polymer chains of thermoresponsive poly(N-isopropylacrylamide) (PNIPAM). By external temperature control, we recently demonstrated [1] the reversible landing, gliding, and releasing of motor-driven microtubules in response to conformational changes of the polymer chains.

Based on recent findings that guided microtubule motility along non-topographical motor patterns is possible [2], we now aim to form switchable tracks. Specifically, we report how we apply electrical currents through micro-structured gold layers in order to locally collapse PNIPAM via Joule heating. Consequently, the kinesin motors become accessible on these tracks only and we show that motility can be guided along the routes where electrical currents are applied. We foresee future applications of this novel guiding technique for lab-on-chip devices in the fields of molecular diagnostics and bio-computation.

[1] L. Ionov et al., Nano Lett., 6, no. 9, pp. 1982-1987, (2006).
[2] C. Reuther, et al., Nano Lett., 6, no. 10, pp. 2177-2183, (2006).

BP 26: Posters: Membranes and Vesicles

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

BP 26.1 Thu 17:30 Poster A

Describing the motions in phospholipid membranes with concepts from glass physics — •Sebastian Busch[1] and Tobias Unruh[1,2] — [1]Physik-Department E13 and FRM II, Technische Universität München, Garching bei München, Germany — [2]Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The diffusion of phospholipid molecules in membranes has been described very successfully by the free volume theory for many decades. This theory had originally been developed in the 1960s for glass physics. Although the *macroscopic* predictions of the theory are very well met, it became clear in recent years that the *microscopic* images of the motions on a molecular scale that are included in the free volume theory cannot be taken very literally.

In this contribution, we give a very short overview over the developments in glass physics since the 1960s and suggest that the microscopic description of the dynamics in phospholipid membranes could profit from an anew loan of their concepts such as soft modes and dynamical heterogeneities.

With these concepts, it is possible to explain the motions of phospholipid molecules on the pico- to nanosecond time scale which occur in transient clusters of molecules that move in a flow-like fashion. It rationalises also the small change of the motions on a 60 ps time scale when crossing the main phase transition.

BP 26.2 Thu 17:30 Poster A

Influence of charge density on bilayer bending rigidity in lipid vesicles: a combined dynamic light scattering and neutron spin-echo study — •Beate-Annette Brüning[1], Ralf Stehle[1,2], Peter Falus[3], and Bela Farago[3] — [1]Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [2]Universität Bayreuth, Postfach 10 12 51, 95440 Bayreuth, Germany — [3]Institut Laue-Langevin, B.P. 156, 6 rue Jules Horowitz, 38042 Grenoble, France

We report a combined dynamic light scattering and neutron spin-echo study on vesicles composed of the uncharged helper lipid DMPC and the cationic lipid DOTAP. Mechanical properties of a model membrane and the corresponding fluctuation dynamics can be tuned by changing composition. We compare the bilayer undulation dynamics in lipid vesicles composed of DMPC/DOTAP to vesicles composed of DMPC and the also uncharged reference lipid DOPC. We find, that on the local scale, lipid headgroup composition and charge change the vesicle fluctuations less than acyl chain packing inhomogenities between the composite lipids. We discuss this result on the basis of domain formation in the lipid mixtures containing charged (DMPC/DOTAP) and uncharged reference lipid (DMPC/DOPC). First, we investigate lipid vesicle size and mass diffusion using dynamic light scattering, then we study collective bilayer undulations and bulk diffusion on two distinct time scales around 25ns and 150ns, using neutron spin-echo spectroscopy. Finally, we estimate bilayer bending rigidities κ_B for the charged and uncharged lipid vesicles.

BP 26.3 Thu 17:30 Poster A

Mathematical modelling of the surface change of erythrocytes due to mechanical influences — •Elisabeth Eckle and Richards Grzhibovskis — Applied Mathematics, Saarland University, Germany

Interactions of erythrocytes with artificial surfaces (e.g. specially prepared glass or a mesh of microfibers) attract a lot of attention from both experimental and modeling communities. Besides rapid changes in the shape of the cell, these phenomena feature forming of contact areas between the cell and the surface in question.

In spite of the overwhelming biochemical complexity of an erythrocyte, simple bilayer membrane models are widely used to gain an insight into a variety of processes it is involved in. We consider the classical Helfrich model of bilayer membranes with additional contact energy terms as well as total volume and surface area constraints. The equilibrium shapes of the cell are obtained numerically through a proper FEM discretization of the weak formulation of the gradient flow for the resulting energy functional. Computations are performed in three space dimensions. We study properties of the model by exploring its results for different physical parameters, discretizations, and configurations of the artificial surfaces.

BP 26.4 Thu 17:30 Poster A

Protein aggregation driven by hydrophobic mismatch — Maxim Manakov[1], Khariton Matveev[1], •Thorsten Auth[2], and Gerhard Gompper[2] — [1]Research-educational Centre "Bionanophysics", Moscow Institute of Physics and Technology, 141700 Dolgoprudniy, Russia — [2]Forschungszentrum Jülich, Institute of Complex Systems and Institute for Advanced Simulation, 52425 Jülich, Germany

The fluid mosaic model for biological membranes proposes a homogeneous distribution of integral proteins in the lipid bilayer. However, cluster formation can be observed if an attractive interaction is taken into account. For asymmetric proteins, bilayer deformation leads to a curvature-mediated interaction. Whereas weakly-curved proteins in a planar membrane repel each other, many-particle interactions can lead to an effective attraction. For symmetric integral proteins, a mismatch of the hydrophobic length of the protein and the thickness of the lipid bilayer induces an interaction that is mediated by monolayer deformation. This system can be modeled using cylindrical inclusions for the proteins and a continuum membrane model for the monolayers; the membrane model is based on the monolayer bending rigidity and the bilayer compressibility. Numerical calculations allow us to obtain pair potentials, many-protein interactions, as well as the interaction of a single protein with a protein cluster. Both membrane-mediated attraction and translational entropy determine the ratios between monomers, dimers, trimers, and bigger aggregates that can be compared with experimental and MD simulation data.

BP 26.5 Thu 17:30 Poster A

Shape as a determinant of membrane protein cluster formation — •Gernot Guigas and Matthias Weiss — Experimental Physics I, University of Bayreuth

Clustering of membrane proteins is a key event in many vital cellular processes, for example during protein sorting or signal transduction. Recent studies have shown that protein clustering can be caused by non-specific attractive interactions between proteins which arise from a hydrophobic mismatch between the membrane and the hydrophobic domain of transmembrane proteins. Here, we show by means of mesoscopic membrane simulations that protein interactions due to a hydrophobic mismatch do not necessarily need to be attractive but can also be repulsive. Key parameter for the character of the interaction is the geometrical shape of the interacting proteins' hydrophobic domains. Attraction of two proteins is observed when they can establish a maximum interfacial contact by adsorbing to each other along the full length of their hydrophobic domains. In contrast, two proteins repell each other when only a pointwise interfacial contact is possible. A geometry-dependent attraction and repulsion hence can fine-tune protein oligomerization events.

BP 26.6 Thu 17:30 Poster A

Modeling vesicular exocytosis in chromaffin cells — •Daungruthai Jarukanont[1], Martin Garcia[1], Imelda Bonifas[2], and Ricardo Femat[2] — [1]Institut für Physik Universität Kassel — [2]División de Matemáticas Aplicadas, IPICyT, San Luis Potosí, Mexico

In cell communications, the transport of vesicles is essential for storage and release of chemical messenger molecules via exocytosis. To understand vesicular exocytosis, current signals induced by transmitter molecules from single cells experiments were measured. Each exocytotic event is characterized by a current spike, and therefore a measurement is represented by a time-series. By performing a series of experiments on chromaffin cells, including cells with pharmacological manipulation of transmitter level with L-DOPA and reserpine, and a careful statistical analysis, we found that the probability for exocytosis events follows a gamma distribution. Combining this with the results from other studies by microscopy method [1], we developed a model for the mechanism of vesicular release and were able to simulate these processes in good agreement with experiment.

[1] Steyer,J. A., Horstmann,H. and Almers,A.,Transport, capture and exocytosis of single synaptic vesicles at active zones, *Nature* 406, 849-854 (2000)

BP 26.7 Thu 17:30 Poster A

Dual emission GFP as highly sensitive fluorophore for the determination of intracellular pH with fluorescence lifetime imaging microscopy (FLIM) — •Franz-Josef Schmitt, Cornelia Junghans, Marco Vitali, and Thomas Friedrich — Biophysical Chemistry, Berlin Institute of Technology, Germany

The determination of the pH in the cell cytoplasm or in intracellular organelles is of high relevance in cell biology. During infection with the influenza virus, cells produce the M2 proton channel, which is encoded by the viral genome and represents a crucial component of the viral reproduction cycle. Influenza treatment utilizes drugs like amantadine, which are targeted against the M2 channel. We present a novel multi-parameter FLIM setup that permits the simultaneous imaging of the fluorescence amplitude ratios and lifetimes of a pH-sensitive dual-emission GFP (deGFP) enabling the determination of the activity of a fusion protein of an membrane intrinsic influenza M2 channel with tagRFP (M2-RFP) monitored by deGFP fluorescence. Both proteins (M2-RFP and deGFP) were expressed in chinese hamster ovary cells (CHO-K1) and monitored with spatial resolution of 500 nm in 2 color channels with time resolution of < 100 ps. It was shown that the presence of M2 leads to an acceleration of proton transfer across the cell membrane that is blocked by amantadine. The time-course of M2-dependent intracellular acidification can be described by a general diffusion equation for the intracellular pH in a buffered medium, thus enabling the determination of transversal proton diffusion coefficients in cell membranes.

BP 26.8 Thu 17:30 Poster A

Membrane Undulations in Ion Channel Systems Undergoing Stochastic Resonance — •Eric Stava[1], Siyoung Choi[2], Minrui Yu[2], Hyuncheol Shin[2], and Robert Blick[1,2] — [1]Universität Hamburg, Hamburg, Deutschland — [2]University of Wisconsin-Madison, Madison, Wisconsin, USA

Stochastic resonance (SR) is the process by which the signal-to-noise ratio of a system is enhanced by an increase in noise. It has been shown that Alamethicin ion channels undergo SR when appropriate levels of voltage noise are applied to them [1,2]. However, changes in the tension of the lipid membrane must also be taken into account. The converse flexoelectric effect enhances the tension in the lipid membrane in the presence of an applied voltage [3]. When voltage noise is applied to the system, this effect causes the lipid membrane to undulate. These membrane undulations enhance the time-averaged membrane area and system capacitance. From the real-time admittance of Alamethicin ion channels undergoing SR, we quantified the effects of voltage noise on the lipid membrane. We find a frequency-dependent enhancement in the system admittance with increasing voltage noise. This increase in admittance correlates with an increase in membrane tension, which enhances the time-averaged ion channel conductance. This results in improved signal transduction over a range of noise intensities.

[1] S. M. Bezrukov and I. Vodyanoy, Nature, 378, 362-364 (1995). [2] E. Stava, et al., submitted for publication. [3] A. T. Todorov, A. G. Petrov, and J. H. Fendler, J. Phys. Chem., 98, 3076-3079 (1994

BP 26.9 Thu 17:30 Poster A

Membrane Adhesion via Lipid-Anchored DNA Oligonucleotides — •Russi Gurov, Reinhard Lipowsky, and Rumiana Dimova — Department of Theory and Bio-Systems, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Cells interact via receptor and ligand molecules located at the surface of their membranes. The binding affinities of these molecules are an important characteristic of the membrane-membrane interactions and can be expressed in terms of the dependence of the bound receptor-ligand complexes on the concentrations of unbound receptors and ligands. In the present study, we use fluorescently-labeled complementary DNA oligonucleotides anchored to the membranes of giant unilamelar vesicles to mimic cell adhesion. By measuring the fluorescence intensities in the adhesion and in the non-adhesion regions of the vesicles we estimate the respective concentrations of bound and the unbound receptors and ligands. The obtained results on the binding affinities are compared to predictions of earlier theoretical studies on the law of mass action (Soft Matter, 2009, 5:3354). We also investigate the partitioning of two types of receptor-ligand pairs in the adhesion zone of the vesicles and discuss the implications of the results for T-cell activation.

BP 26.10 Thu 17:30 Poster A

How to tailor giant proteoliposomes — •Susanne F. Fenz[1], Rita Sachse[2], Stefan Kubick[2], and Thomas Schmidt[1] — [1]LION, Leiden University, The Netherlands — [2]Zellulaere Biotechnologie, Fraunhofer IBMT, Potsdam-Golm, Germany

In this project we address the challenge to incorporate transmembrane proteins in the membrane of giant unilamellar vesicles (GUVs). The reconstitution of biologically relevant transmembrane proteins, like receptors or channel proteins, into GUVs makes them easily accessible to further biochemical and physical investigation. Our strategy combines two approaches: in vitro eukaryotic protein expression and electroswelling. The in vitro protein expression system is based on insect lysates. It provides endoplasmic reticulum (ER)-based vesicles which enable signal-induced translocation and post-translational modification. Starting from these vesicles of approximately 1 mum diameter we applied electro-swelling to achieve giant proteoliposomes. Our recent work showed that the efficiency of this method can be improved substantially by the presence of synthetic lipids in the electro-swelling process. As an example, we introduced the one-transmembrane protein heparin-binding epidermal growth factor-like factor Hb-EGF-eYFP in GUV membranes aided by the lipid DOPC. We applied single-molecule fluorescence microscopy to detect and further characterize the protein. In addition, we introduced biotinylated lipids that enabled us to immobilize the protein-decorated GUVs to streptavidin coated surfaces. We envision this achievement as an important first step toward systematic protein studies on technical surfaces.

BP 26.11 Thu 17:30 Poster A

Translocation of polymer chains through self-assembled lipid bilayers: A Monte Carlo study — •Marco Werner[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden - Institute for Theoretical Physics

Recent experiments have shown that amphiphatic polymers may translocate through phospholipid bilayers using an ATP-independent mechanism [1]. This allows for interesting applications using flexible polymers as gene vectors, drug carriers or in cell imaging techniques. However, the mechanism of translocation is not known. We use a lattice-Monte Carlo model with explicit solvent to study self-assembled lipid bilayers interacting with single polymer chains, where all monomers of a polymer have an effective hydrophobic interaction. Under variation of the polymer hydrophobicity we observe an adsorption transition of the polymer at the surface of the bilayer. Close to the transition point the polymer induces significant perturbations of the orientational order of the lipids and the solvent permeability of the membrane is strongly increased locally. Furthermore, our simulation results indicate that for a critically adsorbed chain there is an additional free energy barrier to translocate through the bilayer's core. For polymer chains with appropiately matched hydrophobicity the bilayer becomes energetically most transparent and we observe a maximum in the translocation frequency.

[1] T. Goda et al., *Biomaterials* 31(8): 2380-2387 (2010)

BP 26.12 Thu 17:30 Poster A

Hydration strongly affects the molecular and electronic structure of phospholipid membranes — Alireza Mashaghi[1], pouya partovi[2], •tayebeh jadidi[2], Nasser Nafari[2], Philipp Maass[2], M. Reza Rahimi Tabar[2], Mischa Bonn[3], and Huib Bakker[1] — [1]FOM Institute AMOLF, Science Park 104, 1098XG Amsterdam, The Netherlands — [2]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany — [3]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We investigate the structure and electronic properties of phosphatidylcholine (PC) under different degrees of hydration at the single-molecule and monolayer level by linear scaling ab initio calculations. Upon hydration, the phospholipid undergoes drastic long-range conformational rearrangements which lead to a sickle-like ground-state shape. The structural unit of the gel-phase PC membrane appears to be a water-bridged PC dimer. We find that hydration dramatically alters the surface potential, dipole and quadrupole moments of the lipids and consequently guides the interactions of the membrane with other molecules and the communication between cells.

BP 26.13 Thu 17:30 Poster A

Unpacking the influenza virus at low pH — •Sai Li[1], Frederic Eghiaian[1], Christian Sieben[2], Andreas Herrmann[2], and Iwan Schaap[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität, Göttingen — [2]Institut für Biologie, Humboldt-Universität zu Berlin, Berlin

The genome of the influenza virus is enveloped in a shell made out of a lipid bilayer which inside is covered by a layer of M1 matrix protein. During infection the virus is taken up in the endosomes of the target cell. For the release of the genome the viral composite shell must undergo large conformational changes to allow for membrane fusion with the host-cell endosome. We performed AFM indentation experiments under conditions that mimicked the gradual acidification from early to late endosomes, and we have found that the softening the viral envelope starts as early as at pH 6 and is completed at pH 5.5. We propose that this softening is related to the irreversible destabilization of the M1 layer. In addition, membrane fusion being enhanced after pre-incubation of viruses at pH6, we speculate that stripping the M1 matrix off the lipid envelope during an exposure to this intermediate pH of early endosomes is essential to achieve efficient infection.

BP 26.14 Thu 17:30 Poster A

Measuring particle fluctuations near cell membranes — •Felix Jünger and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Köhler-Allee 102, 79110 Freiburg, Germany

Thermal fluctuations are omnipresent in the world of living cells and are mainly determined by elastic and viscous forces. It is well known that the viscous drag γ increases when a particle approaches a stiff wall, but is unclear, whether this is still true close to a lipid bilayer or close to a living cell. In our work we investigate how the viscous drag changes when a spherical particle approaches a biological cell and to what extent a cell can vary the bead's temporal thermal fluctuations and the viscous drag γ in its extra-cellular space. We use photonic force microscopy (PFM) to investigate the fluctuations of an optically trapped bead, which is approached to a cell membrane. The motion of the bead is tracked interferometrically in three dimensions with nanometer precision and on a microsecond time scale. The viscous modulus $G''(\omega, d)$, but also the elastic modulus $G'(\omega, d)$ as a function of the particle distance d to the cell surface can be obtained by analyzing the fluctuation data on a broad spectral bandwidth ω. We have measured several bead-cell arrangements and present first results.

BP 26.15 Thu 17:30 Poster A

Clustering of Peripheral Membrane Proteins on Model Membranes — •Tobias Distler, Gernot Guigas, and Matthias Weiss — University of Bayreuth, Bayreuth, Germany

Peripheral membrane proteins (PMP) contribute in various vital cellular functions. In many cases they have to form clusters to accomplish their tasks. Coarse-grained molecular dynamics simulations have predicted PMP cluster formation due to membrane-mediated interactions. Here, we present a measurement setup based on fluorescence correlation spectroscopy (FCS) to probe this prediction. Prior to experiments we have studied the potential measurement signals by means of FCS simulations. These calculations showed that the detection of protein clustering via FCS cross-correlation requires the usage of PMPs with a radius of at least 1.5 nm, and a concentration of 100 Proteins/μm^2. Therefore, we have utilized the fairly large fluorescently labeled cholera toxin subunit B (CTB) bound to the lipid GM1 as a PMP in a free-standing black lipid membrane. Preliminary data indicate that cluster formation of CTB indeed can be detected with this setup.

BP 26.16 Thu 17:30 Poster A

Aggregation of Human Antimicrobial Peptide Fragments at Model Membranes — •Claudia Dannehl[1], Thomas Gutsmann[2], and Gerald Brezesinski[1] — [1]Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam — [2]Research Center Borstel, Center for Medicine and Biosience, 23845 Borstel

Antimicrobial peptides (AMPs) are short, amphiphilic, proteins and part of the host immune defense. They protect organisms against bacteria, viruses and fungi simply by disrupting their membrane. In our work, we focus on two fragments of the human cathelicidin and lipid monolayers as model membranes to get insight into this peptide-lipid interaction. Both peptides adopt an alpha-helical conformation and lead to a fluidization of a negatively charged DPPG monolayer, indicated by an increased transition pressure from a liquid-like to a liquid-condensed phase (seen by GIXD and IRRAS), but the increase in surface pressure and the change in the amide band upon adsorption is peptide specific. We assume that the stronger peptide-lipid interaction of one peptide is accompanied by a peptide aggregation at the interface, as studied by IRRAS on monolayers and CD spectroscopy with SDS in bulk (above the CMC). No changes in the spectra were recorded with IRRAS for zwitterionic lipids (DPPC, DOPC) and CD for the cationic CTAB , which means that the aggregation of the peptide is dominated by the charge density of the target.

BP 26.17 Thu 17:30 Poster A

elastic model for endocytosis of clathrin plaques — •yu-hsein lin[1], david jasnow[2], and hsuan-yi chen[3] — [1]Graduate Institute of Biophysics, National Central University, Taiwan R.O.C — [2]Department of Physics,University of Pittsburgh, Pittsburgh, USA — [3]Department of Physics, National Central University, Taiwan R.O.C

There are two distinct structures of the clathrin- coated vesicles in the early process of the clathrin-mediated endocytosis, one is spherical pits and the other one is flat plaques. Both of them finally form vesicles and enter the cell.

From the observation of experiments, plaques are only found on the cell membrane which is adherent to the substrates, but pit can be found everywhere on the cell membrane. Experiments show that the actin polymerization is essential for both the formation and the invagination of a plaque. But the details of the process, how a coated membrane is lifted on the cell membrane, remain unknown.

In order to understand the mechanism of the invagination of a plaque, we built a model in which the release of the elastic free energy of the growing actin network lead to the detachment of the membrane domain with clathrin plaque from the substrate. Our study suggests a new role played by the actin network on the subcellular process.

BP 26.18 Thu 17:30 Poster A

Statics and dynamics of stalks studied by minimal coarse-grained models. — Giovanni Marelli, •Yuliya Smirnova, and Marcus Müller — Institut für theoretische Physik, Georg August Universität Göttingen

The stalk is a lipid bridge between two lipid membranes and a fundamental step in the process of membrane fusion. The formation and evolution of the stalk is a collective phenomenon which involves the interaction and change of conformation of many lipids. We use our coarse-grained solvent-free model to simulate a stalk between two opposed membranes. The absence of solvent molecules avoids the non trivial problem of re-equilibrating the number of solvent molecules between the two bilayers present in explicit solvent models. Depending on the type and architecture of lipids we can change the stability and morphology of the stalk. Radial stalks are mostly metastable and we calculate the average density profile and fluctuations of their thickness. Small hydrophobic chains (oil) added in the hydrophobic layer of the membrane preferentially go to the lower and upper ends of the stalk, where the membrane is slightly indented, and relax the total tension. Linear stalks formed by more asymmetric lipids are stable and span the simulation box over the pbc. We calculate their line tension. In case of mixed lipid membranes we observe the segregation of lipids with different spontaneous curvatures to curved and planar portions of the morphology. Finally we compare the thickness profile and the bilayer repulsion with different models and experimental data.

BP 26.19 Thu 17:30 Poster A

STED-FCS on near-critical lipid membranes — •Jens Ehrig, Eugene P. Petrov, and Petra Schwille — Biophysics, BIOTEC, Technische Universität Dresden, Dresden, Germany

Dynamic phase separation in cell membranes is believed to play an important role in many membrane-associated cellular processes. This microheterogeneity is one of the reasons for anomalous diffusion of lipid molecules which is frequently observed in cell membranes. We have recently shown via Monte Carlo simulations that the presence of near-critical fluctuations in a lipid membrane may lead to transient anomalous diffusion of lipid molecules [1]. It is therefore extremely interesting to test whether anomalous diffusion due to critical fluctuations can be observed experimentally in model membranes under appropriate conditions. We report results of our experiments on model lipid membranes exhibiting near-critical fluctuations using STED-FCS [2], an experimental technique which can provide valuable information on diffusion dynamics on spatial scales from a few tens to few hundreds of nanometers on time scales ranging from microseconds to seconds.

[1] J. Ehrig, E. P. Petrov, and P. Schwille, Biophys. J. **100** (2011) 80
[2] L. Kastrup, H. Blom, C. Eggeling, and S.W. Hell, Phys. Rev. Lett. **94** (2005) 178104

BP 26.20 Thu 17:30 Poster A

Testing for domain formation in ER-mimicking and native ER membrane GUV. — •Mária Hanulová, Gernot Guigas, Julia Hoffmann, and Matthias Weiss — Experimentalphysik 1,

Uni Bayreuth, Universitätsstr. 30, 95444 Bayreuth

Proteins that are correctly folded are trafficked from the endoplasmic reticulum (ER) to the Golgi apparatus via COPII vesicles. The vesicles bud off from specialized micrometer-sized membrane domains, so-called ER exit sites, after being coated with COPII proteins. Structurally and functionally distinct domains in cellular membranes such as ER exit sites can be based on lipid immiscibility or induced by binding of proteins. Using fluorescence microscopy, we tested for possible lipid-based domain formation in GUV electroformed from ER-mimicking lipid mixtures and native ER membranes. Native ER membranes were isolated from Hela cells by gradient centrifugation. Both types of GUV were homogeneous and the diffusion coefficients measured by FCS were similar to pure liquid-disordered lipid membranes.

BP 26.21 Thu 17:30 Poster A

Influence of charge density on bilayer bending rigidity in lipid vesicles: a combined dynamic light scattering and neutron spin-echo study — •Beate-Annette Brüning[1], Ralf Stehle[1,2], Peter Falus[3], and Bela Farago[3] — [1]Helmholtz Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [2]Universität Bayreuth, Postfach 10 12 51, 95440 Bayreuth, Germany — [3]Institut Laue-Langevin, B.P. 156, 6 rue Jules Horowitz, 38042 Grenoble, France

We report a combined dynamic light scattering and neutron spin-echo study on vesicles composed of the uncharged helper lipid DMPC and the cationic lipid DOTAP. Mechanical properties of a model membrane and the corresponding fluctuation dynamics can be tuned by changing composition. We compare the bilayer undulation dynamics in lipid vesicles composed of DMPC/DOTAP to vesicles composed of DMPC and the also uncharged reference lipid DOPC. We find, that on the local scale, lipid headgroup composition and charge change the vesicle fluctuations less than acyl chain packing inhomogenities between the composite lipids. We discuss this result on the basis of domain formation in the lipid mixtures containing charged (DMPC/DOTAP) and uncharged reference lipid (DMPC/DOPC). First, we investigate lipid vesicle size and mass diffusion using dynamic light scattering, then we study collective bilayer undulations and bulk diffusion on two distinct time scales around 25ns and 150ns, using neutron spin-echo spectroscopy. Finally, we estimate bilayer bending rigidities κ_B for the charged and uncharged lipid vesicles.

BP 26.22 Thu 17:30 Poster A

Simulation of vesicles at surfaces - rupture, fusion and spreading — •Marc Fuhrmans and Marcus Müller — Universität Göttingen, Institut für Theoretische Physik, Göttingen, Deutschland

Adsorption of unilamellar vesicles to an attractive surface is a frequently used way to form supported bilayers. Although this approach is known to produce continuous bilayers, the mechanism of their formation and its dependence on factors like surface roughness, membrane tension, lipid composition and vesicle size is poorly understood. Theoretical considerations based on elastic theory predict rupture of the vesicles caused by adsorption-induced deformation with an exposure of the inner membrane. While some experiments support this mechanism, others result in an exclusive exposure of the outer monolayer or an even exposure of both the inner and outer monolayers. In addition, in some experiments a critical vesicle concentration on the surface is required to initiate the condensation of a supported bilayer, suggesting an involvement of neighboring vesicles in the rupture process.

We have used dissipative particle dynamics simulations to assess the different mechanisms of vesicle spreading on attractive surfaces, placing special emphasis on the initial location and subsequent development of the rupture pore. In addition, we have studied fusion of neighboring adsorbed vesicles and the involvement of free bilayer edges in vesicle rupture and membrane condensation. Making use of the universality of lipid-associated phenomena, we employed a solvent-free coarse-grained model, enabling us to cover the relatively large system sizes and time scales necessary to observe these collective processes.

BP 26.23 Thu 17:30 Poster A

Partitioning of cytochrome c in multicomponent lipid membranes with domains — •Salome Pataraia — Max-Planck-Institute of Colloids and Interfaces Theory & Bio-Systems Potsdam

We characterized the binding of cytochrome c (cyt c), a mitochondrial inner membrane protein, to multicomponent lipid membranes and resolved the role of the bilayer surface charge and lipid composition. As a model system, giant unilamellar vesicles (GUVs) were used. To mimic the membrane composition of the inner mitochondrial membrane we employed lipid mixtures of the charged dioleoyphosphatidylcholine (DOPG), sphingomyelin (SM) and cholesterol. We first characterized the phase behavior of this mixture from confocal microscopy observations on fluorescently labeled GUVs. We localised the region of coexistence of liquid ordered (Lo) and liquid disordered (Ld) phases, mimicking raft-like domains and their environment in cell membranes. We then investigated the change in the phase state of these membranes induced by cyt c at physiological concentrations. Our studies revealed that in the presence of cyt c, the area of the Lo-Ld coexistence region increases on the expense of the single-phase Ld region. By means of fluorescent intensity studies, we also studied the preferential partitioning of cyt c between the Ld and Lo phases. Our results indicate that cyt c strongly prefers the DOPG-rich Ld domains. The specific affinity of the protein to each of the fluid phases are thermodynamically quantified with isothermal titration calorimetry on large unilamellar vesicles with compositions characteristic of either the Lo or the Ld phase.

BP 26.24 Thu 17:30 Poster A

Nonlinear pattern formation in biomimetic membranes — •Chris Händel[1], Bernd Kässemodel[1], Undine Dietrich[1], Sergio Alonso[2], Markus Bär[2], and Josef Käs[1] — [1]Division of Soft Matter Physics, Faculty of Physics and Earth Sciences, University of Leipzig, Linnéstraße 5, 04103 Leipzig , Germany — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany

The MARCKS (Myristoylated alanine-rich C kinase substrate) protein is an actin filament cross-linking protein which reveals relevant functions in different organisms. It is located at the plasma membrane and interacts via electrostatic forces with the membran lipid PIP2 (1,2- Dipalmitoylphosphatidylinositol 4,5-diphosphate). In a biomimetic membrane, designed by a mixed DPPC/PIP2- monolayer, binding of MARCKS peptide to the membrane increases the lateral pressure, whereas unbinding dynamics modulated by PKC (Protein kinase C) generates a nonlinear reaction-diffusion system. This mechanism leads to oscillations of the lateral pressure which can be correlated to changes in the ratio of ordered and disordered phase in the membrane. Employing a theoretical model, we could calculate the dynamic distribution of acidic lipids in response to cytosolic proteins and regulating enzymes. The present work confirms these theoretical assumptions of this reaction-diffusion system by using model membranes. We obtained oscillations in lateral monolayer pressure which correlate with changes in shape and size of the crystalline lipid domains and the ratio of the area requirement of the liquid and the crystalline phase of the monolayer.

BP 27: Posters: Cytoskeletal Filaments

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

BP 27.1 Thu 17:30 Poster A

Cell plasticity is tightly linked to elastic stresses in the cytoskeleton — •Achim Schilling, Navid Bonakdar, Michael Kuhn, Richard Gerum, and Ben Fabry — Biophysics Group, FAU

Cells show pronounced non-linear visco-elastic and visco-plastic properties under large deformations and forces that are important for protecting the cell against mechanical damage. We used a high-force magnetic tweezer setup to deliver unidirectional forces with high precision of up to 30 nN to fibronectin-coated magnetic 5um beads bound to cell surface adhesion receptors. To probe cells with bidirectional forces, the cell culture plate was placed on a rotational/translational stage such that the magnetic bead remained at a constant distance to the magnetic tweezer tip after a 180° rotation. Bead displacements were measured during application of force steps (creep response) and after the force was removed (recovery response). With increasing force magnitude, the cells stiffened, and the recovery became increasingly incomplete, indicating the emergence of plastic behavior. This plas-

ticity was a constant fraction (20%) of the total bead displacement. We attribute the plastic behavior to a buildup of excess slack in the cytoskeletal fibers; when the force direction was suddenly reversed, the beads jumped by twice the slack length in the opposite direction. The creep and the recovery response were fully characterized by a simple power-law vs. time with only 2 force-dependent parameters (elasticity and creep exponent). Our results show that plastic energy dissipation during large cell deformations is tightly linked to elastic stress dissipation and provides additional protection against mechanical damage.

BP 27.2 Thu 17:30 Poster A

Molecular motors can sharpen the length distribution of treadmilling filaments — •Denis Johann, Christoph Erlenkämper, and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

The assembly of actin filaments and microtubules depends on the hydrolysis of nucleotide tri-phostohates. Together with their structural polarity this can lead to treadmilling, a process during which the filaments, on average, grow at one end and shrink at the other. The distribution of proteins binding to a treadmilling filament increases towards the shrinking end. For proteins affecting the removal rate of filament subunits such a gradient implies an effectively length-dependent depolymerization rate, which can lead to a unimodal length distribution unknown to polymers at equilibrium [1]. Using Monte-Carlo simulations, we show that the width of the length distribution can narrow substantially if the depolymerizing proteins are molecular motors, moving directionally towards the shrinking end. We present expressions for the width of the length distribution in the limits of vanishing and infinite motor speeds.

[1] C. Erlenkämper, K. Kruse, *Phys. Biol.* **6**, 046016 (2009)

BP 27.3 Thu 17:30 Poster A

Length Regulation is an Intrinsic Property of Treadmilling Actin Filaments — •Christoph Erlenkämper and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken

Actin polymers constitute a major part of the cell cortex. The polymerisation of these filaments relies on the consumption of chemical energy through the hydrolysis of Adenosin-tri-phosphate (ATP). Together with the structural polarity of actin monomers, this can lead to treadmilling. In this state, the monomers are removed from one end of the filament at the same rate at which they are added at the other end. To investigate the conditions of treadmilling and the accompanying actin-length distribution, we formulate a three-state model of actin dynamics. It accounts for random dephosphorylation of actin-bound ATP along filaments and for the dependence of the various assembly rates on the nucleotide bound to actin monomers. For a range of experimentally accessible parameters, we find that treadmilling goes along with a stationary unimodal length distribution, which is due to a length-dependent monomer removal rate. In this case, the spontaneous disappearance of filaments is largely suppressed. We present analytical estimations of the typical filament length as well as for the variance of the ensuing length distributions and dicuss possible scenarios for *in vivo* length regulation.

BP 27.4 Thu 17:30 Poster A

Cortical dynamics with viscoelasticity — •Arnab Saha[1], Stephan Grill[1,2], Guillaume Salbreux[1], and Frank Jülicher[1] — [1]Max Planck Institute (Physics for complex system) — [2]Max Planck Institute (Molecular cell biology and Genetics)

The cell cortex is a thin layer beneath the cell membrane that largely consists of cross-linked actin filaments, non-muscle myosin motorprotein and various actin binding proteins (ABPs). It can actively contract and generate stress in presence of ATP-consuming motor proteins and treadmilling processes, that drive the cortex far away from thermal equilibrium. Here we present a two dimensional hydrodynamic model for cell cortex valid at long length scale and short to long time scales (incorporating both elastic and viscous regimes), using basic symmetry principles and conservation laws. Using the model, then we probe the elastic regime of cortical dynamics along with the experimental observations from laser ablation of cortex.

BP 27.5 Thu 17:30 Poster A

Measurements of F-actin tube conformation — Evelin Jaschinski, Inka Lauter, Bernd Hoffmann, and •Rudolf Merkel — Forschungszentrum Jülich GmbH, Wilhelm-Johnen-Straße, 52428 Jülich

Actin is a major component of the cytoskeleton of almost all eukaryotic cells. In thermal equilibrium in vitro polymerized actin filaments (F-actin) are fluctuating. These fluctuations are restricted by surrounding filaments which form a tube like volume. The propability distribution of the tube dimension has been measured by means of confocal fluorescence microscopy in our group [1, 2]. Based on these results we are analyzing the F-actin tube conformation under specific external conditions like enforced alignment exerted by shear force as well as counterions.

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

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

BP 27.6 Thu 17:30 Poster A

Dynamics of semiflexible ring polymers in shear fow — •Philipp Lang and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München

The dynamics of semiflexible ring polymers is studied both in equilibrium and subject to external shear flow. We give a comprehensive analytical description of the relaxational dynamics of internal and global modes in the case of persistence lengths greater or equal than the contour lengths. A relaxation behavior similar to linear polymers is found, yet crossover times and amplitudes are different due to smaller internal fluctuations.

The non-equilibrium dynamics in shear flow is investigated by Brownian dynamics simulations of inextensible rings and interpreted in terms of the relaxational dynamics. We find two distinct types of tumbling events: rapid turnover, and tread-milling in a metastable state. The main tumbling frequency is found to scale with the Weissenberg number $Wi = \kappa \cdot \tau_L$ as $Wi^{3/4}$ with the time scale τ_L given by the global rotational relaxation time.

BP 27.7 Thu 17:30 Poster A

How a polymer breaks a bond — •Sebastian Sturm, Jakob Bullerjahn, and Klaus Kroy — Institut für theoretische Physik, Universität Leipzig, Vor dem Hospitaltore 1, 04103 Leipzig

The unbinding kinetics of crosslinking proteins is a crucial ingredient to the rheological behavior of reversibly crosslinked polymer networks and cells. Whereas current models of cell rheology do account for the influence of crosslinker bindings on single-filament dynamics [1,2], the converse effect of polymer dynamics on unbinding kinetics has so far received less attention. Here we address this issue by investigating the unbinding kinetics of polymer-bound crosslinkers based on a rigorous description of subdiffusive monomer dynamics in terms of memory friction [3].

[1] L. Wolff, P. Fernandez, and K. Kroy, New Journal of Physics (2010)
[2] O. Lieleg, K. M. Schmoller, M. M. A. E. Claessens, and A. R. Bausch, Biophysical Journal 96, 4725-4732 (2009)
[3] J. Bullerjahn, S. Sturm, L. Wolff, and K. Kroy, epl (2011), doi 10.1209/0295-5075/96/48005

BP 27.8 Thu 17:30 Poster A

The role of fluctuations in cytoskeletal wave formation — •Florimond Collette, Marc Neef, and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

Spontaneous cytoskeletal waves have been reported in a number of different cell types and under various conditions. Actin waves observed in the slime mold *Dictyostelium discoideum* [1] and in human neutrophils [2] presumably originate from similar mechanisms: Proteins nucleating actin filaments get activated on the membrane, generate new filaments, and are in turn inactivated by actin filaments through an unknow mechanism. We extend a meanfield description of this system [3] to consider stochastic effects in the dynamics of filament nucleators and solve the equation numericaly. When varying the number of nucleators, we observe bifurcations of stationary states into travelling waves. In the case of travelling waves, we find spontaneous switching between waves moving into opposite directions.

[1] T. Bretschneider, *et al.*, *Curr. Biol.* **14**, 1 (2004).
[2] O. D. Weiner, *et al.*, *PLoS Biology* **5**, e221 (2007).
[3] K. Doubrovinski and K. Kruse, *EPL* **83**, 18003 (2008).

BP 27.9 Thu 17:30 Poster A

Active Microrheology: A new approach to determine mechanical properties of assembled networks — •Tobias Paust[1], Ines Martin[1], Michael Beil[2], Harald Herrmann[3], and Othmar Marti[1] — [1]Institute for Experimental Physics, Ulm University, Ulm, Germany — [2]Internal Medicine I, Ulm University, Ulm, Germany — [3]German Cancer Research Center, Heidelberg, Germany

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

In this work we explore the possibility of two point microrheology to determine locally the complex tensorial elastic response of heterogeneous networks. We use the measurements to find possible differences between macro- and microrheology. A careful analysis of the data provides additionally the frequency response of the complex elastic tensor.

As a test system we have investigated keratin 8/18 network extracted from epithelial pancreatic cancer cells. We compare the data to measurements of in vitro assembled keratin 8/18 networks.

BP 27.10 Thu 17:30 Poster A

Super-resolution study of paracrystalline actin in auditory receptor cells — •Valeria Piazza, Britta Weinhausen, Tim Salditt, and Sarah Köster — Institute for X-Ray Physics & CRC Physics, University of Göttingen, Germany

In most cell types microfilaments coalesce into networks and bundles with variable degrees of orientation and size. In statoacustical receptor cells, however, actin bundles inside stereocilia show an unusually "extreme" level of organization: thousands of filaments are tightly packed in a paracrystal array to form stiff cylinders (200-500 nm in thickness and with lengths ranging from 2 to 30 μm) with a supportive function for mechanotransduction. We study the peculiar packing symmetry and molecular composition of these cell protrusions by means of fluorescence nanoscopy and X-ray diffraction. With STED (STimulated Emission Depletion microscopy) coupled to immunofluorescence we test when and where each of the two actin isoforms - β and γ - is incorporated in cochlear stereocilia throughout development. Moreover, using spatially-resolved X-ray nano-diffraction we characterize the spacing of the actin filaments within individual stereocilia. The X-ray measurements are performed on hair cells that are chemically fixed in different conditions (for example, different developmental stages), to test whether the filament array changes or it is constantly maintained in one specific state. Eventually the imaging data will be combined with the X-ray analysis to correlate molecular composition to structure in discrete regions of stereocilia.

BP 27.11 Thu 17:30 Poster A

Network elasticity of stiff rods with semi flexible cross-linkers: simulation and experiment — •Meenakshi M Prabhune[1], Knut M Heidemann[2], Florian Rehfeldt[1], Max Wardetzky[2], and Christoph F Schmidt[1] — [1]Drittes Physikalisches Institut,Georg-August-Universität Göttingen, Göttingen — [2]Institute of Num. and Appl. Math, Georg-August-Universität Göttingen, Göttingen

Mechanical stress plays crucial roles in cellular functions such as adhesion, cell division, motility and many others. Experimental approaches, such as the use of elastic substrates, exist to estimate the forces exerted at the boundaries of cells. Mapping cell-internal stress fields still remains a challenge owing to the heterogeneity of the cytoskeletal filaments and to a lack of appropriate sensors. To model a strongly heterogeneous composite, we construct networks of microtubules cross-linked by dsDNA of variable length. We measure the linear and non-linear shear-elastic response in these networks by macro- and microrheology. Simultaneously, we compare the experimental data to numerical simulations that we have developed for networks of stiff slender rods connected by semi-flexible linkers.

BP 27.12 Thu 17:30 Poster A

Vimentin Filaments in Small Configuration Spaces — •Bernd Nöding, Susanne Bauch, and Sarah Köster — Institute for X-Ray Physics and CRC Physics, University of Göttingen, Germany

The eukaryotic cytoskeleton mainly consists of three types of fibrous proteins. While microtubules and microfilaments are highly conserved, intermediate filaments (IFs) vary from one cell type to another. Here, we focus our study on vimentin IFs. Investigations of the mechanical properties of individual filaments are a necessary prerequisite for a better understanding of the mechanics of biopolymer networks and eventually whole cells. The mechanical rigidity of a polymer is characterized by its persistence length L_p. We perform time-resolved measurements of fluorescently labeled filaments in solutions of different viscosities without any interaction with a substrate whatsoever. To this end, we confine the filaments in microchannels of variable widths and heights ($\sim \mu$m). The purpose of using the channels is threefold: first, they mimic the crowded environment of the cell. Second, they reduce the configuration space occupied by the filaments, thereby markedly improving statistics. Third, they realize the Odijk confinement regime. We find that IFs behave as ideal worm-like chains. Inclusion of data for microfilaments, which are also confined in the Odijk regime, shows that both filament systems behave according to a single scaling law. Furthermore, we find that fluctuations in perpendicular directions decouple as predicted by the worm-like chain model. For freely fluctuating individual vimentin filaments we determine $L_p \sim 2$ μm.

BP 27.13 Thu 17:30 Poster A

Formation of regular actin bundle networks by counter-ion condensation and entropic forces — Florian Huber, •Dan Strehle, Jörg Schnauss, Matti Gralka, and Josef Käs — Universität Leipzig

Actin is a major constituent that contributes mechanical integrity and function to living cells. Filamentous actin is organized in structures spanning networks of filaments, bundles of filaments to networks of bundles. In this work we explore the mechanisms that determine this resulting architecture. In our experimental bottom-up approach we combine actin filaments with uniform attractive interactions. Counterion-condensation as well as depletion-force agents aggregate a homogeneous F-actin solution into regular actin-bundle networks connected by aster-like centers. Both, partial nematic or flow-induced alignment, drastically change the observed network architecture to ladder-like patterns. Complementing the experimental data we aim at elucidating the mechanism on the basis of coarse-grained modeling. Due to the fundamental nature of the interactions considered, we expect that the investigated type of network formation further implies severe consequences to cytoskeletal network formation on the more complex level of living cells.

BP 27.14 Thu 17:30 Poster A

Contractile force generation by entropic softening of actin networks — •Carsten Schuldt, Tom Golde, and Josef Käs — Universität Leipzig

One major constituent of the cell's cytoskeleton is the globular protein actin, organized in filaments subjected to steady assembly and disassembly. We study the depolymerization of actin bundles of cross-linked single actin filaments and networks. In particular, the forces associated with this process are of interest.

Retraction at the rear of a cell is a fundamental part of its migration process. This contraction can be accomplished by actin-myosin interaction. However, myosin knock-out cells have been shown to be still capable of migrating. Alternatively, the depolymerization of the cytoskeleton was proposed to cause contractile forces only by a gain in entropy in the absence of molecular motors. This concept has been demonstrated on polymer meshworks of nematode's major sperm protein [1].

We employ a microrheology approach in conjunction with severing proteins to measure both softening and contraction of the depolymerizing network.

[1] Wohlgemuth et al., Biophys. J, 88, 2462 (2005)

BP 27.15 Thu 17:30 Poster A

Diameter of Keratin 8/18 — •Ines Martin[1], Anke Leitner[1], Masoud Amirkhani[1], Vladislav Krzyzanek[2], Michael Beil[3], Harald Herrmann[4], Paul Walther[5], and Othmar Marti[1] — [1]Institute for Experimental Physics, Ulm University, Ulm — [2]Institute of Medical Physics and Biophysics, Münster University, Münster — [3]Internal Medicine I, Ulm University, Ulm — [4]Division of Molecular Genetics, German Cancer Research Center, Heidelberg — [5]Central Facility of Electron Microscopy, Ulm University, Ulm

The cytoskeleton of epithelial cells consists of three types of filament systems: microtubules, intermediate filaments (IFs) and actin filaments. In our work, we have a closer look at intermediate filaments, which are responsible for the stiffness of cells and responses to mechanical stimuli.

Because of their heterogeneous nature, it is not exactly known how IFs are arranged over their cross-section, even though some measurements of diameter, mass per length and cross-section exist. There-

fore we compared the diameter of filaments with different techniques: Transmission Electron Microscopy with negative staining, Scanning Electron Microscopy of freeze-dried samples with tungsten coating, Scanning Transmission Electron Microscopy (STEM) with and without glutaraldehyde fixation and Small Angle X-ray Scattering (SAXS). Additionally we studied the behavior of Keratin 8/18 adsorbed on a substrate with SEM of freeze-dried samples. Here we could see flattening of some of the filaments, from which one can conclude in agreement with STEM data that the IFs are not very densely packed.

BP 27.16 Thu 17:30 Poster A

Shear-induced wrinkling in random and regular semiflexible polymer networks — •Pascal Müller and Jan Kierfeld — Physics Department, TU Dortmund, Dortmund

Networks of semiflexible polymers such as F-actin are one of the main components in the cytoskeleton and determine the elastic properties of the cell.
We study the elastic properties of filamentous networks by energy minimisation of deformed two-dimensional networks with regular and random geometries. The planar two-dimensional networks are embedded in three-dimensional space, and our main focus is the investigation of wrinkling under shear stress by enabling transversal displacements of the network sheet. We compare triangular networks to random networks in order to identify the impact of network geometry on different wrinkle properties such as amplitude, wavelength, and the critical shear stress that is required to induce wrinkling.

BP 28: Posters: Imaging

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

BP 28.1 Thu 17:30 Poster A

Morphological analysis of MDCK Epithelial tissue on different substrates — •Sara Kaliman[1], Christina Jayachandran[2], Ana-Sunčana Smith[1], and Florian Rehfeldt[2] — [1]Institute for Theoretical Physics and Cluster of Excellence: EAM, FA University Erlangen, Germany — [2]3rd institute of Physics-Biophysics, University of Göttingen, Germany

Significant progress in comprehending the morphology and the internal organization of single cells has been achieved over the last decade. However, cell agglomerates and tissues are understood to a much lesser extent. Here we study the positioning and the orientations of the cell nuclei with respect to the cell body, as well as the organization and the correlations between the cells in two-dimensional epithelial tissues. For this purpose, epithelial Madin-Darby canine kidney (MDCK) cells are grown on collagen coated polyacrylamide gels of various elastic moduli (1-34 kPa) and on stiff glass substrates. Upon fixation and double staining, all cell-lines were imaged in fluorescence, the results of which were processed by a self-made MATLAB program. We find a similar organization in tissues with equivalent local density, irrespective of the substrate elasticity, even though the dynamics of the tissue growth depends on the underlaying matrix. In all cases, we find little deviations from random distributions. Furthermore, favorable comparison between true cell body and the Voronoi construction based on the nuclei shape suggests that the intracellular interactions dominate those of cells with the substrate. Consequently, the morphology of cells in tissues differ significantly from that of individual cells.

BP 28.2 Thu 17:30 Poster A

Fluorescence spectral coding for identification of molecules at low concentration — •Zdeněk Petrášek, Jens Wiedemann, and Petra Schwille — Biotechnologisches Zentrum, TU Dresden, Tatzberg 47/49, 01309 Dresden, Germany

We investigate how a combination of 2-3 distinct fluorescent dyes could be used to produce multiple spectral codes for unique species identification. As an experimental model we use non-fluorescent beads to which different fluorescent molecules are attached. The emission from immobilized beads is dispersed by a prism and imaged by a camera.

We study how the noise level influences the ability to resolve two different spectra, using both simulations and experiments. The effects of the spectral overlap and of the number of spectral channels were explored. Introducing convenient expressions for the noise level in the spectrum and the difference between two spectra leads to a simple relationship between the spectral difference (which can be calculated from noiseless reference spectra) and the resolvability, defined as a maximum noise level required to guarantee a given success identification rate. Experiments show that the bead autofluorescence, if not exceeding the probe fluorescence, does not prevent correct identification of the spectral code. Initial results of simulations further suggest that finding the bead in the noisy image may be more difficult than identifying its spectral code, once the bead is found.

BP 28.3 Thu 17:30 Poster A

3-Dimensional Characterization of Fibroblasts with Enhanced Differential Interference Contrast Microscopy — •Malte Ohmstede, Erik Bernitt, and Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen

Circular dorsal-ruffles, a phenomenon found on the dorsal surface of fibroblast cells, are not yet well understood, actin based membrane protrusions. Algorithms for characterization of three-dimensional properties and dynamics have been developed for evaluation of optical sectioning data, which is gained with differential interference contrast. Due to the low optical density of fibroblast specimens, differential interference contrast is used. Optical sectioning data allows for evaluation of living specimens, thus enabling characterization of dorsal ruffle dynamics. Differential interference contrast, however, complicates evaluation of image data due to gradient-like image properties. Complications with image segmentation, i.e. separating image foreground and background, have been resolved by application of a two-dimensional Hilbert Transform on image data to gain bright-field-like images from gradient sources. Further processing was done by executing morphological filters and skeletonization on the binary images gained by segmentation. Contour data gained by skeletonization was then extracted for further evaluation and processing.

BP 28.4 Thu 17:30 Poster A

Measuring the local refractive index of cells with a laser trap based interferometer — •Kai Bodensiek, Paula Sánchez, Yvonne Kretzer, and Iwan Schaap — III Physikalisches Institut, Faculty of Physics, Georg-August Universität, Götingen, Germany

To be able to measure the spatial distribution of the refractive index in individual living cells we constructed a micrometer sized Fabry-Pérot interferometer that was placed in a microscope sample chamber. One mirror of the interferometer is formed by the microscope coverslip and the second movable mirror was positioned with a laser trap in a direction perpendicular to the coverslip. The local cellular refractive index is extracted by simultaneously measuring the local height of the cell and the cell induced phase shift of the interference signal. Because the instrument is implemented in a diffraction-limited optical microscope we can study the local organization of the cell and its nucleus.

BP 28.5 Thu 17:30 Poster A

Sample preparation and delivery for bio-imaging at the European XFEL Facility — •Joachim Schulz — European XFEL GmbH, Hamburg, Germany

Recent success in femtosecond x-ray protein nano-crystallography [Nature 470, p.73 (2011)] and imaging of mimivirus particles [Nature 470, p.78 (2011)] demonstrate the prospects of free-electron lasers for biophysics.

At the European XFEL GmbH in Hamburg (Germany) we design and build a 3.4 kilometres long x-ray free-electron laser. This facility will produce femtosecond x-ray pulses with wavelengths below an Angstrom. The expected brilliance of the facility will be considerably higher compared with other x-ray FELs and the repetition rate of 27.000 pulses per second will be unique. One of the six end-stations of this laser facility will be optimized for imaging experiments on biological samples. The European XFEL Facility will start operation in 2015.

One of the challenges for biological imaging techniques at free-electron laser sources is the preparation and delivering of specimen into the vacuum of the x-ray laser. Lab space and equipment will have to be provided close to the end-stations. The bio-samples have to be efficiently delivered to the beam and hit by the x-ray pulses.

To this end methods have to be developed to keep the samples in the natural state and to avoid too much contamination of the vacuum. In this presentation I will show first considerations concerning the sample delivery system for bio-samples at the European XFEL Facility.

BP 28.6 Thu 17:30 Poster A

Nanotomography of bovine tendon — •Stefan Kubitza[1], Stephanie Röper[1], Anke Bernstein[2], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [2]Department für Orthopädie und Unfallchirugie, Muskuloskelettales Forschungslabor, Universitätsklinikum Freiburg, 79106 Freiburg

Collagen is the most abundant fibrous protein in mammals. It can be found in various types of biological tissue, for example in tooth, bone and tendon. We use atomic force microscopy (AFM) based nanotomography for imaging the nanoscaled structure of this biological material. The specimen is ablated layer-by-layer by wet chemical etching and imaged with tapping mode AFM after each etching step. From resulting series of AFM images the three-dimensional structure is reconstructed. In our experiments we focus on native bovine tendon (collagen type I) and report about the suitability of different etching solutions for nanotomography imaging.

BP 28.7 Thu 17:30 Poster A

Photoemission electron microscopy of magnetotactic bacteria — •Christoph Keutner[1], Ulf Berges[1], Claus M. Schneider[2], and Carsten Westphal[1] — [1]DELTA / Experimentelle Physik I, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44221 Dortmund — [2]PGI-6, Forschungszentrum Jülich, D-52425 Jülich

In their natural environment magnetotactic bacteria (MTB) respond to earth's magnetic field by aligning their direction of motion parallel or antiparallel to the magnetic field. This sensitivity to the magnetic field is caused by a magnetic particle chain contained within the MTB's body, the so called magnetosome chain. Presently, there are first considerations of applying this phenomenon within a biologic propulsion and steering system for nanorobots [1]. Therefore the magnetic properties of these magnetosomes are of particular interest.

In this work first experiments of imaging MTB with photoemission electron microscopy (PEEM) were performed, here the bacteria *Magnetospirillum magnetotacticum* [2]. In order to prepare the MTB in a UHV compatible way, several methods were tested. The best results were obtained with a lyophilized specimen applied on a Si-wafer. So far, first images of *M. magnetotacticum* could be recorded. In order to achieve a higher resolution and to image the internal magnetosome chain, further modifications and experiments are ongoing.

[1] S. Martel, M. Mohammadi, O. Felfoul, Z. Lu and P. Pouponneau, Int. J. Rob. Res. **28**, 571 (2009)
[2] R. Blakemore, Science **190**, 377 (1975)

BP 28.8 Thu 17:30 Poster A

Multifocus Fluorescence Correlation Spectroscopy using a programmable phase modulator — •Thomas Kuckert, Zdeněk Petrášek, and Petra Schwille — Biotechnologisches Zentrum, TU Dresden, Tatzberg 47/49, 01307 Dresden, Germany

Fluorescence Correlation Spectroscopy (FCS) has been used for studying molecular dynamics and interactions in many fields, ranging from physics, chemistry to biology. Many applications, especially those within living cells or tissues where the measurement time is limited, would benefit from the ability to perform measurements at different positions simultaneously. This requires both excitation localized within a number of well-defined volumes, and separate detection of fluorescence from within these volumes. Here we present an ongoing project the goal of which is to construct such a flexible multifocus FCS setup. Previously, multiple excitation spots have been realized by diffractive optical elements designed specifically for a given spot pattern, without the possibility to adapt the pattern to the sample. We use a programmable phase modulator (PPP), which allows flexible formation of a variable number of foci at arbitrary positions. Initially, avalanche photodiodes will be used for detection, to assess the quality of foci produced by the PPP. Eventually, fast EM-CCD is intended for simultaneous detection from all foci to reach full flexibility.

BP 28.9 Thu 17:30 Poster A

Interferometric Particle Tracking — •Dennis Müller and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany

We report interferometric tracking of gold nanoparticles with spatial resolution in the nanometer range and sub-millisecond temporal resolution. This technique combines a dark-field microscope with laser illumination with a Mach-Zehnder-like interferometer which follows the camera exit of the microscope. In the interferometer scattered light from the object particle is superimposed with scattered light from a reference particle which has been immobilized in the object plane. Readout is done by avalanche photodiodes. The phase of the resulting interferogram is a very sensitive measure for displacements of the object particle relative to the reference particle. This configuration eliminates effectively the effect of microscope drift on the measurement and makes this technique a promising candidate for applications like motor protein tracking experiments.

BP 28.10 Thu 17:30 Poster A

Approaches for improved dual color Photoactivated Localization Microscopy — •Paolo Annibale, Mattia Greco, Marco Scarselli, and Aleksandra Radenovic — LBEN, IBI EPFL Lausanne 1015 Switzerland

Dual color PhotoActivated Localization Microscopy (PALM) presents unique challenges due to the specific photo-physical behavior of the fluorescent proteins used as a tags and to the asynchronous nature of the photoactivation and localization of the molecules belonging to each fluorophore pair. We systematically investigate the effect of molecular photoblinking and fluorescence dark times on a typical dual color PALM experiment. This allows us to propose a method to identify potential photoblinking-originated artifacts by screening for concomitant spatial and temporal clusters, a prerequisite for the correct localization and co-localization of oligomeric sub-diffraction limit cellular structures [1]. Using a setup axially stabilized to better than 5 nm we compare the performance of three different dual color fluorescent protein pairs using as positive controls fusion constructs imaged both in-vitro and on the plasma membrane of HeLa cells. We present an application of these methods to the imaging of a pair of plasma membrane proteins involved in cell signaling.

[1] P. Annibale et al. Nature Methods 8 (2011) 527-528

BP 28.11 Thu 17:30 Poster A

Mechanical Properties of Primary Cilia — •Christopher Battle and Christoph F. Schmidt — 3te Physikalisches Institut, Georg-August Universitaet, Goettingen, Germany

Recent studies have shown that the primary cilium, long thought to be a vestigial cellular appendage with no function, is involved in a multitude of sensory functions. One example, interesting from both a biophysical and medical standpoint, is the primary cilium of kidney epithelial cells, which acts as a mechanosensitive flow sensor. Genetic defects in ciliary function can cause, e.g., polycystic kidney disease (PKD). The material properties of these non-motile, microtubule-based 9+0 cilia, and the way they are anchored to the cell cytoskeleton, are important to know if one wants to understand the mechano-electrochemical response of these cells, which is mediated by their cilia. We have constructed two optical-trapping microscopes for this purpose, one upright instrument with access for patch-clamping pipettes using back-scatterered force and displacement detection, and one inverted microscope with optimized DIC imaging capabilities in conjunction with a double optical trap. With these instruments we can probe the activation of ciliated MDCK cells in confluent monolayers and the mechanical properties of the cilium.

BP 29: Posters: Regulation

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

BP 29.1 Thu 17:30 Poster A

Autocatalytic processes in primordial reactions — •Sabrina Scherer — Universität des Saarlandes, Biologische Experimentalphysik

Stanley L. Miller made a revolutionary experiment in 1952. He discovered amino acids in a reaction of methane, ammonia, hydrogen and water, triggered with electric discharges and heat. We reproduced Miller's experiment to understand the physical and chemical processes, which take place in the first biochemical reactions. Catalysts lead to the selection of specific reactions and push the corresponding reaction rates. To analyse the samples we use mass spectrometry. In our spectra, we detect two different states. One of them consists of hundreds of different masses. In contrast, the other state displays well-ordered spectra with many equidistant peaks. The alternating appearance of these two states over time points to a competing system in which several catalytic cycles could be involved. We suspect self-reproductive and autocatalytic cycles to play a significant role in chemical evolution.

BP 29.2 Thu 17:30 Poster A

Evolution of increasingly complex molecules — •Philipp Zimmer[1], Emanuel Worst[2], Eva Wollrab[2], Albrecht Ott[2], and Karsten Kruse[1] — [1]Universität des Saarlandes, Theoretische Biologische Physik, Postfach 151150, 66041 Saarbrücken — [2]Universität des Saarlandes, Biologische Experimentalphysik, Postfach 151150, 66041 Saarbrücken

Darwinistic evolution of species started on the level of molecules. It is still unknown under which conditions evolution of molecules of increasing complexity can occur in chemical mixtures that are out of thermodynamical equilibrium. We examine a simple scenario, in which molecular units assemble into chains either by spontaneous or by template-driven, assisted concatenation. We show that, beyond a critical rate of assisted concatenation, the fractions of chains of increasing length grow exponentially. An experimental realization of this system is proposed.

BP 29.3 Thu 17:30 Poster A

Atomspektren gewonnen aus einem zellbiologischen Mechanismus — •Manfred Kunz — Reinhardtstraße 11, 04318 Leipzig

Spektren werden aus Übergangsenergien berechnet. Man kann diese ohne direkte Bezugnahme auf die Atomphysik berechnen, wozu lediglich die Masse des Elektrons mit Atomkern und die Feinstrukturkonstante in einer relativistischen Interpretation gebraucht werden. Vorausgesetzt werden Teilchen oder relativistische Scheinmassen, deren Wechselwirkung unter Anwendung der Erhaltungssätze für Energie und Impuls mit ganzen Zahlen zu Spektralserien führen. Die Hinzunahme biologischer Mechanismen erweist sich als hilfreich. Eine modifizierte Keimzellteilung lässt sich auf eine Dreiecksmatrix mit einheitlichen Gliedern reduzieren. Bezeichnet man die Anzahl der Zeilen mit n, dann erfolgt der Wachstumsvorgang im Prinzip durch Kopieren der vorausgegangenen Dreieckszeile und durch ein symmetrisches Anfügen je eines weiteren einheitlichen Gliedes. Jede Dreieckszeile soll aus 2n-1 Gliedern bestehen, das Dreieck beinhaltet demzufolge insgesamt n^2 Glieder. Bei der Lyman-Serie repräsentiert die längste Dreieckszeile zahlenmäßig den Impuls P. Der Gesamtinhalt des Dreiecks verkörpert die Energie E. Die Größen P und E sind nicht frei wählbar. Jede Dreieckszeile lässt sich anordnen als ein räumlich übereinander liegendes Sternpolygon oder Polygon, entfernt vergleichbar mit einer Bohrschen Bahn. Die Glieder können als Punkte eines interessanten Algorithmus belebt werden.

BP 29.4 Thu 17:30 Poster A

Reversible Enzyme Regulation as a Source of Bistability in Covalent Protein Modification Systems — •Ronny Straube and Carsten Conradi — Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

Goldbeter and Koshland have shown that covalent protein modifications can generate highly sigmoidal response behavior (known as ultrasensitivity) when the converter enzymes (e.g. kinase and phosphatase) operate in saturation [1]. However, in vivo, the converter enzymes are often themselves subject to regulation, e.g. by an allosteric effector or by additional covalent modifications. As a result, they typically exist in inter convertible states of high and low activity which may compete for substrate. Here, we show that this competition is structurally sufficient to generate a bistable system response already at the level of a single protein modification cycle, i.e. without the requirement for multisite modifications or additional positive feedback loops. In contrast to mechanisms based on multisite modifications bistability is even predicted to occur when substrate molecules and enzymes are present in equal amounts. Our results provide an alternative and challenging view on the origin of bistability in the Cdk1-Cdc25-Wee1 system [2] which governs the M-phase transition of the cell cycle in fission yeast.

[1] Goldbeter A, Koshland, DE Jr. An amplified sensitivity arising from covalent modification in biological systems. Proc. Natl. Acad. Sci USA 78, 6840-6844 (1981). [2] Ferrell JE Jr. Feedback regulation of opposing enzymes generates robust, all-or-none bistable responses. Curr. Biol. 18, R244 (2008).

BP 29.5 Thu 17:30 Poster A

Cell polarisation's impact on local and global calcium signals during T-cell activation — •Martin Peglow and Heiko Rieger — Universität des Saarlandes

A crucial step for the successful T-cell activation is the stimulation of calcium (Ca^{2+}) entry across the plasma membrane through the so called Ca^{2+} release-activated Ca^{2+} (CRAC) channel. Recently Quintana et. al (The EMBO Journal (2011) 30, 3895 - 3912) have shown, that cell polarisation (the rearrangement of several cell organelles) is a very important step in T-cell- and CRAC-channel-activation. With our model we want to verify if different relativ positions between CRAC-channels, mitochondria and plasma membrane calcium-ATPases (PMCA)-pumps are sufficient to explain the different Ca^{2+} -signals in T-cells. And indeed we can shown, that mitochondria near to the CRAC-channel lead to a higher global Ca^{2+}-concentration and a lower Ca^{2+} microdomain near the CRAC-channel. A nice result is, that an accumulation of PMCA-pumps near the CRAC-channel is essential for high global Ca^{2+}-signals and so for T-cell activation and that in contrast a uniform distribution of PMCA-pumps in the PM lead to lower cytosolic Ca^{2+} -signals. This prediction should be investigated in some new experiments.

BP 29.6 Thu 17:30 Poster A

Molecular Mechanisms of Pattern Formation: Inward Rotating Spiral Waves in Glycolysis — •Ronny Straube[1] and Ernesto M. Nicola[2] — [1]Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg — [2]Institute for Cross-Disciplinary Physics and Complex Systems, Palma de Mallorca

We have recently observed a novel type of spiral wave behavior called inward rotating spiral waves or anti-spirals [1]. To elucidate the underlying molecular mechanism leading to this unusual wave behavior we compare two mechanisms of product activation for the allosteric enzyme phosphofructokinase using amplitude equations. We find that a sequential activation mechanism as in the Monod-Wyman-Changeux (WMC) model is able to generate inward propagating waves while a simple Hill function, as employed in the Selkov model, is not [2]. We show that the occurrence of inward propagating waves does not depend on the magnitude of the enzyme cooperativity (as is true for the occurrence of homogeneous oscillations), but on its sensitivity with respect to changes in the activator concentration. Our results provide an explicit example which shows how the macroscopically observable patterns in a spatially extended system depend on the molecular details of the underlying reaction mechanism.

[1] Straube R, Vermeer S, Nicola EM, Mair T (2010). Inward rotating spiral waves in glycolysis. Biophys. J. 99, L4-L6.

[2] Straube R, Nicola EM (2010). Diffusive coupling can discriminate between similar reaction mechanisms in an allosteric enzyme system. BMC Syst. Biol. 4:165.

BP 29.7 Thu 17:30 Poster A

Dynamics of bacterial persistence — •Pintu Patra and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces Wissenschaftspark Golm 14424 Potsdam, Germany

Persistence is a survival mechanism of bacterial populations that allows them to tackle environmental stress such as antibiotic killing. The phenomenon is the result of reversible phenotype switching between two distinct phenotypic states which are characterized by slow and fast growth or decay. Therefore these cells generate two distinct

sub population during their evolution. We analyse the transient and evolutionary behaviour of a population consisting of two sub population, persister and normal cells, with reversible switching between the two phenotypes. We derive an analytical expression for the fitness of each sub population in fixed and varying environmental conditions. We calculate different time scales in which the total population evolves during its growth and decay which can be used to experimentally measure the phenotypic switching rates. Moreover we show that there is an evolutionary optimal phenotype switching rate for periodic environmental variations. We calculate the total population growth rate to map out the conditions under which the population grows or decays in periodically changing environments. Our study provides a theoretical underpinning for studying phenotypic switching.

BP 29.8 Thu 17:30 Poster A

Effects of receptor location and transport mechanism on bacterial quorum sensing — •Bastian Drees[1,2] and Ilka B. Bischofs[1,2] — [1]Zentrum für Molekulare Biologie der Universität Heidelberg, DKFZ-ZMBH Alliance, Im Neuenheimer Feld 282, 69120 Heidelberg, Germany — [2]BioQuant, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany

In a process known as quorum sensing (QS) bacteria produce, secrete and sense autoinducer molecules (AI) to communicate and get information about their environment, such as cell density and the extent of AI loss by diffusion or flow. QS systems found in different bacteria differ in the way the AIs are secreted and in the way they are sensed. We theoretically investigate the sensitivity and robustness of different QS architectures and the environmental conditions under which these architectures show optimal sensing behavior. We find that active export barely has any effect on external sensing, while any kind of active transport (import or export) increases the noise in internal sensing systems. Furthermore, our model suggests that systems with extracellular sensors are preferred at low AI concentrations, while internal sensing might be preferred at intermediate AI concentrations; a result supported by experimental data.

BP 29.9 Thu 17:30 Poster A

Nonenzymatic Replication of Polynucleotides — •Benedikt Obermayer[1], Kevin Leu[2], Rebecca Turk[2], Sudha Rajamani[2], Irene Chen[2] und Ulrich Gerland[3] — [1]Department of Physics, Harvard University, Cambridge, USA — [2]FAS Center for Systems Biology, Harvard University, Cambridge, USA — [3]Ludwig-Maximilians-Universität München

In the early "RNA world" stage of life, RNA-like polynucleotides stored genetic information and catalyzed chemical reactions. Replication of such molecules suffers from high error rates, limiting the amount of information that can be reliably propagated. We study the fidelity of RNA and DNA replication using experimental non-enzymatic polymerization, and compare to lower bounds on these error rates calculated from a thermodynamic model. We find that RNA replication is intrinsically error-prone compared to DNA, suggesting that transitioning to DNA as genomic material could be of evolutionary advantage [1]. Moreover, we observe a strong context-dependence of polymerization rates, leading to a high probability of successive (cooperative) mutations and markedly slowed polymerization after mismatches. In an intriguing deviation from equilibrium expectations, these effects lead to a drastically lower effective error rate, alleviating its deleterious consequences.

[1] K. Leu, B. Obermayer, S. Rajamani, U. Gerland, I. A. Chen, Nucl. Acids Res. **39**:8135 (2011)

BP 29.10 Thu 17:30 Poster A

Quantum mechanical light in biological systems — •Michael Drexel, Fritz-Albert Popp, and Rajendra P. Bajpai — International Institute of Biophysics, Neuss

Light emanating from living systems ("biophotons") was analyzed and characterized as quantum mechanical, squeezed light. Methods for detecting ultra weak intensity (some photons per square-meter and second) at visible spectral region are described and measurements from biological samples like humans are shown. The three squeezed state parameters (r, Θ and Φ) are estimated for 10 bin sizes (50, 100, ..., 500 milliseconds) by merging the counts at contiguous bins of the observed signal. Coherency index of a signal was established, it can be estimated by a novel method for background corrected measurements, and its practicability to characterize and quantify the deviation from the squeezed state of signals are presented.

The noninvasive measurement of visible- spectral biophoton- signals can be used for reliable characterization and pointing out changes in quantum nature of all emitting systems, as for instance it is done for controlling recovering process of human health, which can be correlated with other physical body parameters like temperature.

A session of colorpuncture treatment improved the coherency indices of signals from different sides and provided relief to the subject suffering from multiple sclerosis. Both improvement of the coherency indices and relief were temporary. More lasting improvement in coherency indices required many sessions of treatment.

BP 30: Symposium SYOL: Origin of Life (with CPP and DY)

Time: Friday 9:30–11:30 Location: H 0105

Invited Talk BP 30.1 Fri 9:30 H 0105

From sequence to function: Random polymerization and modular evolution of RNA — •Susanna C. Manrubia — Centro de Astrobiología (INTA-CSIC), Madrid, Spain

A main unsolved problem in the RNA World scenario for the origin of life is how a template-dependent RNA polymerase ribozyme emerged from short RNA oligomers obtained by random polymerization on mineral surfaces. A number of computational studies have shown that the structural repertoire yielded by that process is dominated by topologically simple structures, notably hairpin-like ones [1]. A fraction of these could display RNA ligase activity and catalyze the assembly of larger, eventually functional RNA molecules retaining their previous modular structure: molecular complexity increases but template replication is absent [2]. This allows us to build up a stepwise model of ligation-based, modular evolution that could pave the way to the emergence of a ribozyme with RNA replicase activity, step at which information-driven Darwinian evolution would be triggered.

[1] Stich, M., Briones, C. and Manrubia, S. C. (2008) On the structural repertoire of pools of short, random RNA sequences. Journal of Theoretical Biology 252, 750

[2] Briones, C., Stich, M. and Manrubia, S. C. (2009) The dawn of the RNA world: Towards functional complexity through ligation of random RNA oligomers. RNA 15, 743

Invited Talk BP 30.2 Fri 10:00 H 0105

Spontaneous autocatalysis and periodic switching in a prebiotic broth — •Eva Wollrab[1], Sabrina Scherer[1], Karsten Kruse[2], and Albrecht Ott[1] — [1]Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken — [2]Theoretische Biologische Physik, Universität des Saarlandes, Saarbrücken

The pioneering experiments of Stanley Miller and Harold Urey have suggested that a large number of today's biomolecules spontaneously emerged under prebiotic conditions. How these organic molecules self-organized to produce the earliest forms of life is poorly understood. Here we perform Miller-Urey-type experiments and monitor the temporal development of the organic mixture using real-time mass-spectrometry. We observe the continuous emergence of a large number of substances during hours, followed by several orders of magnitude faster, autocatalytic growth of polymeric species. In the following these species appear and vanish periodically, while the amplitude of the oscillation increases. Due to the high complexity of the considered chemical dynamics, it will be difficult to determine the precise molecular pathways in the system. However, we will discuss possible, more general mechanisms that lead to the observed behavior. Our results show that upon weak energetic driving, a randomly generated, complex chemical system can spontaneously generate order.

Invited Talk BP 30.3 Fri 10:30 H 0105

Thermal solutions for molecular evolution — •Dieter Braun — Systems Biophysics, Physics Department, Center for Nanoscience, LMU Munich, Germany

Disequilibrium conditions are central for understanding the origin of life. Taking energetic chemicals at high concentrations to synthesize more complex molecules will not be enough to understand early molecular evolution.

Thermal gradients drive two processes. Laminar thermal convection leads to highly regular temperature oscillations that allow the melting and protein-based replication of DNA. In the same setting, molecules move along the thermal gradient (Soret effect), leading with thermal convection to strong accumulation of biomolecules. More complex molecules are exponentially better retained.

Our experiments implement both replication and accumulation in a micrometer-sized chamber. The setting offers an elegant implementation of a Darwinian process of replication and selection that is solely driven by a thermal gradient.

Early replication however has to be implemented without proteins. We demonstrate that a pool of Transfer RNA yields a protein-free route to replication and translation. In addition, Obermayer and Gerland showed that replication-like behavior is already found by selective degradation of single over double stranded RNA. If combined with a length selective thermophoretic trap, complex dynamics are expected. As a first indication, we found the enhanced polymerization of nucleotides in a thermophoretic trap.

Invited Talk BP 30.4 Fri 11:00 H 0105

Systems chemistry: Self-replication and chiral symmetry breaking — •Guenter von Kiedrowski — Chair for Bioorganic Chemistry, Ruhr-University, Bochum, Germany

Self-replication is one of the major principles without life could not exist. Whether the origin of self-replication is identical to the origin of the hypothetical RNA world or whether it existed at an earlier stage of evolution is an open question that has stimulated chemists to search for systems capable of making copies of itselves via autocatalytic reactions. As self-replication means autocatalysis plus information transfer, the reaction products must necessarily be able to store more structural information than their precursors. Templating as a means to transfer structural information has been exploited since the first successful example of a chemical self-replicating system almost two decades ago. Today we have a broad variety of such systems employing oligonucleotides, peptides, and small organic molecules as templates and autocatalytic, cross-catalytic, collectively autocatalytic and non-autonomous (stepwise) schemes of self-replication. Chirality and the spontaneous emergence of optical activity, viz. chiral symmetry breaking may be seen either as the key prerequisite to allow for self-replication of proto-biomolecular structures, or, as a systemic result of self-replication when starting from prochiral precursors. For example, while PNA as well as a recently described small organic replicator are achiral entities, the introduction of variant prochiral building blocks are expected to yield chiral replicators.

BP 31: Imaging

Time: Friday 9:30–11:30 Location: H 1058

Topical Talk BP 31.1 Fri 9:30 H 1058

High-speed imaging of organogenesis in entire zebrafish with SPIM — •Jan Huisken — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

In the past the recording speed of a time-lapse experiment has ultimately been limited by the amount of light the specimen could tolerate. Lately, it has been shown that light sheet microscopy such as Selective Plane Illumination Microscopy (SPIM) reduces photo-toxic effects to a minimum. Due to the illumination of the sample in a thin volume around the focal plane no tissue outside the plane of interest is exposed and bleached. In addition, the fluorescence is collected with very high sensitivity cameras. SPIM benefits from the latest camera technology and is therefore constantly improving in speed and sensitivity.

Experiments have become possible that run at full speed using the best possible hardware, without being limited by the fragility of the sample. The speed advantage of the SPIM over other fluorescence technique can be utilized to image rapid events in developing tissue or to record a large number of views for multi-view reconstruction. The large amount of data that is accumulated when modern cameras are run at high-speed for hours or days is enormous and innovative data processing solutions are needed. One key application of this emerging technology includes the multi-dimensional imaging of the developing zebrafish larvae over extended periods of time. I will give some examples of the unique capabilities of SPIM, especially for monitoring the development of the cardiovascular system and the early endoderm.

M. Weber and J. Huisken, Curr Opin Genet Dev, 21, 566-72 (2011).

BP 31.2 Fri 10:00 H 1058

Revival of prism-based TIR microscopy - Versatile tracking of fluorescent and scattering probes with nm-precision — •René Schneider and Stefan Diez — B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden

Current single-molecule microscopy experiments mostly rely on the fluorescence signal of fluorescent proteins, organic dyes or quantum dots attached to proteins of interest. However, these probes suffer from limitations, namely limited number of photons before photobleaching, photon blinking, and fluorescence saturation. Consequently, the temporal and spatial resolution by which single molecules can be tracked is limited. Promising candidates for replacing fluorescent probes in-vitro are gold nanoparticles (GNPs). GNPs exhibit a large scattering cross section in the optical spectrum due to plasmon resonance, provide long-term stability and allow for versatile surface chemistry. Furthermore, their emission rate does not saturate.

Here, we present a camera-based wide-field imaging technique for GNP-labeled proteins using a novel parabolic prism-type total-internal reflection (TIR) microscope. We demonstrate the advantages of GNPs over commonly used fluorescent probes and discuss the pros and cons of prism-type versus objective-type TIR microscopy. We demonstrate that prism-based TIR microscopy allows imaging of fluorescent and scattering probes with high signal-to-noise and excellent control over a wide range of incidence angles.

Our method allows for precise localization of biomolecules within short acquisition times over long time scales.

BP 31.3 Fri 10:15 H 1058

Cryogenic Colocalization with Nanometer Resolution — •Siegfried Weisenburger and Vahid Sandoghdar — Max Planck Institute for the Science of Light, 91058 Erlangen, Germany

The advent of super-resolution microscopy methods in the past decade caused a stir in the fluorescence microscopy community [1]. In particular, wide-field localization microscopy has pushed the resolution by more than one order of magnitude. Here, the centers of the point-spread functions of individual fluororescent molecules are determined with very high accuracy only limited by the number of collected photons [2]. At room temperature, the localization accuracy typically reaches a few tens of nanometers restricted by photobleaching. From low-temperature optical studies of single biomolecules, it is known that fluorophores are much more photostable at cryogenic temperatures [3] allowing for the detection of more photons. To overcome the accuracy limitation given by photobleaching, we introduce a new method of colocalization microscopy utilizing liquid helium temperature.

We will demonstrate our technique by colocalization measurements of a double-stranded DNA which is specifically labeled with two fluorescent molecules at a distance of ten nanometers. Furthermore, we will discuss the perspectives of this method for other biological applications.

1) S. Hell, *Nat. Methods* **6**, 24 (2009).
2) R. Thompson et al., *Biophys. J.* **82**, 2775 (2002).
3) R. Zodervan et al., *J. Phys. Chem. A* **108**, 1657 (2004).

BP 31.4 Fri 10:30 H 1058

Multimodal imaging of the human cerebellum: phase contrast tomography, magnetic resonance microscopy and histology — •Georg Schulz[1], Timm Weitkamp[2], Irene Zanette[3,4], Franz Pfeiffer[4], Conny Waschkies[5], Christian David[6], and Bert Müller[1] — [1]BMC, Uni Basel, Switzerland — [2]Synchrotron Soleil, Gif sur Yvette, France — [3]ESRF, Grenoble, France — [4]Biomedical Physics, TUM, Garching, Germany — [5]IBT, ETH / Uni Zurich, Switzerland — [6]LMN, PSI, Villigen, Switzerland

To visualize a part of the human cerebellum we use grating based

phase contrast CT, MR microscopy and histology. Phase contrast tomography yields the 3D distribution of the X-ray refractive index and is much more sensitive than conventional absorption imaging. Using a grating interferometer we are able to detect deflection angle differences of around 20 nrad. The CT results were acquired at ESRF Grenoble using a 5 μm pixel size detector. The high sensitivity of the method even provides contrast between structures within the gray matter. The MR microscopy data set was acquired using a T2*-weighted 3D FLASH sequence with an isotropic pixel length of 45 μm. The method allows a clear differentiation between white and gray matter but shows marginal contrast between the two structures within the gray matter. During histology a Nissl staining was applied. While the micrographs have a high spatial resolution of less than a μm and a contrast comparable to the X-ray phase contrast data, they do not provide 3D information. The complementarity of X-ray phase-contrast CT, MR microscopy and histology gives better insights into the morphology of the human brain.

BP 31.5 Fri 10:45 H 1058

Planar structured AlGaN/GaN High Electron Mobility Transistor sensor for recording of Physarum cell activity — •Hartmut Witte[1], Thomas Lippelt[1,2], Christian Warnke[1,2], Marcus J. B. Hauser[2], and Alois Krost[1] — [1]Otto-von-Guericke-Universität Magdeburg, Inst. Exp. Phys., Abt. Halbleiterepitaxie — [2]Otto-von-Guericke-Universität Magdeburg, Inst. Exp. Phys., Abt. Biophysik

Planar multi-electrode AlGaN/GaN High Electron Mobility Transistors (HEMTs) arrangements are very useful for spatial and time resolved stimulation and recording of extended and excitable biological cultures such as neurons or yeast cells. In this contribution, the spatially resolved sensitivity of a multiple AlGaN/GaN HEMT structure is used for detection of migration and growth of Physarum cells in situ. Physarum polycephalum displays remarkably *intelligent* abilities inducing intensive studies for instance on learning and on memory of past events. We have investigated the impact of Physarum cell motion on the source-drain current and impedance of a sensor structure presented by ten circular arranged AlGaN/GaN HEMTs described in detail in Witte et al; J. Phys. D, 44, 355501 (2011). All time tracks were correlated with video pictures of the area around the actual HEMT and the Physarum cell. So, we detected the cell growing across a HEMT sensor. Based on the detailed analysis of the sensor/medium interface we are able to distinguish between the signals from the cell and the medium. Additionally, the cell dispersions were investigated by impedance spectroscopy for more information about the properties of inner structures.

BP 31.6 Fri 11:00 H 1058

4D imaging: a versatile suite for image analysis — •Bhavna Rajasekaran[1], Jean-Yves Tinevez[2], Koichiro Uriu[3], Guillaume Valentin[1], Frank Jülicher[3], and Andrew Oates[1] — [1]Max Planck Institute for Cell Biology and Genetics, Dresden, Germany — [2]Institut Pasteur, Paris, France — [3]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Fluorescence microscopy can capture in vivo time-space visualization of cellular dynamics, changes in spatio-temporal pattern of gene expression within cellular structures, tissue growth and morphogenesis. Computational image analysis techniques serve to translate such image data into meaningful quantitative measurements that can further be analyzed and understood to draw precise description of a biological phenomena or allow hypothesis testing. Here, we demonstrate novel computationally efficient 3D nuclei segmentation algorithm based on image derivatives combined with semi-automated method for post rectification of segmented data to reliably extract individual cell identity and track cells over time based on nearest neighborhood for the developing pre-somitic mesoderm (PSM) tissue in the zebrafish embryo. The PSM undergoes rigorous morphological changes and has juxtaposed cells that exhibit continuous diverse and dynamic cell motions, thus providing a technically challenging platform for image analysis. We use synthetic data and transgenic chimeric embryos to assess and validate the performance of the algorithm. Algorithm development and testing was done in Matlab 7.10.0 (R2010a) and exported to the Fiji library- an open source, user-friendly platform for biological image analysis.

BP 31.7 Fri 11:15 H 1058

In-focus phase contrast electron cryo-microscopy of biological samples with an electrostatic phase plate — •Daniel Rhinow[1], Andreas Walter[1], Manfred Lacher[2], Siegfried Steltenkamp[2], Sam Schmitz[2], Peter Holik[2], and Werner Kühlbrandt[1] — [1]Max-Planck-Institut für Biophysik, 60438 Frankfurt, Deutschland — [2]caesar research center, 53175 Bonn, Deutschland

Although the instrumental resolution limit of the latest generation of transmission electron microscopes reaches 0.5 Å, a variety of physical factors limit the experimental resolution achievable with biological samples. Biological macromolecules are pure phase objects that are visualized by phase contrast, which in conventional cryoEM is generated by defocusing. Disadvantages of defocusing are weak contrast and incomplete transfer of object information, which impairs data collection and 3D reconstruction. A powerful alternative to defocus phase contrast is the use of a physical phase plate in the back focal plane of the electron microscope. The Boersch phase plate (BPP) comprises an electrostatic einzel lens shifting the phase of the unscattered electron beam by 90°, thus maximizing phase contrast for in-focus TEM. The PACEM (Phase Contrast Aberration-Corrected Electron Microscope) is a TEM prototype developed by Carl Zeiss NTS in collaboration with the MPI of Biophysics. BPPs have been tested in the PACEM. First BPP images of stained, unstained, and cryogenic biological specimens have been obtained.

BP 32: Physics of Cells III

Time: Friday 9:30–13:00 Location: H 1028

BP 32.1 Fri 9:30 H 1028

Margination of white blood cells in microvessels — •Dmitry A. Fedosov, Julia Fornleitner, and Gerhard Gompper — Institute of Complex Systems, Forschungszentrum Juelich, Juelich, Germany

Margination of white blood cells (WBCs) towards microvessel walls is an essential pre-condition for their efficient adhesion to the vascular endothelium, which is a crucial step in the organism's immune response. WBC margination depends on hydrodynamic interactions of blood cells with the vessel walls as well as on their collective behavior and deformability. Numerical simulations with 2D and 3D blood flow models using the Dissipative Particle Dynamics method reveal a non-trivial dependence of WBC margination on blood hematocrit, flow rate, WBC deformability, and red blood cell (RBC) aggregation properties. In particular, WBC margination appears to be optimal within certain intermediate ranges of hematocrit and flow rate values, while beyond these ranges WBC margination is substantially attenuated. Moreover, RBC aggregation is found to enhance WBC margination in microvessels. We will present margination state diagrams, which identify WBC margination behavior for a wide range of flow and cell suspension conditions. These findings will help us better understand WBC margination and adhesion in microcirculation.

BP 32.2 Fri 9:45 H 1028

Insights into equilibrium shape from in-silico modeling of red blood cells — •Ulf Schiller[1,2] and Anthony Ladd[2] — [1]Theoretical Soft Matter and Biophysics, Institute of Complex Systems, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Chemical Engineering, University of Florida, Gainesville FL 32611-6005, USA

We present a novel computational model for deformable particles such as red blood cells. It is based on a finite-element like model of an elastic membrane with director degrees of freedom. The model resembles a two-dimensional liquid crystal coupled to an elastic network. We outline the connection to Helfrich's curvature model, and demonstrate how a coarse-grained worm-like chain model can account for the spectrin network elasticity. One of the advantages of our model is that we have full control over the reference state of the elastic surface. This allows us to probe its influence on the equilibrium shape of RBCs, which in most other models is implicitly built in via the parametric shape function put forward by Evans and Fung. We show simulation results that indicate that the Evans-Fung shape is not a strain-free minimum if a spherical reference configuration is used. The remaining strains drive the RBC away from the discocyte shape and into the stomatocyte

shape. The discocyte shape thus requires a-priori assumptions to be stabilized, which is to be contrasted with the relaxation of remaining strains due to dynamic reorganization of the spectrin network. We discuss the relevance of these findings with respect to possible extensions of computational RBC models.

BP 32.3 Fri 10:00 H 1028

Quantification of Depletion Induced Adhesion of Red Blood Cells — •Patrick Steffen[1], Claude Verdier[2], and Christian Wagner[1] — [1]Universität des Saarlandes, Sarbrücken, Germany — [2]CNRS - Universite de Grenoble I, Laboratoire Interdisciplinaire de Physique

Under physiological conditions, red blood cells are known to form aggregates in the forms of rouleaux due to the presence of plasma proteins. Roleaux formation can be also induced in vitro by the adddition of macromolecules to washed red blood cells. Current data on the adhesion strength between red blood cells in their natural discocyte shapes are limited. Here we present measurements on the dextran induced aggregation of red blood cells by use of atomic force microscopy based single cell force spectroscopy (SCFS). The effects of dextran concentration and molecular weight on the interaction energy of adhering RBCs was determined. The results are in excellent agreement with a model based on the depletion effect and former experimental studies.

BP 32.4 Fri 10:15 H 1028

'Wound Healing in vitro': Blood Platelets on Structured Substrates — •Rabea Sandmann[1], Sarah Schwarz G. Henriques[1], Florian Rehfeldt[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics & CRC Physics, University of Göttingen, Germany — [2]Third Institute of Physics, University of Göttingen, Germany

Blood platelets are anuclear, adherent cells primarily responsible for blood clotting and their activation can be triggered by, e.g., soluble factors like thrombin. Whenever a wound arises, the endothelial cell layer inside blood vessels is disrupted and underlying proteins become exposed, which creates a micro- and nanostructured surface. It is therefore important to understand how platelets react to micro- and nanostructured surfaces. Our results show that isotropic structures in the μm-range do not have an influence on the orientation of cells or the ordering of the stress fibers. However, the degree of surface coating determines the size of the platelets. Furthermore, platelets build distinct geometrical shapes on unstructured glass. Quite similar shapes can be observed on microstructured PDMS substrates. Therefore, the process of shape formation may be governed by underlying nanostructures. We examine the effect of such nanostructured substrates, which have the potential to alter the ordering of stress fibers by confinement of the focal adhesions' positions. Our experiments contribute to the fundamental understanding of cell behavior in general, and may have direct applications in medicine due to the importance of platelets in wound healing.

BP 32.5 Fri 10:30 H 1028

Active fluctuations of the red blood cell membrane violate the fluctuation dissipation theorem — •Timo Betz, Hervé Turlier, Jean-François Joanny, and Cécile Sykes — Institut Curie, UMR 168, 11 rue Pierre et Marie Curie, 75005 Paris, France

Red blood cells are extremely elastic objects, able to recover their shape even after large deformation as when passing through tight capillaries. Despite many decades of intensive research, the influence of active mechanical of red blood cells is still under debate. Here we present direct evidence that the red blood cell fluctuations violate the fluctuation dissipation theorem (FTD). We directly measure the mechanical response function using optical tweezers, and compare it to the thermal fluctuation spectrum represented by the power spectral density (PSD). In equilibrium thermodynamics, the dissipative part of the response function and the PSD are related by the fundamental relation of the fluctuation-dissipation theorem, which we directly tested with our measurements. The experimental investigation of the FDT shows a violation at the low frequency range (f<10Hz), while at higher frequencies the FDT is confirmed. This has important implications for the analysis of red blood cell mechanics, as the FDT is commonly used to extract mechanical parameters from membrane fluctuations. Using classical equilibrium membrane theory, we can show that the effect of the active fluctuations is manifested in an apparent lower membrane tension as compared to the direct measurement using the response function. Our results suggest that the active fluctuations help the RBC to pass through capillaries and to prevent adhesion.

BP 32.6 Fri 10:45 H 1028

Towards the understanding of bond organization in adhesion domains: Coexistence of the dilute and the dense packing — •Daniel Schmidt[1], Timo Bihr[1], Udo Seifert[1], and Ana-Sunčana Smith[2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart — [2]Institut für Theoretische Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg

We study the optimal arrangement of ligand-receptor bonds in microdomains that form during the adhesion of biological membranes. In our model-domains, the bonds are placed on a regular lattice and described by harmonic springs. The membrane also interacts with the substrate by a nonspecific potential. Additionally, we explicitly consider the effects of fluctuations of both the membrane and the bonds as well as the membrane tension. The stability of domains emerges from the analysis of the appropriate free energy density. We determine the phase diagram of the system as a function of key parameters such as the stiffness of the bonds, the ligand-receptor binding affinity, and the distance between the bonds.

In a parameter range typical for experiments, we find the commonly observed densely packed domains and a regime in which the bonds are sparsely distributed. The two regimes are separated by an energy barrier, which may signify unstable specific adhesion at intermediate densities, if one of the binding partners is immobile. If both ligands and receptors can freely diffuse through the opposing membranes, we predict a coexistence between the two domain types, which agrees with recent experimental observations.

BP 32.7 Fri 11:00 H 1028

Direct observation of catch-bonds in focal adhesions of living cells — •Navid Bonakdar, Achim Schilling, Claus Metzner, Michael Kuhn, Richard Gerum, and Ben Fabry — Biophysics Group, University of Erlangen, Germany

Single molecule force spectroscopy data have demonstrated that the chemical bonds between extracellular matrix proteins, integrins, and several proteins of the focal adhesion complex show catch-bond behavior: the binding strength increases under mechanical load. It remains unknown, however, whether catch-bond mechanisms are of any relevance for stabilizing matrix adhesions in living cells. To measure adhesion strength, we bind RGD-coated magnetic beads to integrin adhesion receptors of living cells and apply forces of up to 80 nN with a magnetic tweezer. In the case of a pulling force that increases linearly with time, the characteristic bead detachment force is expected to increase logarithmically with the loading rate for thermally activated Bell-type molecular bonds. We find that the detachment force tends to increase faster than logarithmically, demonstrating that the adhesion bonds strengthen under force. This may be indicative of catch bonds, but could also arise from a complex binding energy landscape. To distinguish between these two possibilities, we applied a staircase-like mechanical load with the same average loading rate but with forces that at all times exceeded those of the linear ramp protocol. We find significantly increased detachment forces under a staircase-like loading protocol compared to a linear force ramp, which rules out other mechanisms except catch-bond behavior.

15 min break

BP 32.8 Fri 11:30 H 1028

The Hair Bundle's Viscous Losses in Response to Tip-Link Forces — •Johannes Baumgart — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden

The ear can sense air vibrations smaller than the Bohr radius. One important step of this highly sensitive process is the mechanotransduction, which takes place in the hair bundle. Therein active forces along the tip links can amplify the motion. Here we investigate which viscous forces counteract this active forces.

One individual bundle consists of closely apposed stereocilia surrounded by a viscous liquid, which are coupled by stiff horizontal top connectors and softer tip links. This configuration ensures a highly coherent motion over broad frequency ranges, as was shown by experimental data in conjunction with a detailed three-dimensional finite-element model incorporating the fluid-structure interaction[1].

We investigate with the same numerical model how the bundle responds to a force at all tip links with the same phase and amplitude. This forces can displace the free standing bundle coherently, if the stiff horizontal top connectors below the tip links ensures the coupling. For this mode of motion the assigned viscous drag coefficient is similar

to the one for displacing the bundle at the kinociliary bulb, which is mainly due to the external liquid. If the horizontal top connectors are removed, the bundle splays and the related drag coefficient increases by up to thirtytimes for frequencies below a few Hertz.

[1] A.S. Kozlov, J. Baumgart, T. Risler, C.P.C. Versteegh & A.J. Hudspeth, *Nature*, 2011, **474**, 376–379.

BP 32.9 Fri 11:45 H 1028

Temperature-dependent auditory tuning can arise from transduction channel gating — •Björn Nadrowski[1] and Martin Göpfert[2] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Dept. of Cellular Neurobiology, Schwann-Schleiden Research Centre, Julia-Lermontowa-Weg 3, 37077 Göttingen, Germany

Ears achieve their exquisite sensitivity by means of active mechanical feedback. This feedback depends on metabolic energy, which might explain why temperature affects the mechanical tuning of ears. Spontaneous otoacoustic emissions from reptile ears, for example, get faster when the ambient temperature rises, and self-sustained oscillations in mosquito ears likewise speed up when temperature is increased. By analyzing the resulting frequency-shifts in terms of the Arrhenius equation, activation energies of the molecular motors that promote the mechanical feedback have been deduced. Here, we show that apart from motor characteristics the gating of auditory transduction channels can influence auditory mechanics in a temperature-dependent manner, providing an alternative explanation for the temperature-dependent tuning of ears. The link between auditory tuning and channel gating is established using physical models of sensory hair bundles and the Drosophila hearing organ. In both systems, opening or closing all the transduction channels requires larger stimulus forces as temperature rises, decreasing mechanical nonlinearities and causing best-frequency shifts.

BP 32.10 Fri 12:00 H 1028

Rupture dynamics of cytoskeletal networks — •Philip Guthardt Torres[1,2] and Ulrich S. Schwarz[1,2] — [1]Bioquant, University of Heidelberg — [2]ITP, University of Heidelberg

In cell adhesion and migration, mechanical stability of cytoskeletal networks under force has emerged as an important factor. For example, the transition from lamellipodium to lamella at the front edge of migrating tissue cells and the dissociation of the treadmilling actin gel at the back of rapidly migrating keratocytes might both be determined by the mechanical stability of the actin network contracted by myosin II motors. In contrast to traditional fracture mechanics, rupture in cytoskeletal networks is not dominated by stability thresholds, but rather by stochastic rupture events with exponentially distributed waiting times. Moreover, load sharing in such networks is strongly determined by their spatial organization, which can be very variable in the cellular context. We use a simple two-dimensional model for cable networks to study the rupture dynamics of cytoskeletal networks.

BP 32.11 Fri 12:15 H 1028

Measurement of adhesion forces of bacteria on controlled hydroxyapatite surfaces — •Christian Zeitz[1], Peter Loskill[1], Markus Bischoff[2], Mathias Herrmann[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]Saarland University Hospital, Microbiology and Hygiene, D-66421 Homburg/Saar, Germany

The aim of the study presented here is to probe the adhesive properties of bacteria on hydroxyapatite (HAP) surfaces. However, "real" surfaces like teeth are very complex due to their natural variation in structure, roughness and chemical composition. Therefore, artificial HAP samples have been prepared, a characterization of which is presented in this work. The sample surface is very smooth (local RMS roughness below 1 nm) and, thus, allows controlled AFM adhesion measurements with bacterial probes. The HAP samples can be fluoridated [1] and the adhesion strength of *Staphylococcus epidermidis*, *Streptococcus oralis* and *Streptococcus mutans* can be probed on both types of surfaces. The results suggest an alternative explanation for the efficiency of fluoridation of teeth for the prevention of cavities.

[1] F.Müller et al., Langmuir, 2010, 26 (24), p 18750

BP 32.12 Fri 12:30 H 1028

Ballistic motion of bacterial membrane proteins — •Holger Kress[1,2], Rostislav Boltyanskiy[2], Alexia A. Belperron[3], Cecile O. Mejean[2], Charles W. Wolgemuth[4], Linda K. Bockenstedt[3], and Eric R. Dufresne[2] — [1]University of Bayreuth — [2]Yale University — [3]Yale University School of Medicine — [4]University of Connecticut Health Center

The mechanical behavior of proteins in bacterial membranes is not well understood. We investigated this behavior in *B. burgdorferi* bacteria with functionalized microparticles and optical tweezers. We attached particles to membrane proteins and tracked the subsequent particle motion. Although *B. burgdorferi* have a symmetric morphology, the particles were transported ballistically with a well defined speed and stall force to a preferred end of the bacteria. Mutant *B. burgdorferi* which lack flagella did not show directed protein transport, but only diffusive motion. We hypothesize that the transport is enabled by the bacterial motility machinery and that it indicates a defense mechanism against immune cells [HK and RB contributed equally].

BP 32.13 Fri 12:45 H 1028

Energy switching of helical bacteria trapped in a light tube — Matthias Koch and •Alexander Rohrbach — University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

A bacterium can undergo continuous transitions between ground states and excited states of mechanical energy. In the case of the wall-less - and therefore flexible - helical bacterium spiroplasma melliferum (SM), the deformations encode a state of mechanical energy storage, which can express a health state of the bacterium. SM has an extreme structural simplicity and is among the smallest cells in size (~500 genes, ~200nm thin, 3-5μm long). It infects various plants and insects and thereby has done tremendous harm to agriculture industry. Their motility, defined by helicity changes, kinking and propelling is very complex, and enables propagation in complex environments. However, it is unclear which molecular mechanisms work at which forces on which time scales?

We address these questions by optically caging the whole bacterium in an object adapted optical trap, which consists of a high speed scanning line optical trap: the light tube. Tiny phase changes from scattered laser light are recorded at several Kilohertz and allow imaging the whole bacterium at about 1000 Hz with 3D super-resolution. The measured dynamics is analysed and modelled with Fourier-techniques. We show experimental and simulation results, including energies and forces involved in its motility, as well as first models describing the switching of mechanical energy of the bacterium.