Overview of Invited Talks and Sessions
(Lecture Rooms: H 1028 and H 1058; Posters: A)

Plenary Talks related to BP

PV I  Mon  8:30– 9:15  H 0105  Force and Function: Single Molecule Biophysics of Molecular Interactions — •Hermann E. Gaub
PV IX Tue  13:00–13:45  H 0105  Nanoscopy with focused light — •Stefan Hell
PV XX Wed  20:00–21:00  Urania  Musikalische Rhythmen und Algorithmen: Physiker auf anderen Wegen — •Theo Geisel
PV XXVIII Fri  8:30– 9:15  H 0105  Nanocrystalline Junctions and Mesoscopic Solar Cells — •Michael Graetzel

Invited Talks of BP sessions

BP 1.1 Mon  9:30–10:00  H 1028  Light sheet-based fluorescence microscopy for quantitative biology — •Ernst H.K. Stelzer
BP 7.1 Mon  14:30–15:00  H 1028  Super-resolution imaging of small, fast moving cellular structures — •Alexander Rohrbach
BP 18.1 Tue  9:30–10:00  H 1028  Multifaceted BAR-domain proteins to shape cell membranes — Co- line Prévost, Mijo Simunovic, Henri-François Renard, Emma Evergren, Harvey McMahon, Ludger Johannes, Jacques Prost, Andrew Callan-Jones, •Patricia Bassereau
BP 19.1 Tue  9:30–10:00  H 1058  Emerging social behaviour during aggregation in Dictyostelium discoideum — Giovanna De Palo, Darvin Yi, Thomas Gregor, •Robert Endres
BP 33.1 Wed  9:30–10:00  H 1058  Feeling for cell function: Mechanical phenotyping at 100 cells/sec — •Jochen Guck
BP 34.7 Wed  11:30–12:00  H 1028  Efficiently extracting thermodynamics and kinetics from molecular simulation data at multiple thermodynamic states — •Frank Noe
BP 35.1 Wed  15:00–15:30  H 1028  Caged Hyperpolarized Xenon in Phospholipid Membranes for NMR Sensing Applications — •Leif Schröder
BP 37.1 Wed  15:00–15:30  EW 202  The cost of moving optimally — •Dinant Kistemaker
BP 41.1 Thu  9:30–10:00  H 1058  Probing the downhill folding kinetics of Lambda repressor variants with optical tweezers — Ann Mukhtarwa, Andreas Hartmann, •Michael Schlief
BP 42.1 Thu  9:30–10:00  H 1028  Microtubules adapt to mechanical stress through spontaneous intralattice repair — Laura Schaedel, Karin John, Jeremie Gaillard, Maxence Nachury, Laurent Blanchon, •Manuel Thery
BP 42.7 Thu  11:30–12:00  H 1028  Cellular chirality arising from the self-organization of the actin cytoskeleton — •Alexander Bershadsky
BP 44.1 Thu  15:00–15:30  H 1058  Molecular Systems Engineering with DNA: Four pieces, one rule, and many possibilities. — •Hendrik Dietz
BP 49.1 Thu  16:45–17:15  H 1028  Directional bias in the kinesin superfamily of molecular motors — •Robert Cross
## Invited talks of the joint symposium SYNP

See SYNP for the full program of the symposium.

| SYNP 1.1 | Tue | 9:30–10:00 | H 0105 | Connectomics: The dense reconstruction of neuronal circuits — **Moritz Helmstädtter** |
| SYNP 1.2 | Tue | 10:00–10:30 | H 0105 | Whole-brain imaging and analysis of network activity in behaving zebrafish — **Misha Ahrens** |
| SYNP 1.3 | Tue | 10:30–11:00 | H 0105 | Circuit neurophysics: Theory and biophysics of information-flow through large-scale neuronal systems — **Fred Wolf** |
| SYNP 1.4 | Tue | 11:15–11:45 | H 0105 | Cognitive devices based on ion currents in oxide thin films — **Stuart Parkin** |
| SYNP 1.5 | Tue | 11:45–12:15 | H 0105 | Distributed neuro-physical interfaces: technology and ”exciting” biophysics — **Shy Shoham** |

## Invited talks of the joint symposium SYPS

See SYPS for the full program of the symposium.

| SYPS 1.1 | Wed | 9:30–10:00 | H 0105 | Anticipating and avoiding tipping points — **Timothy M. Lenton** |
| SYPS 1.2 | Wed | 10:00–10:30 | H 0105 | Climate investment under uncertainty: the two degree target and the desire for dynamic consistency — **Hermann Held, Delf Neubersch** |
| SYPS 1.3 | Wed | 10:30–11:00 | H 0105 | What are the resources required to fulfil human needs? — **Julia Steinberger** |
| SYPS 1.4 | Wed | 11:15–11:45 | H 0105 | Design of Sustainable Supply Chains for Sustainable Cities — **Anna Nagurney** |
| SYPS 1.5 | Wed | 11:45–12:15 | H 0105 | Ecological econophysics for degrowth — **Salvador Pueyo** |

## Sessions

| BP 1.1–1.12 | Mon | 9:30–13:00 | H 1028 | Imaging |
| BP 2.1–2.13 | Mon | 9:30–13:00 | H 1058 | Neurophysics I |
| BP 3.1–3.9 | Mon | 9:30–12:15 | BH-N 243 | Statistical Physics of Biological Systems I (joint DY/BP/CPP) |
| BP 4.1–4.12 | Mon | 9:30–12:45 | C 130 | Colloids and Complex Liquids I (joint CPP/DY/BP) |
| BP 5.1–5.12 | Mon | 9:30–13:00 | C 243 | Nanoparticles and Composite Materials I (joint CPP/BP) |
| BP 6.1–6.4 | Mon | 12:15–13:15 | MA 001 | Networks: From Topology to Dynamics I (joint SOE/DY/BP) |
| BP 7.1–7.9 | Mon | 14:30–17:15 | H 1028 | Superresolution Optical Microscopy (focus session) |
| BP 8.1–8.9 | Mon | 14:30–17:00 | H 1058 | Neurophysics II |
| BP 9.1–9.10 | Mon | 14:30–17:15 | EB 202 | Biomaterials and Biopolymers I (joint BP/CPP) |
| BP 10.1–10.14 | Mon | 15:00–18:45 | C 130 | Colloids and Complex Liquids II (joint CPP/DY/BP) |
| BP 11.1–11.14 | Mon | 15:00–18:45 | C 243 | Nanoparticles and Composite Materials II (joint CPP/BP) |
| BP 12.1–12.3 | Mon | 15:00–15:45 | MA 001 | Evolutionary Game Theory I (joint SOE/BP/DY) |
| BP 13.1–13.15 | Mon | 17:30–19:30 | Poster A | Posters: Imaging and Superresolution Optical Microscopy |
| BP 14.1–14.12 | Mon | 17:30–19:30 | Poster A | Posters: Neurophysics |
| BP 15.1–15.12 | Mon | 17:30–19:30 | Poster A | Posters: Multi-cellular systems |
| BP 16.1–16.33 | Mon | 17:30–19:30 | Poster A | Posters: Cell adhesion, mechanics and migration |
| BP 17.1–17.22 | Mon | 17:30–19:30 | Poster A | Posters: Protein structure and dynamics |
| BP 18.1–18.10 | Tue | 9:30–12:30 | H 1028 | Membranes and vesicles I (joint BP/CPP) |
| BP 19.1–19.11 | Tue | 9:30–12:45 | H 1058 | Multi-cellular systems |
| BP 20.1–20.11 | Tue | 9:30–12:30 | BH-N 128 | Microswimmers, Active Liquids II (joint DY/BP/CPP) |
| BP 22.1–22.23 | Tue | 14:00–16:00 | Poster A | Posters: Cytoskeletal filaments |
| BP 23.1–23.3 | Tue | 14:00–16:00 | Poster A | Posters: Molecular Motors |
BP 24.1–24.16 Tue 14:00–16:00 Poster A Posters: Membranes and vesicles
BP 25.1–25.9 Tue 14:00–16:00 Poster A Posters: DNA/RNA and related enzymes
BP 26.1–26.15 Tue 14:00–16:00 Poster A Posters: Statistical Physics of Biological Systems
BP 27.1–27.8 Tue 14:00–16:00 Poster A Posters: Complex Fluids and Soft Matter
BP 28.1–28.6 Tue 14:00–16:00 Poster A Posters: Biomaterials and Biopolymers
BP 29.1–29.4 Tue 14:00–16:00 Poster A Posters: Systems biology
BP 30.1–30.2 Tue 14:00–16:00 Poster A Posters: Biotechnology and bioengineering
BP 31.1–31.1 Tue 14:00–16:00 Poster A Posters: Modelling of non-linear dynamics in biological movement
BP 32.1–32.9 Tue 14:00–16:15 MA 001 Evolutionary Game Theory II (joint SOE/BP/DY)
BP 33.1–33.12 Wed 9:30–13:15 H 1058 Cell adhesion, mechanics and migration I (joint BP/CPP)
BP 35.1–35.12 Wed 15:00–18:30 H 1028 Membranes and vesicles II (joint BP/CPP)
BP 36.1–36.12 Wed 15:00–18:30 H 1058 Cell adhesion, mechanics and migration II
BP 37.1–37.5 Wed 15:00–16:30 EW 202 Modelling of non-linear dynamics in biological movement (focus session)
BP 38.1–38.9 Wed 15:00–18:00 C 130 Electrolytes at Interfaces - Stern Layer (focus session, joint CPP/BP)
BP 39.1–39.6 Wed 16:45–18:30 MA 001 Physics of Sustainability and Human-Nature Interactions I (joint SOE/DY/jDPG/BP/AKE)
BP 40 Wed 19:00–20:00 H 1058 BP Mitgliederversammlung (Annual General Meeting of the Biological Physics Division)
BP 41.1–41.11 Thu 9:30–13:00 H 1058 Protein structure and dynamics I
BP 42.1–42.11 Thu 9:30–13:00 H 1028 Cytoskeletal filaments (joint BP/CPP)
BP 43.1–43.5 Thu 12:00–13:15 MA 001 Networks: From Topology to Dynamics II (joint SOE/DY/BP)
BP 44.1–44.7 Thu 15:00–17:00 H 1058 DNA/RNA and related enzymes
BP 45.1–45.5 Thu 15:00–16:15 H 1028 Systems biology
BP 46.1–46.11 Thu 15:00–18:00 C 264 Biomaterials and Biopolymers II (joint CPP/BP)
BP 47.1–47.7 Thu 15:45–18:00 PC 203 Microswimmers, Active Liquids I (joint CPP/BP/DY)
BP 48.1–48.5 Thu 17:00–18:30 MA 001 Physics of Sustainability and Human-Nature Interactions II (joint SOE/DY/jDPG/BP/AKE)
BP 49.1–49.7 Thu 16:45–18:45 H 1028 Molecular motors
BP 50.1–50.5 Thu 17:30–18:45 H 1058 Biotechnology and bioengineering
BP 51.1–51.2 Thu 18:00–18:30 C 264 Physics of Food (joint CPP/BP)
BP 52.1–52.7 Fri 9:30–11:45 H 1028 Protein structure and dynamics II
BP 53.1–53.10 Fri 9:30–12:15 H 1058 Complex Fluids and Soft Matter (joint BP/DY/CPP)
BP 54.1–54.7 Fri 9:30–11:30 C 264 Microswimmers, Active Liquids III (joint DY/BP/CPP)
BP 55.1–55.12 Fri 9:30–12:45 BH-N 128 Networks: From Topology to Dynamics II (joint DY/BP/SOE)
BP 56.1–56.6 Fri 9:30–12:00 BH-N 334 Aging in Physical and Biological Systems (focus session, joint DY/BP)

BP Mitgliederversammlung (Annual General Meeting of the Biological Physics Division)
Mittwoch 19:00–20:00 H 1058
• Award of the EPL poster prizes for biological physics
• Report of the current speakers
• Election of new BP speaker and co-speaker(s)
• Lessons learned and spring meeting Regensburg 2016
• Miscellaneous
Light sheet-based fluorescence microscopy for quantitative biology — EXHIBIT H.K. STELZER — Physical Biology, BMLS, Goethe-Universität, D-60438 Frankfurt am Main

As long as we rely on epifluorescence microscopes, we are faced with serious challenges. Fluorophores and specimens are essentially wasted during the observation process, since all fluorophores and many endogenous organic compounds in the specimen are excited whenever we record a single plane. Obviously, the situation becomes even more challenging when we perform complex biological experiments and observe the behavior of multiple targets in three dimensions as a function of time. In light sheet-based fluorescence microscopy (LSFM), planar optical sectioning in the excitation process minimizes fluorophore bleaching and phototoxic effects. Since biological specimens survive long-term three-dimensional imaging at high spatio-temporal resolution, LSFM has become the tool of choice in developmental biology. LSFM makes a sincere and honest effort to reduce bleaching and phototoxicity. LSFM allows one to record millions of pixels in parallel. Laser light sheet-based devices, including a macroscope, had been built several times, but their capability to perform at a microscopic level was unknown until we described a diffraction-limited microscope in 2002, observing living biological samples and evaluated multiple-view imaging. This developed from theta microscopy (1993) and a systematic evaluation of diffraction-limited microscopes with two to four lenses, in theory and practice.

3D-Refractive Index Measurements of Single Cells by Optical Diffraction Tomography — •PAUL MÜLLER1, MIRIAM SCHÜRMANN2, CHRISTOPH FAIGLE1, MIRKO KREYNSK2, and JOCHEN GUCK2 1Biotechnology Center of the TU Dresden — 2Max Planck Institute of Molecular Cell Biology and Genetics

The refractive index is an inherent property of biological cells. The 3D distribution of the refractive index within a cell determines its light scattering properties. It is possible to reconstruct the refractive index distribution, and thus the internal structure of a cell, from scattering data using optical diffraction tomography (ODT). ODT combines computerized tomography (CT) with the Born approximation to address the wavelike propagation of light through a specimen. In ODT, the phase of the scattered field behind a rotating specimen is measured. From these 2D phase images one can reconstruct the 3D refractive index map of the specimen. Here, we demonstrate quantitative 3D ODT imaging of single biological cells with sub-cellular resolution. The technique does not require a marker and the acquisition of images is contact-free. In this particular study, suspended cells are held in an optical trap and rotated using microfluidic flow or, all-optically, by means of an optical cell rotator (OCR). The phase of the scattered field is measured using digital holographic microscopy (DHM), a quantitative phase microscopy technique. The resulting 3D refractive index map allows us to determine properties such as cell volume, dry mass, or density and refractive index of sub-cellular compartments. Many future applications in biology and medicine are envisioned.

Label-free optical detection of single proteins — •KATHARINA KÖNIG, MAREK PILIARIK, and VAIDH SANDOGHDAR — Max Planck Institute for the Science of Light, Erlangen, Germany

Detection of small amounts of biomolecules down to the single molecule level is highly desirable in a variety of fundamental and technological investigations. Conventional modern methods rely on strong fluorescence or absorption properties of marker molecules. However, labeling strategies have many disadvantages since they are nontrivial to implement and can often alter the behavior of analyte molecules. In this work we report on the direct, optical detection of single proteins without the need for any labels. This sensitivity is achieved via intermodulation detection of the scattering (iSCAT) from a single protein. Here we report a method to reveal single molecules at various imaging depths and thicker tissues. We adapted and optimized reflected light-sheet microscopy (RLSM) as one of the most popular candidates. However, RLSF has the major limitation that it is constrained to the imaging depth of only several hundred nanometers close to the coverslip surface. The need for alternative imaging techniques is therefore evident.

Single laser beam photothermal microscopy — •ANDRE HERBER, MARKUS SELMKE, MARCO BRAUN, and FRANK CICCHOS — Molecular Nanophotonics Group, Institute of Experimental Physics I, Leipzig University, 04103 Leipzig, GERMANY

Photothermal microscopy enables the selective detection of single absorbing nanoparticles and molecules in the presence of scatterers. It is based on refractive index changes upon optical excitation. Typically, it utilizes the incoherent scattering on a discrete nanogap to induce and detect changes of the optical properties in the vicinity of an absorbing nanoobject. Here, we show that a single modulated heating laser with an intensity offset suffices to selectively image absorbers. The modulated optical heating creates a thermal wave around the absorber and results in a retardation of the refractive index field. The out-of-phase component of the scattering on the heated nanoparticle and the refractive index profile provides a selective contrast for absorbers. The use of a single laser beam simplifies the application of photothermal microscopy in existing microscopy schemes.

Helium Ion Microscopy of Biological Cells — •NATALIE FRESE1, ANDRE BEYER1, MATTHIAS SCHÜRMANN2, BARBARA KALTSCHMIDT4,
Fluorescent molecules behave as electric dipole emitters with fixed but typically distinct excitation and emission dipole orientations. In the vicinity of dielectric or conducting surfaces, the emission properties of a dye molecule such as the emission rate (Purcell effect) and angular distribution of radiation are dramatically changed. Utilizing these effects, we develop a first-ever method, by combining radially-polarized laser scanning together with imaging on a defocused EMCCD camera in a way that provides excitation and emission patterns of each individual dye molecule, which gives us the three-dimensional orientations of both the excitation and emission dipole. Furthermore, using the orientation information of the emission dipole with respect to the interface, we localize single emitters axially from the interface with nanometer accuracy, a technique which we term as single-molecule metal-induced energy transfer (smMiET). This method is ideal for investigating the dimensionality and orientations of the TDMs of quantum dots, which are substantially modified in the vicinity of metal nanostructures.

Three-dimensional orientation imaging of single fluorescent emitter transition dipoles — N. Karedla, A. Chizhik, I. Gregor, A. Chizhik, and J. Enderlein — Physikalisches Institut, Georg-August-Universität Göttingen

In this presentation HIM images of biological cells are presented. The presented study focuses on neuronal differentiated human inferior turbinate stem cells, mouse neurons and mouse fibroblasts. The cells were prepared by critical point drying and a flood gun was used to compensate charging, so no conductive coating was necessary.

Therewith, extremely small features at native cell surfaces were imaged with an estimated edge resolution of 1.5 nm. Due to the size of the structures and the preparation methods of the cells the observed features could be an indicator for lipid rafts. This hypothesis will be discussed.
### General Anaesthesia: From experiments to theory — AXEL HÜTT — INRIA Nancy, Frankreich

The talk will introduce into general anaesthesia, starting from a clinical perspective in human medicine showing the link to animal experiments. Anaesthetic effects on the macroscopic scale of evoked potentials elucidates the complexity of the neural mechanism originating from the interaction bridge between single neurons and populations and networks of populations. In the last part, the talk will introduce to recently developed neural population models involving nonlinear delayed interactions. This model permits to reproduce the major anaesthetic effects on a macroscopic scale. A final reduced model proposes an interaction mechanism explaining few signals in EEG.

### Synthetic Neuronal Networks on Glass Using Topological and Chemical Cues — ANDREAS SCHLEGEL1, AUNE KOITMAA1, PAUL GWOZDZ1, JANN HARBERTS1, CHRISTIAN HEUSINGER1, GABRIELLE LOERES2, and ROBERT H. BLICK3 — 1Center for Hybrid Nanostructures (CHYN) and Institute of Nanotechnology and Solid State Physics, University of Hamburg, Germany — 2Center for Molecular Neurobiology, Hamburg University Medical Center Hamburg-Eppendorf, Germany — 3Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

The understanding of neuronal signal transduction is of interest for research of biological networks. We present a method to achieve directional guidance of neurite outgrowth with the goal of providing synthetic neuronal circuits.

We use glass microstructured with an excimer laser (geometrical confinement). In a second step patterns of Poly-L-Lysine (PLL) are printed onto the glass (chemical guidance). The topological pattern consists of lines with alternating units of containers (diameters ~ 20 µm) and channels (width ~ 4 µm, length 30 ~ 200 µm). The distance between the lines varies between 10 and 200 µm. The depth of the structures is 4 µm. PLL is printed inside the containers to promote cell adhesion.

The neurites prefer to grow within the microstructures over several hundred µm. Neurons situated inside containers grow neurites along channels and connect to multiple neurons in line over a millimeter range. Crosslinking of neurites between separated lines becomes less common with increasing distance. A transition from partially random behavior to controlled growth is observed.
spatially detect or image neurotransmitters. Therefore, the chemical events in synapses and neural circuits remain largely unexplored. Optical nanoscale sensors/probes could provide non-invasive, fast, high-resolution and parallel imaging of neurotransmitters. Nanomaterials are promising building blocks for such probes. For example, semiconducting single-walled carbon nanotubes (SWCNTs) are hollow cylinders of one-atom-thick sheets of carbon. They provide an intrinsic bandgap, which results in near infrared (nIR) fluorescence (900-1600 nm) that is beneficial for biomedical applications. The molecular environment of SWCNTs strongly affects their nIR-fluorescence, which can be used for molecular recognition and signal transduction. We have developed carbon nanotube-based label-free fluorescent sensors/probes for neurotransmitters. These probes change their fluorescence in the presence of neurotransmitters. Parallel imaging of many of these probes provides an image that corresponds to the neurotransmitter concentration. We also demonstrate spatiotemporal imaging of dopamine release from cells during exocytosis. In summary, this method enables chemical imaging in biological systems and can provide completely new insights into communication between neurons.

15 min break

Probing a quantum mechanical model of olfaction in insects — Marco Paoli1, 2, Elisa Rigos1, 2, Gianfranco Anfora1, Giorgio Vallortigara1, Renzo Antolini1, 3, and Albrecht Haase1, 4

1Center of Mind/Brain Sciences, University of Trento, Rovereto, Italy — 2Biotech center, University of Trento, Trento, Italy — 3Research and Innovation Centre, Fondazione Edmund Mach, S. Michelle all’Adige, Italy — 4Department of Physics, University of Trento, Trento, Italy

One of the first examples for a possible manifestation of quantum effects in biological systems is the vibration theory of olfaction. In contradiction to the widespread assumption that smell is a purely chemical sense, it proposes phonon assisted electron tunneling as the trigger mechanism for signal transduction. This would induce a sensitivity of olfactory receptors not only to molecular shape and binding properties, but also to the vibrational spectrum of the odorant. This would mean that these receptors do not perform classical electronic recognition but present first in viva functional imaging experiments in the honeybee brain showing evidence for the bees’ ability to distinguish isopopes by smell. A possible correlation of these results with the odorants’ vibrational spectra is discussed.

Dense neural networks with self-organizational dynamics which allow flexible changes between different network configurations can provide completely new insights into communication between neurons. The analysis is based on spiking multi-unit activity which had been simultaneously recorded from 32 positions along and across isofrequency laminae of the ICC on 11 species-specific vocalizations to guinea pigs. Using neural discrimination and cross-correlation it was found that small groups of neurons reliably encode the spectrotemporally rich set of vocalizations. Combination of a few multi-unit recording sites frequently trapped in the spines which slows down their propagation in the dendritic channel. Anomalous diffusion of tracer particles has been reported in dendrites, which is strongly dependent on spines morphology and also on their spatial arrangement. Here we analytically show a diffusion process composed of different modes of motility, a motion and a waiting mode. We investigate how the overall transport properties depend on the structural properties of the dendrites and spines, and on the fraction of time spent in each state. The analytical predictions are in agreement with available experimental data as well as the results of extensive Monte Carlo simulations.

The effects of positive interspike interval correlations on neuronal information filtering properties. — Osvn Blankenburg1, 2 and Benjamin Lindner1, 2

1Department of Physics Humboldt University Berlin, Germany — 2Bernstein Center for Computational Neuroscience Berlin, Germany

Neurons encode time-dependent stimuli in sequences of action potentials (spike trains). The neuron can encode either preferentially slow components of the stimulus (low-pass filter), high frequency components (high-pass filter), or a specific frequency band (band-pass filter) depending on the characteristics of the stimulus as well as the intrinsic neuronal dynamics. The standard integrate-and-fire model acts as a low-pass filter of information, irrespective of the firing regime (regular, Poisson-like, or bursting) of the neuron. However, experiments reveal band-pass filtering in some neurons, requiring theoretical explanation. In this study, intrinsic stochastic adaptation is identified as a possible mechanism. For our analytically tractable model system we show that positive ISI correlations, such as those caused by stochastic adaptation can result in a pronounced band-pass filtering of information for time-dependent stimuli.

Nonlinear population dynamics for finite-size spiking neural networks with spike-frequency adaptation — Tilo Schwalger

Brain Mind Institute, École polytechnique fédérale de Lausanne, CH-1015 Lausanne

Bridging the scale from the microscopic dynamics of single neurons to the global population activities of pulse-coupled neurons is crucial for multi-scale modeling of the nervous system. Current theories mostly consider the limit of large networks. However, this approximation is limited to the mean activity and neglects fluctuation effects. In realistic neural circuits, the number of neurons of a given type can be rather small (N = 50–1000), which requires a theory for the fluctuating population dynamics. Existing finite-size theories are either based on rather simplified neuron models or rely on heuristic assumptions. Using network-field models, in Ref. [1, 2] we allow for stochastic population equations for the large class of generalized integrate-and-fire neurons with spike-frequency adaptation. Our theory goes beyond the Gaussian approximation and thus applies to
rather small populations. We study spontaneous transitions between up and down states in a bistable network induced by finite-size noise. Furthermore, for the asynchronous state, we analytically calculate the power spectrum of the fluctuations. This allows us to investigate in-
formation filtering by coupled populations of adapting neurons [2].

BP 3: Statistical Physics of Biological Systems I (joint DY/BP/CPP)

Invited Talk
BP 3.1 Mon 9:30 BH-N 243
Chemical warfare and survival strategies in bacterial range expansions — MARKUS F WEBER, GABRIELE POXLEITNER, ELKE HERRICH, ERWIN FREY, and MADELINE OPTZ — Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany

Spreading of species into uncolonized territory is a fundamental eco-
logical process in the evolution and maintenance of biological diver-
sity. Although interactions between species have experimentally been iden-
tified as major determinants of species coexistence in spatially ex-
tended populations, their role in spatially expanding populations is
largely unknown. Here, we address the roles of resource and inter-
ference competition by genetically tuning a bacterial model system of
three Escherichia coli strains: a toxin (colicin) producing strain, a
sensitive strain, and a resistant strain. We show that maintenance of
biodiversity is determined by three strongly interdependent ecological
factors: the relative ratio of the competing strains, their growth rates
and the strength of toxicity. Our mathematical analysis suggests, that
develop general expectations, a non-hierarchical interaction network is
not a necessary prerequisite for biological diversity. Moreover, we find
that robust three-strain coexistence requires a balance between growth
rates and a small enough toxicity range or, alternatively, a reduced in-
itial ratio of the colicin-producing strain. We expect that the approach
presented in this study will be useful to identify further mechanisms
for the maintenance of biodiversity in microbial communities.

BP 3.2 Mon 10:00 BH-N 243
A New Dimension: The Influence of Two Dimensional Niche
Space on Evolutionary Food Web Models — DANIEL RITTER-
skamp and BERND BLASCHUS — ICBM, University Oldenburg, Germany

Food webs encode feeding interactions of ecological communities, orig-
inating from an intricate interplay of evolutionary and ecological pro-
cesses. This dynamic can be described by evolutionary food web mod-
els, in which feeding interactions between species are related to the
relative distance of their adaptive traits (e.g., body size) on a niche
axis. However, not much is known about evolutionary food web dy-
namics in space.

Here, we go beyond traditional approaches and develop an evolu-
tionary food web model in a two dimensional niche space, where the
additional niche axis might describe a spatial coordinate or an envi-
ronmental variable. Using numerical simulations, we investigate popu-
lation dynamics, evolutionary behaviour and the emerging community
structure in space. The model is able to produce both static and dy-
namic food webs, depending on the width of the interaction kernel;
whereas food web complexity is determined mainly by the interaction
strength.

We observe rich dynamics including: spatio-temporal patterns, arms
races, red queen dynamics, as well as sub-food webs moving in space.
By sampling the spatial axis, local food webs are recovered, which
can be related to empirical data. We conclude that the additional
nichedimension is essential to capture realistic patterns of spatially
structured food webs.

BP 3.3 Mon 10:15 BH-N 243
Biodiversity and ecosystem functioning in evolving food webs
— KORINNA T. ALHOFF and BARBARA DROSSL — TU Darmstadt,
Germany

We analyze an evolutionary food web model where each species is char-
acterized by three traits, namely its own body mass, its preferred prey
body mass, and the width of its potential prey body mass spectrum.
Population dynamics includes feeding and competition interactions and
determines which species are viable and which ones go extinct.
On a timescale much slower than population dynamics, new species
emerge as modifications of existing species. The network structure
emerges according to the interplay between population dynamics and
evolutionary rules and shows an ongoing species turnover. The model
gives thus insights into how the functional diversity changes during
the initial network build up as well as due to extinction avalanches.
We investigate the relation between the functional diversity and five
community level measures of ecosystem functioning. These are the
metabolic loss of the predator community, the total biomasses of the
basal and the predator community and the consumption rates on the
basal community and within the predator community.

BP 3.4 Mon 10:30 BH-N 243
Efficiency of cellular information processing — DAVID HAR-
tich, ANDRE C. BARTO, and UDO SEIFERT — II. Institut für Theor-
etische Physik, Stuttgart, Germany

We study theoretical models inspired by the E. coli sensory network,
using the framework of stochastic thermodynamics for bipartite sys-
tems [1]. More precisely, we model the sensory system by an internal
process measuring an external process, which is a ligand concentration
jumping at random between two values. We show that the rate of con-
ditional Shannon entropy reduction, characterizing the learning of the
internal process about the external process, is bound by the thermo-
dynamic entropy production [2]. This approach allows for the definition
of an informational efficiency that can be used to study cellular in-
formation processing. We start with a simple model for which ATP
must be consumed so that a protein inside the cell can learn about the
external environment. A further discussion illustrates, inter alia, that
a non-zero learning rate without dissipations in the cell can only be
obtained if the external process compensates for it.

BP 3.5 Mon 10:45 BH-N 243
Tackling your free energy estimates with pyfeat — ANTONIA
MEY, CHRISTIAN WEMEYER, FABIAN PAUL, HAO WU, and FRANK
NOER — Institut für Mathematik, FU Berlin

Understanding the equilibrium properties of physical systems is of
general interest in many different areas of physics. In complex systems,
equilibrium properties can only be evaluated by means of numerical
simulations, which are frequently plagued by rare event dynamics.
One approach to circumvent rare event dynamics is to use enhanced
sampling methods (e.g. replica exchange methods or umbrella sam-
ing).

The range of established analysis methods to optimally estimate
equilibrium properties from multi-ensemble simulations often requires
an expert user for their implementation or even usage. Here, we
introduce a new software package, the python free energy analysis
toolkit – pyfeat, that facilitates the analysis of multi-ensemble sim-
ulation. Pyfeat provides an easy-to-use interface to well established
methods such as WHAM or MBAR, as well as the recently introduced
transition-based reweighting analysis methods (TRAM), which borrow
ideas from Markov state models. The software’s straightforward us-
ability makes comparing different estimation method applied to the
same input data trivial.

Generally, any multi-ensemble simulation can be used for the anal-
alysis ranging from all-atom protein molecular dynamics simulations to
simulations of condensed matter systems. Pyfeat is available for down-
load at: https://github.com/markovmodel/pyfeat.

15 min. break

BP 3.6 Mon 11:15 BH-N 243
Lateral domain formation in membranes coupled to curva-
ture — SINA SADREGHI, MARCUS MÜLLER, and RICHARD VINK
— Institute of Theoretical Physics, Georg-August-Universität Göttingen,
Göttingen, Germany

The lateral heterogeneity in the plasma membrane of eukaryotic cells

REFERENCES
is an important factor for regulating biological functions. As opposed to plasma membranes, model membranes (either artificially prepared membranes, or membranes extracted from living cells) typically phase separate. To address this paradox, we present computer simulations of a coarse-grained membrane model that undergoes macroscopic phase separation at low temperature. Considering a coupling between local composition and local curvature of the membrane, we show that the system exhibits composition fluctuations with a nontrivial length scale, resembling microemulsion. The latter is identified as a region where lipid rafts can form. We furthermore probe the nature of phase transition between the phase-separating regime and the mixed state. This transition is continuous and belongs to the two-dimensional Ising universality class for weak coupling to curvature, but becomes first-order for strong curvature-composition coupling.

DNA denaturation transition: environmental effects on scaling — Christian von Ferber and Yuri Holovatch

1 Coventry University, UK — 2 Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, UA

The Poland and Scheraga model for the DNA denaturation transition is reconsidered taking into account environmental effects. We apply field theoretical methods to discuss environmental effects on the nature of the transition. In particular we discuss variants of the transition that may occur due to particular properties of the environment. These are the presence of uncorrelated and power-law long-range correlated disorder which influences the transition as function of the power law exponent, the quality of the solution which may affect the self- and mutual interaction of both single and double strands and combination of these. All these have significant effects on the transition.

Variational approach to molecular dynamics — Bettina Keller — Freie Universität Berlin, Institut für Chemie und Biochemie, Takustraße 3, 14195 Berlin

The eigenvalues and eigenfunctions of the classical molecular dynamics propagator contain the essential information about the molecular thermodinamics and kinetics. A matrix representation of the propagator can be constructed by partitioning the conformational space into discrete states and estimating the state-to-state transition probabilities from molecular dynamics simulations, yielding a so-called Markov state model (MSM). The precision of an MSM depends sensitively on how well the discretization reproduces the shape of the dominant eigenfunctions. The difficulty to find a suitable discretization has limited the routine use of MSMS. Moreover, most discretizations are data-driven, impairing the comparison between MSMS and the interpretation of the eigenvectors in terms of structural transitions.

To circumvent the recently published variational approach, it is possible to construct a matrix representation of the propagator using an arbitrary basis set, allowing to use basis functions with gentle slopes. This reduces the discretization error. More importantly, the user can define basis sets which have a chemical meaning and can be used for entire classes of molecules, thereby allowing for direct comparison of the kinetic models. I will give an overview of the variational principle for the classical molecular dynamics propagator and propose a basis set for peptide dynamics which is based on the dominant eigenfunctions of individual amino acids.

Simple association-dissociation-aging process: recursive solution — Thomas Niedermaier and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The simple association-dissociation-aging process (SADAP) is characterized by the coupling of stochastic growth and shrinkage of one-dimensional structures to the random aging of the constituting subunits. Most prominently, SADAPs capture the essential features of the polymerization and degradation of actin filaments and microtubules. Previously employed mean field methods fail to describe the dynamics of SADAPs. We found an ansatz for the full master equation which allows us to study SADAPs analytically and derive a recursion relation for the steady state solution which enables the calculation of all emergent quantities with increasing accuracy. In particular, our method allows, for the first time, the precise calculation of the boundary between the growth and shrinkage regime, in excellent agreement with results from stochastic simulations.

Disclination lines at homogeneous and heterogeneous colloids immersed in a chiral liquid crystal — Sergei Schlothauer

1 Technische Universität Berlin, Berlin, Germany — 2 North Carolina State University, Raleigh (NC), USA — 3 Universidad Autonoma Metropolitana-Iztapalapa, Iztapalapa, Mexico

We perform Monte Carlo simulations in the isothermal-isobaric ensemble to study defect topologies formed in a cholesteric liquid crystal due to the presence of a spherical colloidal particle. Topological defects arise because of the competition between anchoring at the colloidal surface and the local director. We consider homogeneous colloids with either local homeotropic or planar anchoring to validate our model by comparison with earlier lattice Boltzmann studies. The presence of a Janus colloïd in a cholesteric host fluid reveals a rich variety of defect structures. Using the Frank free energy we analyze these defects quantitatively indicating a preferred orientation of the Janus colloïd relative to the cholesteric helix.

Anisometry versus anisotropy in systems of colloidal magnetic cubes — Joe Donaldson

1 Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — 2 Ural Federal University, Lenin av. 51, 620083, Ekaterinburg, Russia

Contemporary colloidal science provides numerous ways of synthesising particles with non-spherical geometries. Indeed, a whole spectrum of shapes is now readily accessible, cubes being one such example. The directionally dependent interactions of these particles are key tools in the development of new soft materials. An additional internal anisotropy is introduced into the system when these particles are constructed from a magnetic medium. Consequently, the interplay between anisometry and anisotropy, and its influence on how magnetic particles self-assemble, can be studied. Two different magnetic orientations within the cube have been considered; the first is represented by a dipole aligned along the [001] crystallographic axis, and the second by a dipole aligned along the [111] axis. We have determined the ground state structure of isolated clusters for both systems and have shown for the [001] orientation a preference for a ground state dominated by chain formation. In contrast, clusters of [111] oriented particles tend to arrange in lattices within which dipoles form ring structures consisting of four dipoles. We shall discuss the consequences of these structural configurations on the bulk properties of such systems, including preliminary predictions of the magnetic properties of dilute suspensions.

Active microrheology of a nematic liquid crystal — Tillmann Streicher

1 Technische Universität Berlin — 2 University of Chicago — 3 MPIDS Göttingen

The knowledge of rheological properties of soft matter is of great importance on the one hand because it is essential for understanding complex systems and on the other hand because many systems can be modeled by macroscopic rheological behavior. At the same time it is of great importance to understand how small changes in the microstructure can influence these macroscopic properties. The focus of this work is nematic liquid crystals (LC) which are characterized by a high degree of orientational order along a specific direction. If now a colloid is immersed into such a nematic host phase properties of the later are effected greatly at the nanoscale. The colloid perturbs orientational order of the nematic LC in its vicinity. This causes defect topologies to arise.

BP 4: Colloids and Complex Liquids I (joint CPP/DY/BP)

Time: Monday 9:30–12:45

Location: C 130
We present nonequilibrium molecular dynamics (MD) simulations of a homogenous colloid with either planar or perpendicular anchoring of LC molecules at the colloid’s surface. This leads to well known defect topologies such as the Boojum defect or the Saturn ring. The colloid is moved periodically, comparable to a typical experimental setup where one uses optical tweezers. The phase shift and the magnitude of the measured force response is used to investigate viscoelastic properties of the LC host phase. Specifically, we are interested in calculating the dynamic modulus \( G = G' + iG'' \), where \( G' \) and \( G'' \) are storage and loss moduli. For both quantities we present analytic expressions that can be used to analyse our MD data.

**BP 4.4** Mon 10:15 C 130

**Characterizing Dissipation during the Crystallization Process**
— **Sven Dorosz** — 162a avenue de la faïencerie, L1511 Luxembourg

I present computational results on the compression of a hard sphere liquid into the solid phase in finite time.

I will discuss the consequences of the resulting work distributions and in particular focus on the correlations between the dissipated heat during the process and the detected structures in the solid resp. melt.

**BP 4.5** Mon 10:30 C 130

**Colloidal Plastic Crystals of Hard Dumbbells under Shear**
— **Nils Heptner** — 2, Fangfang Chao**1,2, **Matthew Ballauff**1,2, **and Joachim Deubella**1,2 — Helmholtz-Zentrum Berlin, Germany

We study the structural response of plastic crystals of colloidal dumbbells to an oscillatory shear field using Brownian Dynamics (BD) computer simulations. Under increasing shear strains, a discontinuous transition is found from a twinned-fcc like crystal to a partially oriented highly ordered sliding-layer state via a disordered intermediate state. In this novel partially oriented sliding-layer phase, sheared hard dumbbells exhibit a small but finite collective orientational order. We show that the orientations of only weakly anisotropic particles play a crucial role in non-equilibrium transitions. Our findings from simulations are compared to data obtained by rheo-SANS experiments and reveal the nature of a second rheological yielding event which has not been observed for crystalline suspensions of hard spheres.

**BP 4.6** Mon 10:45 C 130

**Experimental determination of structural and dynamical heterogeneities in a metastable colloidal fluid**
— **Sebastian Golde**3, **Markus Franke**3, **Thomas Palberg**3, and **Holger Stark**
— Technische Universität Berlin, D-10623 Berlin

We present nonequilibrium molecular dynamics (MD) simulations of a homogenous colloid with either planar or perpendicular anchoring of LC molecules at the colloid’s surface. This leads to well known defect topologies such as the Boojum defect or the Saturn ring. The colloid is moved periodically, comparable to a typical experimental setup where one uses optical tweezers. The phase shift and the magnitude of the measured force response is used to investigate viscoelastic properties of the LC host phase. Specifically, we are interested in calculating the dynamic modulus \( G = G' + iG'' \), where \( G' \) and \( G'' \) are storage and loss moduli. For both quantities we present analytic expressions that can be used to analyse our MD data.

**BP 4.7** Mon 11:15 C 130

**Dense Colloidal Suspensions in Microfluidic Flow**
— **Philipp Kanel** and Folger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Dense colloidal suspensions in a pressure driven flow accumulate in the center of the microchannel. Bidisperse mixtures partially demix depending on their densities [1]. In very dense colloidal systems, one observes oscillations in the colloidal flow velocity which is attributed to transient jamming. The oscillations ultimately become irregular when density is further increased [2].

To develop a theoretical understanding of all these effects, we simulate hard spheres under pressure-driven flow in two and three dimensions using the mesoscale simulation technique of multi-particle colloid dynamics which is an efficient solver of the Navier-Stokes equation and includes thermal motion.

In our simulations, we reproduce the experimental observations that a monodisperse suspension enriches the channel center and a binary mixture segregates into its two species. Comparison with our analytical model suggests that Brownian motion is crucial for demixing and that the non-diagonal elements of the collective diffusion tensor determines, which species enriches the center. Qualitative differences between 2 and 3 dimensions are found.

Finally, we present first results on monodisperse suspensions near close packing to understand flow oscillations and transient jamming.


**BP 4.8** Mon 11:30 C 130

**Rheological study of anisometric pigment particle suspensions**
— **Yong Ge**, **Alexey Eremin**, and **Ralf Stannarius** — Rheo- and Guerick-Group, Humboldt Universität zu Berlin, Germany

Rheological properties of colloidal suspensions formed by nanometer size rod-shaped pigment particles dispersed in a non-polar solvent are studied. Experiments have shown that these suspensions possess unusual properties such as liquid crystalline behaviour at high dispersant concentration, field-induced phase separation at low and intermediate concentrations, switching in electric fields, and a reversible response to the adsorbing light affecting current transients in sandwich cells.1 By doping with small amounts of ferrofluid these pigment dispersions can form a basis for magneto-responsive materials. A strong magneto-optical effect has been confirmed. In our studies, we demonstrate a strong shear-induced birefringence and shear thinning behaviour in pure dispersions. We also discuss the effects of magnetic fields on the rheological properties of the pigment/ferrofluid mixtures. This helped to get a deeper insight into the properties of these suspensions and understand the mechanisms of the structural changes under external field such as electric, magnetic and flow.

of the Péclet number (Pe) from 0.01 to 50. To obtain diffusion coefficients, image-time series from a Confocal Scanning Laser Microscope were analysed with a method that, after finding the particle trajectories, subtracts the instantaneous convective displacements and subsequently measures the slopes of the Mean Squared Displacement in the flow (x) and shear (y) directions. The thus obtained Dx and Dy, which should be equal to the free diffusion coefficient (regardless of shear) in the dilute limit, both increase strongly with Péclet number (for Pe > 10) in a concentrated suspension. This effect of shear-induced collisions is counteracted by the contribution of walls, which cause a strong local reduction in Dx and Dy.

**BP 4.11 Mon 12:15 C 130**

*Transport of active particles in low-porosity structures* — **Frank Winzer**, **Christian Scholz**, and **Clemens Bechinger**

Transport of active bacteria in porous media is of importance in many different fields, ranging from bioremediation, groundwater contamination and enhanced oil recovery to blood perfusion inside the body. We study the motion of active particles in artificially created porous media by a semi-experimental approach. In porous media with low porosities the presence of stagnant parts can lead to a temporary trapping of active particles in such regions, which can vastly increase their retention times. We compare the distributions of retention times and the transport properties of active and purely Brownian particles.

**BP 4.12 Mon 12:30 C 130**

*Isotbyric acid and water mixture confined in a silica nanopore* — **Michael Harrach** and **Barbara Drossel** — Institut für Festkörperphysik, TU Darmstadt, Darmstadt, Germany

We analyze the phase behaviour of water and isotburytic acid mixtures of differing weight percentages, in a silica nanopore of roughly 4 nm diameter and a corresponding smooth-walled confinement based on the average potential as given by the pore. While experimental studies have been interpreted as showing evidence for a phase separation of water and isotburytic acid with the water situated at the pore wall we observe the converse, with the water rich part of the mixture preferring the pore center. The comparison of the smooth and rough pore allows us to further determine the importance of potential hydrogen bond sites and their influence on the static and dynamic characteristics of the mixture.

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**BP 5: Nanoparticles and Composite Materials I (joint CPP/BP)**

**BP 5.1 Mon 9:30 C 243**


Iron Oxide Nanocube Monolayers at the Air/Water Interface: Self-Organization on Nano- and Mikroscales

**BP 5.2 Mon 9:45 C 243**

*ZnO nanoparticle stabilization - How much is necessary?* — **Torben Schindler**, **Tilo Schucheltz**, **Wei Lin**, **Doris Segert**, **Wolfgang Peukert**, and **Tobias Unruh**

ZnO nanoparticles tend to aggregate at neutral pH values due to the high negative surface charge, colloidal stability and responsiveness. The aggregation behavior of nanoparticles (GNPs) is widely used in biological systems. Unfortunately, the colloidal variability is neglected in most studies, so that the chemical identity is not coherent with the biological identity. An undefined absorption alters the properties of the particles fundamentally, so that it is not possible to predict or study their biological behavior in dependence of their original physicochemical properties, e.g. surface charge, colloidal stability and responsiveness.

**BP 5.3 Mon 10:00 C 243**

*A Toolbox to Connect the Physicochemical Properties of GNP's with their Biological Behavior* — **Jonas Schubert** and **Munish Chanana** — Department of Physical Chemistry II, University of Bayreuth, 95440 Bayreuth (Germany)

Due to their plasmonic properties and their biocompatibility, gold nanoparticles (GNPs) are widely used in biological systems. Unfortunately, the colloidal variability is neglected in most studies, so that the chemical identity is not coherent with the biological identity. An undefined absorption alters the properties of the particles fundamentally, so that it is not possible to predict or study their biological behavior in dependence of their original physicochemical properties, such as surface charge, colloidal stability and responsiveness.

**BP 5.4 Mon 10:15 C 243**

*Electrochemical growth of ZnO nanostructures for biosensing applications* — **Clemens Bechinger**, **Christiane A. Ahrens**, **Barbara Drossel**, **Michael Harrach**, **Clemens Bechinger**, **Veit Wagner** — Jacobs University, Bremen, Germany

Biosensors have been used in applications such as blood glucose measuring or pregnancy tests already for a long time, and their improvement is of high interest in many fields of research such as medicine (e.g. diagnostics), military (e.g. monitoring of poison gases) and industry (e.g. food and drink process control). The sensitivity of biosensors can be improved by increasing the surface area where the molecules under observation can bind. Therefore, we have employed ZnO nanoparticles (GNPs) as active particles in such regions, which can vastly increase their retention times. We compare the distributions of retention times and the transport properties of active and purely Brownian particles.

**BP 5.5 Mon 10:30 C 243**

*Isotbyric acid and water mixture confined in a silica nanopore* — **Michael Harrach** and **Barbara Drossel** — Institut für Festkörperphysik, TU Darmstadt, Darmstadt, Germany

We analyze the phase behaviour of water and isotburytic acid mixtures of differing weight percentages, in a silica nanopore of roughly 4 nm diameter and a corresponding smooth-walled confinement based on the average potential as given by the pore. While experimental studies have been interpreted as showing evidence for a phase separation of water and isotburytic acid with the water situated at the pore wall we observe the converse, with the water rich part of the mixture preferring the pore center. The comparison of the smooth and rough pore allows us to further determine the importance of potential hydrogen bond sites and their influence on the static and dynamic characteristics of the mixture.
Insulin capped gold nanoparticles-polymer brush composites

1Muriel RoVira-esteva, ZuleYHa yenice, StephAnie Chris-tau, stefAn wellefert, and regine von klitzing — stranski labo-ratorium für physikalische und theoretische chemie, technische uni-versität Berlin, 10623 Berlin, Germany

Polymer brushes are polymers grafted to a surface by one end, with the other end free enough that the polymer chains stretch away from the surface. This stretching is often responsive to environmental conditions, which makes them a suitable candidate for the design of smart coatings, among a number of other applications. Polymer brush-nanoparticle composites allow to combine the responsive properties of the brush with the physico-chemical properties of the particles. Therefore, determination of how the geometric parameters on the brush-nanoparticle interactions was then explored using a number of techniques, such as AFM and reflectometry.

BP 5.5 Mon 12:00 C 243

Drug delivery to cancer cells by nanodiamonds — Anna ermakoV, yuZhou Wu, boris navensov, tanja wehl, and federico leJelekzo — 1Institute of Quantum Optics, University Ulm, Ulm, Germany — 2Institute of Organic Chemistry III, University Ulm, Ulm, Germany

The numbers of new cancer cases increase every year, and only few last years in some country the numbers of deaths were stable or decreased [1], this is result of progress in medicine. The main problem of the cancer therapy is the poor drug delivery to cancer cells, and the action of healthy cells. The direct drug delivery can bring a lot of advantages: reduction of the total amount of uptaken drug, more stable drug level in the specific sides, potential reduction of the drug in healthy unaffected tissues, and reduction of dosages frequency. Nanodiamonds (NDs) are potentially good drug carriers since they are non-toxic [2], their surfaces can be chemically functionalized [3] and they can be easily inserted into cells [4]. Furthermore, colour defect centres in NDs can be used as photostable biomarkers compared to quantum dots and dyes. In our work to release drug we used the property of the tumour tissue to have on average a lower pH level than healthy tissue [5]. We demonstrate a drug release from NDs in the solution, triggered by change in the pH, and inside HeLa cells. We show that only drugs penetrate into a cell nucleus and NDs stay at the cytoplasm. [1]R.Jain, J of Controlled Release,53(1998) [2]A.M.Schrand et al, J Phys Chem B,111(2007) [3]A.Datta et al, Nanotechnology,22(2011) [4]F.Neugart et al, NanoLett.,7(2007) [5]R.Jain, J of Controlled Release,53(1998)
atoms is observed on the neutral block with an exponential growth of metal particle size. The coalescence behavior of the inert metal is mainly dominated by the improved atom mobility within the neutral polymer block. [1] Metwalli et al. ChemPhysChem 15, 2236 (2014)

BP 5.11 Mon 12:30 C 243

Nanocomposites of colloidal triglyceride platelets and DNA — Michael Schmiele, Charlotte Knittel, and Tobias Unruh — Physik Department, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany

Aqueous suspensions of colloidal tripalmitin platelets, stabilized by a mixture of soybean lecithin, Poloxamer 188 (or Polyborate 80) and the cationic surfactant dioctadecyldimethylammonium bromide (DODAB), are prepared by high-pressure melt homogenization. DODAB provides the platelets with a positive surface charge. DNA complexes are prepared by addition of herring DNA to the suspensions. The structure of the DNA complexes, ranging from the molecular to the micron scale, is investigated by small- and wide-angle x-ray and neutron scattering, microcalorimetry, photon correlation spectroscopy, transmission electron microscopy and computer simulations.

Complexes prepared from native suspensions with low concentrations of DODAB and high +/- charge ratios (DODAB:DNA) exhibit sizes in the colloidal range. Higher concentrations of DODAB and charge ratios close to the isoelectric point promote platelet agglomeration, leading to very large complexes of several microns. Small-angle scattering and computer simulations reveal a lamellar arrangement of the platelets in the complexes, with the DNA being most probably sandwiched between the platelets. Such nanocomposites of macromolecules (DNA) and tripalmitin platelets could provide a good protection of the intercalated macromolecules and can be regarded as a potential carrier system for them.

BP 5.12 Mon 12:45 C 243

Nanocomposites composed of HEUR polymer and magnetite iron oxide nanoparticles — Antonella Campanella, Hennrich Frielinghaus, Zhengyu Di, Marie-Sousai Appavou, Alessandra Luchini, Luigi Pauduaro, Alice Klapper, Oleg Petracci, Peter Müller-Buschbaum, and Dieter Richter — 1JCNS0-FRMI, Lichtenbergstrasse 1, 85747 Garching — 2University of Naples, Federico II, Dipartimento di Scienze Chimiche, Via Cintia, 80126 Naples, Italy — 3JCNS-2, Forschungszentrum Jülich GmbH, 52425 Jülich — 4TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Strasse 1, 85748 Garching

We study nanocomposites of a polymer matrix which consists of hydrophobically modified ethoxylated urethane polymers (HEUR) with embedded coated magnetite nanoparticles. Two different kinds of coatings are compared namely, the hydrophobic coating, composed of oleic acid and oleylamine, and the hydrophilic coating composed of a cationic surfactant, C18TAB, as an additional layer to the hydrophobic magnetic nanoparticles. We focused on the structural characterization of such nanocomposites in two different morphologies: as thin dry films and as hydrogels.

BP 6: Networks: From Topology to Dynamics I (joint SOE/DY/BP)

Time: Monday 12:15–13:15

BP 6.1 Mon 12:15 MA 001

How mutational networks shape evolutionary processes — Henning Siemens, Benjamin Maier, and Dirk Brockmann — Robert Koch-Institut, Berlin

Dynamic processes on complex networks have attracted a lot of attention in the past. The majority of the studies focus on understanding how topological network features shape dynamics. Several interesting results have been obtained in the context of epidemics and contagion phenomena recently, for instance the absence of epidemic thresholds in scale free networks, or the context of synchronization phenomena where certain network topologies can sustain chimera states. However, evolutionary processes on networks received comparatively little attention. It is largely unresolved how network topologies influence mutation and selection dynamics. Here, we investigate a network system of genetic strains in which each node represents a strain and links represent possible mutational pathways. We compare generic network topologies ranging from ordinary lattices and Erdos-Renyi networks to small world and scale free networks. We find that network topologies can have a substantial impact on equilibrium strain distributions. We show that locally clustered networks such as small world and lattice topologies tend to generate local maxima composed of communities with high fitness. Furthermore, we find that scale free topologies as opposed to ER networks are more likely to exhibit a lower error threshold.

BP 6.2 Mon 12:30 MA 001

Possible Origin of Stagnation and Variability of Earth’s Biodiversity — Jan Nagler, Thilo Geisel, and Frank Stolzmeier — 1ETH Zurich — 2MPI DS, Göttingen

The magnitude and variability of Earth’s biodiversity have puzzled scientists ever since paleontologic fossil databases became available. We identify and study a model of interdependent species where both endogenous and exogenous impacts determine the nonstationary extinction dynamics. The framework provides an explanation for the qualitative difference of marine and continental biodiversity growth. In particular, the stagnation of marine biodiversity may result from a global transition from an unbalanced to a balanced state of the species dependency network. The predictions of our framework are in agreement with paleontologic databases. [1] Stollmeier, Geisel, Nagler, Phys. Rev. Lett. 112, 228101 (2014)

BP 6.3 Mon 12:45 MA 001

Excitable dynamics and cellular automata dynamics on loop-free networks — Anne-Wiikke Harden, Jens Christian Claussen, and Jens Christian Claussen — 1Institut für Neuro- und Bioinformatik, Universität zu Lübeck — 2Computational Systems Biology Lab, Jacobs University Bremen

Spreading dynamics on graphs or networks have attracted considerable attention in the context of pattern formation and infection dynamics [1]. Here we investigate patterns generated by excitable dynamics [2] comprised by the states of susceptible - excitable - recovered, as well as cellular automata dynamics started from a localized seed on lattices and loop-free graphs [3]. The latter type of dynamics exhibits interesting characteristics as 1/f type spectra [4] and relates to new integer sequences [5]. Finally we investigate cellular-automata (CA) like limiting cases of the SER dynamics.


BP 6.4 Mon 13:00 MA 001

Noise in Coevolving Networks — Marina Diakonova, Victor Eguiluz, and Maxi San Miguel — Instituto de Fisica Interdisciplinar y Sistemas Complexos IFISC (CSIC-UIB), E07122 Palma de Mallorca, Spain

Coupuling dynamics of the states of the nodes of a network to the dynamics of the network topology leads to generic absorbing and fragmentation transitions. The coevolving voter model is a typical system that exhibits such transitions at some critical rewiring. We study the robustness of these transitions under two distinct ways of introducing noise. Noise affecting all the nodes destroys the absorbing-fragmentation transition, giving rise in finite-size systems to two additional regimes: bimodal magnetisation and dynamic fragmentation. Noise Targeting a fraction of nodes preserves the transitions but introduces shattered fragmentation with its characteristic fraction of isolated nodes and one or two giant components. Both the lack of absorbing state for homogenous noise and the shift in the absorbing transition to higher rewiring for targeted noise are supported by analytical approximations.
Invited Talk

BP 7.1 Mon 14:30 H 1028

Super-resolution imaging of small, fast moving cellular structures - Laboratory for Bio-imaging and Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Many new, exciting imaging techniques have emerged during the last decade, providing significantly improved spatial resolution and contrast. However, this extra information comes at the cost of more photons required to illuminate the cell, which requires more time and energy and often damages biological structures. The smaller the structures to be investigated, the faster they usually move inside living cells, because of both Brownian motion and coordinated work of molecular motors. Therefore, alternative imaging approaches have to be developed. In this talk I will demonstrate how fluorescence-based super resolution microscopy uncovers the work of polymerization motors driving the cytoskeleton in bacteria. I will make the switch to ultra-fast, label-free, coherent imaging through scattering of a rotating laser beam, which reveals unexpected biological transport processes at the periphery of macropages. And last, I will show how fast shape changes of a tiny helical bacterium held in a scanning optical trap can be monitored in 3D at 1000 Hz giving insights of molecular processes inside the 200 nm thin cell body.

BP 7.2 Mon 15:00 H 1028

Molecular architecture of native fibronectin fibrils — INGMAR SCHOEN1, SUSANNA FRÖHL1, JONAS RIEß2, and VIOLA VOGEL1 — 1ETH Zurich, Zurich, Switzerland — 2European Molecular Biology Laboratory, Heidelberg, Germany

Fibronectin fibrils within the extracellular matrix play central roles in regulating cell anchorage and behavior, particularly in early development, wound healing, but also in cancer and other pathologies. However, their hierarchical structure at the molecular level remained elusive. Using single-molecule localization microscopy combined with site-specific labeling techniques, we found that the most elemental fibronectin protofibrils consist of overlapping dimeric fibronectin molecules that show a quasi-periodic order. The spatial autocorrelation of regular, punctate label patterns along these fibrils yielded an average spacing of ca. 95 nm which was consistent for different antibody epitopes along the fibronectin molecule. Dual-color cross-correlation revealed alternating N- and C-terminal regions. Single end-labeled fibronectin molecules incorporated into protofibrils displayed an average end-to-end distance of ca. 133 nm. Together, these results suggest a staggered arrangement with an antiparallel 30-40 nm broad overlap of the N-terminal of adjacent molecules involving the first five type I and type III repeats of each molecule. While demonstrated here using fibronectin fibers, this powerful super-resolution approach can be extended to elucidate the build-up of other filamentous protein structures in their physiological environment.

BP 7.3 Mon 15:15 H 1028

Quantitative Analysis of Nuclear Genome Nanostructure using Super-resolution Fluorescence Microscopy — CHRISTOPH CHERNER1,2,3, ALEXANDER SECCHI1, HYUN KEUN LEE1,3, KIRTI PRAKASH1,2, and UDÖ BIUK1,3 — 1Institute of Molecular Biology (IMB), D-55128 Mainz, Germany — 2Institute for Pharmacy and Molecular Biotechnology (IPMB), University Heidelberg & Kirchhoff-Institute for Physics (KIP), D-69120 Heidelberg, Germany — 3Department of Physics, University Mainz (JGU), D-55128 Germany

Numerical models of nuclear genome structure have provided quantitative predictions on various length scales, from the micrometer to the nanometer range. Until recently, experimental tests of such models using far field light microscopy were limited by the conventional resolution limit of about 200 nm in the object plane and 600 nm along the optical axis (*Abbe/Rayleigh-limits*). These limits have been overcome by various super-resolution fluorescence microscopy (SRM) methods, such as Stimulated Emission Depletion (STED) and Photoactivated Localization Microscopy (PALM). Here, we report on quantitative nuclear nanostructure analysis based on complementary SRM approaches. Presently, these approaches allow us to analyze nuclear nanostructures down to few tens of nanometer in 3D using a special variant of localization microscopy, Spectral Precision Distance/Position Determination Microscopy (SPDM).
far not be achieved with standard fluorophores.

Cryo-Fluorescence Microscopy of Single Molecules —

KLAUS NEUSCHWANDER1, 2, DAVID E. WHITNEY3, GORDON B. SMITH3, DAVID FITZPATRICK2, and MATTHIAS KASCHUBE1 — 1Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany — 2Max Planck Florida Inst., Jupiter, FL, USA

The cortex is spontaneously active from the first moments that circuits form and there is ample evidence indicating that early cortical maturation relies on spontaneous activity. Yet, we know very little about how the pattern of spontaneous activity prior to visual experience impacts circuit formation. Here we took advantage of the robust columnar representation of orientation preference in ferret visual cortex to determine how patterns of spontaneous activity before eye-opening are related to stimulus-evoked patterns in the same animal later in development. By using the calcium indicator GCaMP6 we revealed population activity on the sub-second timescale of the developing visual cortex. Novel analysis approaches allowed us to uncover interpretable statistical relations from these data. We found that events of spontaneous activity varied in size over several orders of magnitude. Large events displayed robust columnar patterns that resembled the mature neuron model and roughly scales with the inverse square root of the detected photon number. Therefore, photo-bleaching is the fundamental bottleneck that limits the achievable resolution. One method to suppress photo-bleaching is to cool a sample down to cryogenic temperatures. For that purpose, we designed and built a dedicated cryostat suitable for single molecule fluorescence microscopy. The system is not only capable of cooling the sample to cryogenic temperatures, but gives also optical access to the sample for high-quality imaging with a conventional microscope employing an objective with high numerical aperture. Another important property of our system is its excellent mechanical stability, enabling long-time observations of samples over several hours with negligible drift. Using our system, we successfully performed photo-bleaching studies on single molecules showing a more than two order of magnitude enhancement in photo-stability, which results in an exceptional molecular localization accuracy in angstrom scale.

A Scanning Cavity Microscope —

MAXIMILIAN MAERZ1, 2, JAKOB KRAEMER3, THORSTEN W. HANSSCH1, 2, and DAVID HUNGER1, 2

1Ludwigs-Maximilians-Universität München, Fakultät für Physik, Schellingstraße 4, 80799 München — 3Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching — 2Laboratoire Kastler Brossel, ENS/UPMC-Paris/CNRS, 24 rue Lhomond, 75005 Paris

We present a versatile tool for ultra-sensitive and spatially resolved optical characterization of single nanoparticles.

Using signal enhancement in a scanning optical microscopy made of a micromachined optical fiber and a plane mirror [1] we measure the polarization dependent extinction of a single nanoparticle as well as its birefringence. Harnessing multiple interactions of probe light with a sample within the optical resonator, we achieve a 1700-fold signal enhancement compared to diffraction-limited microscopy. We demonstrate quantitative imaging of the extinction cross section of gold nanoparticles with a sensitivity below 1 nm², we show a method to improve spatial resolution potentially below the diffraction limit by using higher order cavity modes, and we present measurements of the birefringence and extinction contrast of gold nanorods [2].

The information spike trains encode about an external time-dependent stimulus is quantified by Shannon's mutual information rate. However, the numerical estimation of the mutual information rate is demanding and does not reveal which features of the stimulus are encoded. Several studies have identified mechanisms at the cellular and network level leading to low- or high-pass filtering of information, i.e., the selective coding of low- or high-frequency components of the time-dependent stimulus. However, these findings rely on an approximation, specifically, on the qualitative behavior of the coherence function, an approximate frequency-resolved measure of information flow, whose quality is generally unknown.

We developed a numerical procedure to directly calculate a frequency-resolved version of the mutual information rate. This can be used to study how different frequency components of a Gaussian stimulus are encoded in neural models without invoking a weak-signal paradigm or making undue assumptions on the nature of the neural encoding. We demonstrate its application for paradigmatic descriptions of neural firing like an integrator neuron and a simple setup mimicking a coincident detector cell receiving input from two leaky integrate-and-fire neurons.

**BP 8.4** Mon 15:15 H 1058

**Spike timing reliability and information transfer under noisy juxtaplottular stimulation — Experiment and theory** — Jenks Doosel1,2, Guy Doron1,2, Michael Brecht1,2, and Benjamin Lindner1,2 — 1Bernstein Center for Computational Neuroscience — 2Humboldt University of Berlin, Germany

We used nanostimulation, a technique which allows stimulation of identified single neurons in vivo, in order to drive pyramidal cells in anesthetized rat motor cortex. Using this method we find that stimulating with fluctuating stimuli (frozen bandpass-limited white noise) results in increased spike timing reliability. Specifically, we report that parametrically increasing the stimulus variance results in increased spike train synchronization. We also explore how well the spike train as well as statistics like the power spectrum or the spectral coherence function, in response to this stimulus can be captured by a model neuron. In particular, we use the exponential integrate-and-fire neuron, a simple model that has been successfully applied to reproducing spike times of pyramidal cells under noisy current stimulation in vivo.

**BP 8.5** Mon 15:30 H 1058

**Synaptic unreliability facilitates information transmission in balanced cortical populations** — Leon A. Gatys1, Alexander S. Ecker1, Tatjana Tchumatchenko2, and Matthias Bethge1 — 1Centre for Integrative Neuroscience and Institute for Theoretical Physics, Tübingen, Germany — 2Max Planck Institute for Brain Research, Frankfurt, Germany

Synaptic unreliability is one of the major sources of biophysical noise in the brain. In the context of neural information processing, it is a crucial question how neural systems can use this unreliability. Here, we examined how synaptic noise affects signal transmission in cortical circuits, where excitation and inhibition are thought to be tightly balanced. Surprisingly, we found that in this balanced state synaptic response variability actually facilitates information transmission, rather than impairing it. In particular, the transmission of fast-varying signals benefits from synaptic noise, as it instantaneously increases the amount of information shared between presynaptic signal and postsynaptic current. This finding provides a parsimonious explanation why cortex can afford to operate with noisy synapses.

15 min break

**BP 8.6** Mon 16:00 H 1058

**Electro-physiological characterization of the ultra-fast Channel-Rhodopsin Chronos** — Ulrich Frommer1, Andreas Neer2,3, and Christoph F. Schmidt1 — 1Faculty of Physics, George August University, Gottingen, Germany — 2Bernstein Center for Computational Neuroscience, Gottingen, Germany — 3MPI for Dynamics and Self-Organization, Gottingen, Germany

The light-gated ion channels Channel-Rhodopsins (CHRs) have become a major tool in experimental neuro science due to their low invasiveness and the possibility of genetically targeting specific cell types. To address specific issues, various CHRs with a wide array of different properties have been introduced. Here we characterize Chronos an especially light sensitive ChR with improved opening and closing speeds compared to traditional ChRs such as the widely used ChR2. This ChR shows great promise in various applications, such as the creation of neural implants, where good time resolution and low light intensities are favorable. We used patch-clamp recordings to characterize the kinetics of the ensemble of channels, which dictate the performance in applications. We also created Markov models representing the light cycle of Chronos, which enables the extraction of single-molecule properties from the electro-physiological measurements.

**BP 8.7** Mon 16:15 H 1058

**Assessing network states from subsampled activity** — Anna Levina1,2,3, Theo Geisel1,2, and Viola Priesemann1,3 — 1BCCN Göttingen, Germany — 2MPI MIS, Leipzig, Germany — 3MPI DS, Göttingen, Germany

Experimental studies suggest that neural activity self-organizes close to criticality, as various preparations have shown signatures of it. At criticality, the neural network may profit from the optimal information processing associated with a critical state.

The appeal of the criticality hypothesis for the brain lies in its potential to unveil a fundamental principle of collective neural dynamics and offers an opportunity to relate neuronal circuits to well studied physical systems. Wang et al. suggested for criticality in simulated systems the full information about their activity can be used. Data obtained from brain recordings are limited by subsampling, however, since to date it is impossible to assess the activity of every single neuron in the brain.

Here we discuss how subsampling changes avalanche size distributions, and how it is possible to recover information of the actual network state even under subsampling. To this end, we extend methods from statistical physics and analyse scaling laws for subsampled systems. To demonstrate the generality of our novel approach, we evaluate models from different universality classes and support our results by analytical considerations.

**BP 8.8** Mon 16:30 H 1058

**Estimating branching parameters from subsampled systems** — Jens Wilting1, Theo Geisel1,2, and Viola Priesemann1,2 — 1Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — 2BCCN, Göttingen, Germany

Branching processes are frequently used to model time-varying data in economics, finance, epidemiology, population dynamics, physics, and neuroscience. Depending on the expected number of offspring, the process shows either stationary fluctuations (sub-critical) or transient growth (super-critical), and has a deep connections to self-organized criticality. Methods to infer $\varepsilon$ from fully sampled systems are well established. In real-world systems, however, often only a subset of all agents can be sampled. Since under subsampling classical approaches fail, we developed a novel approach based on the auto-correlation function that for the first time allows to robustly infer $\varepsilon$ even under subsampling. Importantly, our method generalizes to auto-regressive processes with both additive and multiplicative noise, making it widely applicable. We demonstrate that our method correctly estimates $\varepsilon$ under sub-sampling in simulated branching processes, and also in the purely deterministic Bak-Tang-Wiesenfeld model. Moreover, applying our method to necessarily subsampled neuronal population dynamics from macaque monkeys, we show that spiking dynamics reflects a sub-critical regime ($\varepsilon = 0.95$).

**BP 8.9** Mon 16:45 H 1058

**Self-consistent spectra in recurrent spiking networks** — Stefan Wieland1,2 and Benjamin Lindner1,2 — 1Bernstein Center for Computational Neuroscience Berlin, Germany — 2Humboldt University Berlin, Germany

Firing patterns in cortical networks are often modeled with Poissonian spike trains. Demanding self-consistency at the level of firing rates, i.e. that spike trains driving a neuron possess the same firing rate as the spike train they evoke, then yields a tractable analytic description of network dynamics. However, output spike trains are usually observed to be non-Poissonian, something a more coherent framework should account for. Here we present iterative schemes that yield self-consistent statistics in recurrent neural networks at the level of spike-train correlations.
BP 9.1 Mon 14:30  EB 202
Determination of Conformational Entropy of Fully and Partially Folded Conformations of Holo- and Apomyoglobin  

Holo- and apomyoglobin can be stabilized in native folded, partially folded molten globules (MGs) and denatured states depending on the solvent composition. In a comparative experimental study we investigated the correlation between protein folding and dynamics on the picosecond time scale using incoherent quasielastic neutron scattering (QENS). The conformational entropy difference $\Delta S_{\text{conf}}$ between the folded conformations and the acid denatured state could be determined from the measured mean square displacements and was compared to the entropy difference $\Delta S$ obtained from thermodynamic parameters. The observed difference between $\Delta S$ and $\Delta S_{\text{conf}}$ was attributed to the entropy difference $\Delta S_{\text{hydr}}$ of dynamically disordered water molecules of the hydration shell. The entropy content of the hydration water is significantly larger in the native folded proteins than in the partially folded MGs. We demonstrate the potential of incoherent neutron scattering for the investigation of the role of conformational dynamics in protein folding.

BP 9.2 Mon 14:45  EB 202
Mechanical rupture of mono- and bivalent coordination compounds  
Manuel Gensler1, Christian Eidamshaus2, Arthur Galstyan2, Ernst-Walter Knapp3, Hans-Ulrich Reissig2, and Jürgen P. Rabe4 — 1Department of Physics, Humboldt-Universität zu Berlin — 2Institute of Chemistry and Biochemistry, Freie Universität Berlin

Biomolecular systems are commonly exposed to a manifold of forces, often acting between multivalent ligands. To understand these forces we studied a monovalent and three bivalent pyridine Cu(II) coordination complexes with varying backbone structures. We performed SFM based single-molecule force spectroscopy in aqueous environment and compared results with ab-initio DFT calculations. According to the Kramers-Bell-Evans theory, all interactions show remarkably long rupture lengths of more than 3 Å. We explain this observation by dissociation mechanisms involving hydrogen-bound intermediate states. Additionally we show that most probable rupture forces of the bivalent systems can be larger, but also smaller than those of the monovalent counterpart. In contrast, when our results are extrapolated to forceless conditions, all bivalent systems show lower thermal dissociation rates. Then, mechanical stability is not solely determined by binding energy, but also by rupture lengths. Thus both parameters should be considered in the rational design of biomolecular ligands.

BP 9.3 Mon 15:00  EB 202
Opposite translocation of long and short oligomers through a nanopore  
Thomas Töws, Sebastian Getfert, and Peter Reimann — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

We consider elongated cylindrical particles, modeling e.g. DNA fragments or nano-rods, while translocating under the action of an externally applied voltage through a solid-state nanopore. Particular emphasis is put on the concomitant potential energy landscape due to the complex interplay of various electrohydrodynamic effects beyond the realm of small Debye lengths. We find that the net potential energy difference across the membrane may be of opposite sign for short and long particles of equal diameters and charge densities (e.g. oligomers). Thermal noise thus leads to biased diffusion through the pore in opposite directions. The specific particle length at which this transport inversion occurs can be controlled by means of a membrane gate electrode.

BP 9.4 Mon 15:15  EB 202
Hydrodynamic Slip on DNA in Nanopore Translocation Experiments  
Lucas Galla1, Andreas J. Meyer1, André Spiering2, Andy Sischo3, Michael Mayer4, Adam R. Hall3, Peter Reimann4, and Danio Anselmetti5 — 1University of Bielefeld, Germany — 2Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany — 3Wake Forest University School of Medicine, USA

In a recent paper, we reported on the observation of hydrodynamic slip on DNA by optical tweezers-controlled translocation experiments in solid-state and lipid-coated nanopores [1]. After a short introduction to the performed experiments, I will present our theoretical model describing the dominating electrohydrodynamic effects, with particular emphasis on the hydrodynamic slip boundary condition.

By solving the Poisson-Nernst-Planck and Stokes equations using finite element methods it is possible to gain insight into the influence of nanopore geometry and composition on translocation experiments. Furthermore, these continuous models of electrohydrodynamics can serve as an appropriate basis for dynamic DNA simulations.


BP 9.5 Mon 15:30  EB 202
How to escape the maze  
Teresa Breh1, Felix Höfling2, and Thomas Franosch3 — 1Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität, München — 2Max Planck Institute for Intelligent Systems, Stuttgart, and Institut für Theoretische Physik, Universität Stuttgart — 3Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Austria

Recently, novel materials such as carbon nanotubes extended the interest in the diffusion dynamics of semiflexible polymers far beyond classical biophysics. Semiflexible polymers form entangled networks when dispersed in solution by virtue of their lengthy nature. Due to their relative stiffness they exhibit a reptation movement to escape their local surrounding maze of crossing polymers, usually modelled as a tube constraining the polymer sterically.

We have investigated the dynamics of a semiflexible polymer via computer simulations of a 2D bead-rod-algorithm. Point obstacles mimic the cross sections of the surrounding polymers with the plane in which the polymer diffuses. Extensive computer simulations are performed to resolve the slow disentanglement processes. In particular we measure the translational and rotational diffusion for a broad density range. Furthermore, we discuss the intermediate scattering function and the chances and limitations of the performed simulations.

BP 9.6 Mon 16:00  EB 202
Theory on linear viscoelasticity of a cytoskeletal network  
Tetsuya Hirawa and Rolfan Netz — Freie Universität Berlin, Germany

Mechanical properties of a cortical cytoskeleton, which is a network consisting of actin filaments and crosslinker proteins located underneath the cell membrane, govern the elastic and viscous resistances of living cells to deformation and are crucial for wide variety of cellular functions. I would like to present a theoretical method to evaluate linear viscoelasticity of a filamentous network like a cortical cytoskeleton based on properties of single segments. Using the method, we can explain the universal power-law in complex moduli, which is also found in several experiments and our numerical simulation.

BP 9.7 Mon 16:15  EB 202
Scaling with persistence length: Expanding the accessible phase space of semi-flexible polymer networks via DNA tubes  
Carsten Schulte1, 2, Jessica Lorenz3, Jörg Schnauss4, Tina Händler1, Martin Glaser1, Josef A. Kas5, and David M. Smith2 — 1University of Leipzig, Soft Matter Physics Division, Leipzig, Germany — 2Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany

Biologically evolved materials are often used as inspiration in both the development of new materials as well as examinations of underlying physical principles governing their general behavior. One prominent
example is actin and its set of accessory proteins. However, a major limitation lies in the molecular toolbox provided by naturally occurring biological systems. The inability to deterministically modulate or "program" basic properties such as stiffness or interaction strengths hinders a meticulous examination of the parameter space, and the subsequent potential for developing new classes of materials.

We overcome these limitations employing model systems assembled from programmable nanomaterials such as DNA. Nanotubes with similar dimensions and mechanical properties as actin filaments can be constructed from small sets of specially designed DNA strands. Properties such as stiffness and inter-filament attraction (i.e. crosslinking) can be controlled through the design of a particular set of DNA strands. Forming networks from these semi-flexible polymers, we test established theories with respect to these parameters for the first time.

BP 9.8 Mon 16:30 EB 202 pH-dependent Ordered Fibrinogen Adsorption on Polyethylene Single Crystals — CHRISTIAN HELRING1, ROBERT SCHULE2, DOMINIK HERING2, and KLAUS D. JANDT1 — 1Chair of Materials Science (CMS), Otto-Schott-Institute of Materials Research (OSIM), Friedrich Schiller University Jena, Jena, Germany — 2Clemenshospital Münster, Münster, Germany

The biological performance of materials is mostly determined by protein adsorption. Protein adsorption can influence the assembly and orientation of adsorbed proteins. The aim of the current study was to control the protein adsorption by nanostructured surfaces. For this, we tested the hypothesis that human plasma fibrinogen (HPF) assemblies can be oriented on the (001) surface nanostructures of Polyethylene Single Crystals (PE-SC).

At a physiological pH of 7.4, HPF assemblies consisted of crosslinked HPF molecules, e.g., protofibrils, networks or sponge-like structures in dependence of the protein concentration. However, at an increased pH of 9.2 spherical-shaped and trinodal-shaped single HPF assemblies were observed. The observation of these multi protein assemblies (pH 7.4) and the single HPF assemblies (pH 9.2) can be explained by activated (pH 7.4) and deactivated (pH 9.2) HPFs αCr domains. While the single trinodal-shaped HPF molecules preferred an orientation along crystallographic [100] and [010] directions on the nanostructured PE-SC surface the HPF protofibrils showed no preferential orientation. The current study deepens the understanding of controlled protein assembly and orientation on nanostructured surfaces.

BP 9.9 Mon 16:45 EB 202 Insights into diatom biomineralization with nanoscale silica-peptide hybrid films — HELMUT LUTZ1, VANCE JÆGER2, JIM PFAENOTNER3, MISCHA BONN4, and THOAS WEIDNER4 — 1Max-Planck-Institute for Polymer Science, Mainz — 2University of Washington, Chemical Engineering, Seattle

Taking clues from diatom silification we have recently shown that amphiphilic peptides consisting of lysine and leucine (LK peptides) are capable of producing silica wires, spheres and tubes, depending on their secondary structure. Precipitating particles, i.e. mineralization in three dimensions is very different from the two dimensional silification required for the cell walls of diatoms. Hence, we studied mineralization in 2D at the air-water interface. At the interface, slightly different peptides can adopt alpha helical or beta sheet structures depending on the hydrophobic periodicity of amino acids. Upon addition of a silica precursor we were able to obtain peptide-silica hybrid films with a thickness of ~4 nm. By means of surface sensitive techniques, such as sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS) we were able to probe the film composition and interactions between peptides and silica at the early stages of biomineralization. Electron and atomic force microscopy show that the fine structure of the film resembles the in-solution silica precipitates of each peptide. We employed molecular dynamics simulations as a technique to complement the experimental insights with a computational model. Our results provide insights into the biomineralization of structured films, which might prove useful in materials design and surface engineering.

BP 9.10 Mon 17:00 EB 202 Mapping internal mineral strains in human dentine under tension: X-ray diffraction insights into the contribution of the mineral nano-particles to the load-bearing capacity of tooth tissue — JENABAPTISTE FORHÉN1, CLAUDIA FLECH2, PETER FRATZ3, and PAUL ZASLAVSKY1 — 1Julius Wolff Institut, Berlin, Germany — 2Technische Universität Berlin, Berlin — 3Max-Planck-Institute of Colloids and Interfaces, Potsdam, Germany

Teeth are hierarchical strong and stiff structures, consisting of a mineralized protein-based composite (dentine). They function under mechanical load, and the nanometer-sized hydroxyapatite mineral particles in the collagen fiber matrix deform as a response to applied external stress (Deymier-Black, 2012). In this study, we report on the mineral response in human dentine to mechanical tensile testing. We track mineral particles following changes in the mineral dimension using X-ray diffraction. It is thus possible to compare the stresses experienced by the mineral particles with the stress applied by the external load. We find that the tissue to mineral strain ratios observed increase until they reach a value of 2, which is three times lower than for bone (Gupta, 2006), and suggests that a different load-partitioning mechanism exists in teeth. We also find that the Poisson’s ratio decreases with increasing load, suggesting that as load increases, there is some dynamic change in the loads transferred to the crystals, similar to what was found for bovine dentine loaded in compression. With increasing load, more strain-energy is oriented along the tensile axis and less is distributed into particles oriented along other orientations.

BP 10: Colloids and Complex Liquids II (joint CPP/DY/BP)

Time: Monday 15:00-18:45

BP 10.1 Mon 15:00 C 130
TIRM at liquid/liquid interfaces — KILIAN DIETRICH — University of Stuttgart, Germany

Total Internal Reflection Microscopy (TIRM) is a well-established method for the direct measurement of interaction potentials between a spherical colloidal particle and a solid wall. It is based on the tracking of the particle’s vertical motion from which interaction forces with the interface can be inferred with a resolution down to 10fN.

In contrast to previous measurements, which were performed at solid/liquid interfaces, here we demonstrate that TIRM can be applied also to liquid/liquid interfaces. These are of special interest not only due to their frequent appearance but they also exhibit an exceptional smoothness. In our study, we present a novel inverted TIRM apparatus which is capable to measure the motion of a colloidal probe particle in water close to an oil-water interface. First measurements indicate the counterplay of electrostatic interactions and van-der-Waals forces for interfaces treated with different ionic and non-ionic surfactants. In each case surface charge densities of particle and interface could be determined. The detailed knowledge of interactions can provide valuable information for the stability of emulsions and dispersions.

BP 10.2 Mon 15:15 C 130
Short Ranged Repulsive Energy in Oscillatory Structural Forces — SEBASTIEN SCHÖN and REGINE VON KLITZING — Technische Universität Berlin Strasse des 17. Juni 124 D-10623 Berlin

Oscillatory structural forces are a genuine feature observed for simple and complex fluids in the vicinity of smooth wall. The origin of these forces is related to the characteristic quality of molecules or nanoparticles to form well-ordered layers in the vicinity of a confining wall. These forces can be described by the following function as proposed by Israelachvili: \[ f(x) = \frac{A}{\cosh^2(\frac{x}{\xi})} \] with \( A \) a force constant, \( x \) the separation. The Amplitude \( A \) describes the strength of the particle interaction, the decay length \( \xi \) is a measure of how fast the force decays and the wavelength \( A \) is directly related to the inter-particle distance. Structural oscillation forces are long ranged compared to the common DLVO forces and can be used in a variety of applications e.g. oil removal or separation of bidisperse particle suspensions. For both it is important to know the strength of the oscillatory forces at very small separations. An additional repulsive term is introduced to describe deviations observed between experimental data and the common fit function, this allows accurate fitting of experimental data down to very small separations and removes systematic limitations from previous measurements.
deviations in $A$, $\lambda$, and $\xi$ depending on the starting point of the fit. The short ranged repulsive energy described by the new term is investigated at different particle concentrations, measurement speed and under the addition of NaOH, HCl and NaCl at different concentrations.

**BP 10.3 Mon 15:30 C 130**

**Complex nanoparticle arrangements via wrinkle-assisted self-assembly** — Christoph Hanske, Moritz Tebbe, Christian Kuttner, Munish Chanana, Tobias König, and Andreas Frey

- Physical Chemistry II, University of Bayreuth, 95447, Germany

**Title**:template-assisted assembly enables the arrangement of colloidal particles into well-defined structures that often demonstrate special optical, biological or catalytic functionality due to the hierarchical internal organization. A major bottleneck so far is the limited scalability of lithographic template fabrication. As an alternative strategy, we utilize wrinkled elastomer substrates exhibiting periodicities on the micron or submicron scale. The topographic features of such templates allow the arrangement of hydrophilic nanoparticles into regular, close-packed chains, which can further be transferred site-selectively onto flat substrates by wetting controlled printing. This versatile method is applicable for polymeric, inorganic and metallic particles with spherical as well as anisotropic shapes. We discuss the influence of interfacial properties originating from the employed particle and substrate coatings and demonstrate the formation of complex structures on chemically patterned substrates.[1] Further, the realization of macroscopic, gold nanoparticle assemblies is shown.[2, 3] Due to small interparticle distances of few nanometers, strong plasmonic coupling is achieved, which grants access to surfaces with tailored optical properties.


**BP 10.4 Mon 15:45 C 130**

**Linking intermolecular interactions, microstructure, and macroscopic rheology in protein suspensions** — Alessio Zacccone, Miriam Siebenbürger, Henning Winter, Frank Schreiber, and Matthias Ballauff

- 1Physics-Department, Technische Universität München — 2Helmholtz-Zentrum Berlin für Materialien und Energie — 3University of Massachusetts Amherst — 4Applied Physics, University of Tübingen

We propose a microscopic framework based on nonequilibrium statistical mechanics to connect the microscopic level of colloidal biopolymer self-assembly with the macroscopic rheology of protein gelation. The method is based on the master kinetic equations for the time evolution of the self-assembled cluster size distribution, from which the relaxation time spectrum during the gelation process can be extracted. The relaxation spectrum is a simple stretched-exponential, with a stretching exponent related to the mass fractal dimension of the self-assembling clusters. In the case of thermoreversible gelation, for weak interparticle attractions, the attraction energy is finite and plays the role of the control parameter driving a nonequilibrium phase transition into a nonequilibrium steady-state (the gel). Our theory is in good agreement with experimental data of different systems published by other authors, for which no theory was available. Further, it allows us to interpret new experimental data on the gelation of BSA which provides a benchmark system to connect the level of coarse-grained protein interactions with the macroscopic oscillatory rheology of the protein suspension.

**BP 10.5 Mon 16:00 C 130**

**Molecular versus macroscopic perspective on the phase separation mechanisms of thermo-responsive solutions** — Martine Philippe, Ralitsa Aleksandrova, Ulrich Müller, Jan K. Krüger, and Peter Müller-Buschbaum

- 1TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — 2Université du Luxembourg, LPM, Luxembourg, Luxembourg


**BP 10.6 Mon 16:15 C 130**

**Cononsolvency in P(S-b-NIPAM) diblock copolymers - a time-resolved SANS study of the aggregation process** — Konstantinos Kyriakos, Martine Philippe, Jean Adelbergher, Sebastian Jaksch, Anatoly V. Berezkin, Dersy M. Lugo, Walter Richter, Isabelle Grillo, Anna Miasnikova, André Laschewsky, Peter Müller-Buschbaum, and Christine M. Papadakis

- 1TU München, Physik-Department, Garching — 2BWT Aachen University, Institut für Physikalische Chemie — 3Institut Laue-Langevin, Grenoble, France — 4Université Potsdam, Institut für Chemie, Potsdam-Golm

In mixtures of water and methanol, the thermoresponsive poly(N-isopropylacrylamide) (PNIPAM) exhibits the cononsolvency effect, i.e. an enhanced tendency for phase separation at certain solvent compositions. We investigate the effect of adding methanol to (i) micellar solutions of polypeptide-b-poly(N-isopropylacrylamide) (PNIPAM) diblock copolymers and (ii) PNIPAM homopolymers in D2O using a stopped-flow instrument. The structural changes on mesoscopic length scales were followed by time-resolved small-angle neutron scattering (TR-SANS) with a time resolution of 0.1 s. In both systems, the pathway of the aggregation depends on the content of deuterated methanol; however, it is fundamentally different for homopolymer and diblock copolymer solutions. We propose a logarithmic coalescence model based on an energy barrier which is proportional to the aggregate radius.


**BP 10.7 Mon 16:30 C 130**

**Cation-activated attractive patches to control protein interactions** — Felix Roosen-Runge, Fajun Zhang, Frank Schreiber, and Roland Roth

- Institut Laue-Langevin, Grenoble, France — Institut für Angewandte Physik, Universität Tübingen — Institut für Theoretische Physik, Universität Tübingen

We present evidence for an explicit ion-activated mechanism to cause a patchy attraction between proteins [1]. Experimentally, ion bridges of multivalent cations between protein molecules have been observed in protein crystals [2]. Modeling this mechanism via particles with ion-activated attractive patches, a broad variety of experimental results for protein solutions with multivalent cation is explained and understood very naturally, including charge reversal, reentrant condensation, metastable liquid-liquid phase separation, cluster formation and collapse of protein crystals [1,3]. The good agreement between theory and experiments indicates that protein-cation solutions represent a natural model system for patchy patches. The mechanism of ion-activated patches can be embedded seamlessly into theory and simulations of charged soft matter, and promises rational design of phase behavior and crystallization pathways in protein solutions based on the statistical physics of patchy particles.


**BP 10.8 Mon 16:45 C 130**

**Buckling of paramagnetic chains in soft gel** — Shilin Huang and Günter K. Auernhammer

- Max Planck Institute for Polymer Research, Mainz, Germany

We study the magneto-elastic coupling behavior of paramagnetic chains in a soft polymer gel. To this end, the laser scanning confocal microscope is used to observe the morphology of the paramagnetic chains as well as the whole gel. Paramagnetic chains in a soft polymer gel show rich morphologies under an oblique magnetic field. Depending on the chain length, the chains rotate, bend and buckle. In a perpendicular magnetic field, longer chains form wave structure with higher number of buckles. A higher magnetic field strength and a lower modulus of gel matrix lead to higher number of buckles. A higher magnetic field strength and a lower modulus of gel matrix lead to higher susceptibility of the gel to magnetic field. The deformation magnetic chain confirms that the polymer network is strongly coupled with the paramagnetic chain. A theoretical model is developed to describe the buckling of the chain.
Environmental compatibility microemulsion at solid surfaces: Wettability behavior and extraction properties — \textit{Salomé Vargas Ruiz}, \textit{Christoph Schulreich}, \textit{Ramasia Sheich}, \textit{Martin Junc}, \textit{Regine von Klitzing}, \textit{Thomas Hellweg}, and \textit{Stefan Welletr} — 1Stranski Laboratory, TU Berlin, Str. d. 17 juni 124, 10623 Berlin, Germany — 2Physical Chemistry III, University Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany. 

Microemulsions based on sugar surfactants and food grade oil are potential decontamination media for the remediation of sorptive surfaces exposed to highly toxic compounds (e.g. nerve agents, pesticides). The main advantage of microemulsions relies on their capability to degrade the solubilized toxic compound by means of active ingredients hosted in the water phase. Although microemulsions have good performance on the detoxification process, the overall efficiency of the decontamination process is also determined by their ability to wet the treated surfaces and to extract the contaminants. In this study, we examined firstly the wettability and penetration properties of microemulsion formulated with sugar surfactant SL55 and methyl oleate oil, and secondly the extraction of the six lipophilic contaminants via spectroscopic and chromatographic techniques. Here, the formulated microemulsions can wet and penetrate hydrophobic and hydrophilic sorptive surfaces and their extraction properties are greatly influenced by their structure and oil content.


Hydrogen bonds are essential for the structure and dynamics of alcohols, aqueous solutions, and water. Due to their low tendency of crystallization and large variability in molecular configuration, monohydroxy alcohols (MAs) are often studied as model systems for hydrogen-bonded fluids in general [1]. MAs are supposed to form supramolecular structures such as chains and rings via hydrogen bonding in the liquid phase. Based on their small dielectric absorption, ringlike arrangements were suggested for neat MAs with a sterically hindered polar hydroxyl group [1], e.g., for 4-methyl-3-heptanol and 2-hexyl-1-decanol. Mixtures of these MAs show a significantly enhanced dielectric absorption which hints at a change of supramolecular topology [2]. We present combined X-ray diffraction and X-ray Raman measurements of MAs mixtures. The X-ray diffraction peak and the shape of the oxygen K-edge, respectively, are sensitive to the local arrangement of MAs. The results are interpreted with a transformation from ringlike to chainlike structures upon mixing. [1] R. Böhmer et al. Phys. Reports 545 125-195 (2014) and references therein; [2] S. P. Bierwirth, et al. Phys. Rev. E 90, 052807 (2014).

The role of the cation and polarization on lithium ion coordination in ionic liquids — \textit{Volker Lesch}, \textit{Zhe Li}, \textit{Dmitry Bedrov}, and \textit{Andreas Heuer} — 1Westfälische Wilhelms- Universität Münster — 2University of Utah.

MD-simulations are only slightly affected. The comparison of the cations shows only small differences for the lithium ion coordination.

A systematic study of the influence of trivalent metal ions on liquid behavior in protein solutions — \textit{Micheal Braun}, \textit{Andra Sauter}, \textit{Marcell Wolf}, \textit{Roland Roth}, \textit{Fajun Zhang}, and \textit{Frank Schreiber} — 1Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — 2Institut für Theoretische Physik, Universität Tübingen.

Thermodynamic phenomena such as reentrant condensation (RC) and liquid-liquid phase separation (LLPS) are involved in various protein-related processes, e.g. protein condensation diseases and protein crystallization. We could show that these transitions are inducible in protein solutions using various trivalent cations [1], [2]. In this work, the influence of cation size on such phase behaviour in bovine serum albumin (BSA) was studied systematically in the presence of salts with increasing cation sizes (YbCl3, YCl3, GaCl3, CeCl3 and LaCl3). The results reveal that charge inversion, the prerequisite of RC and LLPS in these systems, is found independent of cation size. Interestingly, however, salt concentration ranges in which macroscopic LLPS is observed decrease with increasing cations: while Yb3+ leads to the largest LLPS area, Ce3+ features the smallest one. La3+, the largest cation studied, induces RC, but does not lead to LLPS at all. The findings thus underline the crucial role of a protein influences the strength of protein-cation interactions and therefore plays an important role in phase transitions of the protein.

Excess entropy scaling for the segmental and global dynamics of polyethylene melts — \textit{Evangelos Voyiatzis}, \textit{Michael Bohm}, and \textit{Florian Müller-Plathe} — 1For Angewandte Physik, Universität Tübingen, 72076 Tübingen — 2Institut für Theoretische Physik, Universität Tübingen.

The range of validity of the Rosenfeld and Dzugutov excess entropy scaling co-efficient with increasing chain length which contrasts
physical expectations. The origin of this trend can be traced back to the density dependence of the scaling factors. In connection with diffusion coefficients and viscosities, the Rosenfeld scaling appears to be of higher quality than the Dzugutov. An empirical excess entropy scaling is also proposed which leads to a chain length-independent correlation.

**BP 11: Nanoparticles and Composite Materials II (joint CPP/BP)**

**Time:** Monday 15:00–18:45  
**Location:** C 243

**BP 11.1 Mon 15:00 C 243**  

Inorganic/organic hybrid materials receive steadily growing interest due to their capability to show unprecedented properties. Most likely, at the length-scale of single chains, many different phenomena add and form the final material. Due to the small diameters, their specific surface area is very high, and thus may contribute significantly. To predict the material properties, many concepts have been developed to understand the influence of those chains close to surfaces. For example, a very common picture is the assumption of an immobilized or glassy layer when the polymer is very close to solid substrates.

In our contribution, we present macroscopic properties and show that these can be explained perfectly by the concept of a glassy layer. However, for these examples, our macroscopic information by neutron scattering experiments evidence that the underlying assumptions are wrong, but our experiments permit a different explanation.

Based on our toolbox of hybrid materials, we used a well-defined system. As a consequence it allows us to formulate a theorem under which conditions new materials can be designed on the computer based on our results. Therefore, we believe that our achievements represent a major progress toward the prediction of macroscopic properties of nanocomposites based on information at the length-scale of a single chain.

**BP 11.2 Mon 15:15 C 243**  
Dynamics of polymers in composites — **ULRICH SCHLEl** — Leibniz-Institut für Polymerforschung Dresden e.V.

Magnetic resonance is applied to study the dynamics of polymers interacting with inorganic solid surfaces. The dynamics of polymers over a wide range of correlation times is determined using magnetic resonance relaxation experiments for the investigation of systems in contact with solids and inorganic materials. In highly dispersed systems, these are nanoparticle-coated thin films that have been investigated. Measurement of T2 or T1rho is ideally suited for the dynamics of chain segments, which is mostly affected by the interaction with the solid surface. Because of sensitivity issues only proton NMR signals have been detected. In order to obtain sufficient chemical resolution for instance to exclude solvent signals in swelling experiments high-resolution solid-state and NMR based on CRAMPS has been applied.

These line narrowing techniques permit the selection or suppression of the solvent signal and thus one can focus on the polymer dynamics. It is seen, that there is much stronger motion and dynamics and putting the brushes compared to polymers of the same molecular weight. To investigate that further dedicated techniques for the selective excitations at the interface part based on magnetization transfer from the inorganic particle to the polymer has been applied. Spin-labels on polyelectrolytes permit the selective study of the dynamics of the polymer in the vicinity of the label. Because of the high sensitivity of EPR dynamics of individual layers in a multilayer system can be studied.

**BP 11.3 Mon 15:30 C 243**  
Disentanglement in polymer-star mixtures — **HENDRIK MEYER** — Institut Charles Sadron, CNRS UPR22, 67034 Strasbourg, France

We present a molecular dynamics simulation study of entangled melts mixed with particles of the order of the micro-meter. The choice of compact stars represents a model system of nanocomposites without polymer-particle adsorption. The matrix particles remain well dispersed over the whole concentration range and the stars are sufficiently compact that the pure system is jammed. For this system, we observe a weak compression of the matrix chains with increasing volume fraction of stars. Short (unentangled) matrix chains get slowed down by adding particles to the system. When the matrix chains become significantly longer than the entanglement length, this trend is inverted and the matrix chains become faster because the particles dilute the entanglement network. The center-of mass (CM) dynamics exhibits regimes of anomalous diffusion in accordance with viscoelastic hydrodynamic interactions (VHI) [1]. At low and intermediate star-particles concentration, the particles themselves vary little in mobility, only at high concentration (above percolation), they become slowed down because of colloidal packing. As a result, the viscosity as a measure of the collective mobility drops when adding few particles to the melt because of disentanglement, and at high particle volume fraction the viscosity increases again because of colloidal caging. [1] J. Farago et al. PRL 107, 178301 (2011); PRE 85, 051807 (2012).
ent morphologies analysed by UV-Vis spectroscopy, SAXS and TEM — •TILO SCHMUTZLER, TORBEN SCHINDLER, MARTIN SCHMIELE, and TOBIAS UNRUH — Friedrich-Alexander-University Erlangen-Nuernberg, Chair for Crystallography and Structural Physics, Staudtstrasse 3, 91058 Erlangen, Germany

An nanoparticles (NPs) have been the subject of widespread research in the last two decades. Therefore, numerous studies dealing with the synthesis leading to exact shape and size control were made. Applications are expected in biological imaging, drug delivery and phototherapeutics.[1]

Especially anisotropic Au NPs show interesting optical behaviour due to their ability to absorb light at different wavelengths for more than one surface plasmon resonance. Via a modified seed-mediated growth synthesis route for gold nanorods[1] we were able to synthesise a variety of morphologies of Au NPs with defined absorption bands (500-800 nm) in the UV-Vis spectrum and narrow distributions of the particle dimensions which could be determined by small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM).

The particle formation of Au nanorods in contrast to other morphologies like star-like nanoaggregates under different conditions (temperature, concentration of precursors, ...) was investigated by Vis-UV spectroscopy, SAXS and TEM to understand indirectly the formation mechanism of such particles.


BP 11.10 Mon 17:30 C 243
Local Chemical Characterization of Nanoporous Materials with Atom Probe Tomography — •CARSTEN NOWAK, PHILIPP SAUERBIEH, and BJÖRN PFEIFFER — Georg-August-Universität Göttingen, Institute for Materials Physics, Göttingen, Germany

Because of their high surface-to-volume-ratio and their chemical activity, nanoporous materials and nanoparticles often have a lot of interest in the areas of catalysis and electrochemistry. To obtain a detailed insight into reaction mechanisms, knowledge of the local chemical composition and structure, particularly at the surface of the material, is desirable.

Here we present experimental results on the local chemical characterization of nanoporous gold with atom probe tomography. The gold nanoparticles and with pore and ligament size of 50 nm, chosen as model system, is converted into a compact material by electron beam induced deposition of metalorganic precursors. Subsequently, the material is characterized with atom probe tomography which essentially is a combination of single molecule time of flight spectroscopy and atomic scale microscopy, thus allowing to characterize the local chemical composition of the filled material and particularly its former surface with sub-nanometer spatial resolution.

Although the preparation involves a chemical reaction of the surface with the precursor and thus alters the active surface of the nanoporous material, this approach offers the potential to detect chemical species at the surface of irregularly shaped nanoparticles with sub-monolayer sensitivity.
Interrelation of fluorescence and morphology of molecular aggregate structures — Mohammadmehraa Bahrami1, Tasham Bohamad1, Clemens Schindler1, Lukas Rathie2, Hannes Hartmann1, J.A.A.W. Elemans3, Ingo Barke1, and Sylvia Speller2 — 1University of Rostock, Institute of Physics, 18051 Rostock, Germany — 2Radboud University Nijmegen, Institute for Molecules and Materials, 6525 AJ Nijmegen, The Netherlands

Metallo-porphyrins are widespread in nature and act as a key component in photosynthesis as well as in oxygen transport in blood cells. They have attracted much attention in view of applications like molecular wires, fluorescence switches, and light-energy conversion [1]. We study the spatially resolved photoluminescence from Copper-based, porphyrin [2] aggregates as one of the deexcitation pathways of excitation. Among the different observed morphological motifs of the aggregates we here focus on branched strands with typical diameters of 50 - 100 nm. Fluorescence microscopy images show varying intensity along strands and junctions. In combination with atomic force microscopy we correlate fluorescence and structural properties to elaborate possible reasons of such morphology-dependent fluorescence. We further present fluorescence data on a composite system of silver nanostuctures in the vicinity of molecule aggregates, and address the role of these metal systems as local sources of electromagnetic fields.


Electric detection of ortho and para water in fullerene cages — Benno Meier, Salvatore Mamone, Javier Alonsovaldezueiro, Maria Concistrate, Andrea Krachialmicooff, Richard J. Whitty, and Malcolm H. Levitt — School of Chemistry, University of Southampton, SO17 1BJ Southampton, United Kingdom

Water, like molecular hydrogen, exhibits spin isomerism, a phenomenon in which the entanglement of spatial and spin states leads to ortho and para spin isomers with different symmetry. The physical properties and the interconversion of the two isomers of molecular hydrogen are central to fields as diverse as astrophysics and nuclear magnetic resonance, but much remains unknown about the different isomers of water, owing to the difficulty of separating the two isomers. Here, we use fullerene cages to provide freely rotating water molecules at cryogenic temperatures in the form of the supramolecular endofullerene H2O@C60. Unlike molecular hydrogen, water has an electric dipole moment and we show that the dielectric constant, a bulk property, that is linked to the spin states via their molecular polarizabilities, changes upon ortho-para conversion that is induced by a sudden temperature change. Our findings are in excellent agreement with previous NMR studies and suggest the possibility to detect and eventually manipulate H2O@C60 molecules selectively depending on the nuclear spin state of the comprised water molecule.

Effective mechanical properties of graphene obtained by computational mechanical tests — Markus A. Hartmann1, Melanie Todt2, and Franz G. Rammerstorfer2 — 1Institute of Physics, Montanuniversität Leoben, 8700 Leoben, Austria — 2LB, Vienna Institute of Technology, 1040 Vienna, Austria

Carbon nanostructures combine a high stiffness with low weight and an exceptional toughness making carbon a promising candidate for applications in structural mechanics. Understanding the mechanical properties of these structures on every length scale is of utmost importance to be able to exploit the full potential these materials. In the presented work the effective mechanical parameters of graphene are assessed that are the necessary input parameters for large scale finite element calculations. Of special interest is the "effective thickness" in combination with the "effective Young's modulus" of monolayer graphene. Potentials obtained by ab initio calculations [1] were used in subsequent Monte Carlo simulations to assess the effective mechanical properties of graphene [2]. The membrane stiffness and the bending stiffness (and consequently the effective thickness) of graphene were evaluated. The results showed that the elastic modulus as well as the Poisson ratio corresponds well to values known from literature. For structures too small the continuum approximation breaks down and the effective thickness decreases, while it attains a constant value of approximately 0.132 nm for structures larger than 5 nm.


When playing simple games humans sometimes fail to achieve maximization, often due to random events. Here I present a mathematical formalism describing behavior and change over time, some rules of which being formulated first by Darwin. We develop this concept of competing agents within finite populations which can reproduce far less than required for optimizing mean payo ot." Such behaviour has been attributed to accessory objectives or processes too small the continuum approximation breaks down and the effective thickness decreases, while it attains a constant value of approximately 0.132 nm for structures larger than 5 nm.
rate/death rate) as fitness. A special ‘gene setting’ passed to offspring determines a particle’s behavior in encounters. Following Dawkins, particles sharing the same gene setting (here called gene-relatives) should favor each other or exempt from harm in an encounter, but type one and type two errors hamper a correct behavioural decision. Inserting pay-off matrices characterizing aggression, altruism, co-operation or grouping into the formalism reveals, how the respective social particles’ frequency develops in domains with limited resources.

**BP 13: Posters: Imaging and Superresolution Optical Microscopy**

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

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**BP 13.1 Mon 17:30 Poster A**  
**Detecting rare Events for sure: Stitched Field-of-view Imaging on the Intelligent Programmable Array Microscope (iPAM)**  

Imaging rare events by confocal microscopy in populations of live cells requires a macroscopic field of view (FOV) of several millimeters in diameter. Standard laser scanning confocal microscopes or spinning disk systems are too slow to capture FOVs that large. Using the scripting capabilities of the driving software of our iPAM [1,2] we are able to seamlessly image regions of the size of 1 mm². The total FOV is subdivided into regular array of tiles corresponding to the size of the FOV of the microscope which depends on the number of pixels in the camera. Usually, the array is of the size of 30 x 30 where at each position a z stack of 10 to 30 images is recorded within a couple of seconds. The scripting facility of the iPAM allows us to record the images concurrent to the acquisition so that after a first scan of the total area only those tiles or retained where cells of interest have been detected. As sample application we discuss the recording of UV-triggered protein transport from the endoplasmatic reticulum to the Golgi apparatus.


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**BP 13.2 Mon 17:30 Poster A**  
**Wide Field Detection and Imaging of Atomic Spins using Nitrogen-Vacancy Centers**  
—FLORENTAN ZIEM, PHILIPP SCHEIER, HELMUT FEDDER, and JÖRG WRACHTRUP — Physicalisches Institut und SCoPE, Universität Stuttgart

Electron and nuclear magnetic resonance provide information ranging from composition over structure to function of diverse samples in material and life sciences, as well as medical diagnostics. Applied at micro- and nanoscale dimensions, these technique provide label-free imaging and eventually single molecule analysis, e.g. revealing the structure of proteins or membrane channel mechanisms. Traditional induction based magnetic resonance sensing schemes are blind to such vanishing conditions by optically detected magnetic resonance. In a wide field microscope, parallel magnetic detection and imaging on the microscale are demonstrated.


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**BP 13.3 Mon 17:30 Poster A**  
**X-ray waveguide optics for nanoscale phase contrast tomography**  
—MARTIN KRENZEL, ANDREAS KREUSCH, MATTHIAS BARTELS¹, CHRISTIAN DULIN², FRANKE ALVES², and TIM SALDITT³ — ¹Institute for x-ray physics, University Göttingen, Germany — ²University Medical Center, Göttingen, Germany

We use propagation based hard x-ray phase contrast tomography to explore the three dimensional structure of soft biological tissues from the organ down to sub-cellular level. As in classical absorption tomography nano-scale structures only barely absorb the radiation, the much stronger phase shift can be used to enhance the contrast.

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**BP 13.4 Mon 17:30 Poster A**  
**Calibration of the diffusion coefficients of the FCS standard Rhodamine 6G in aqueous solutions**  
—GÜNTER MAJER — Max Planck Institute for Intelligent Systems, Stuttgart, Germany

Precise diffusion measurements of rhodamine 6G (R6G) dissolved in D₂O at various concentrations were carried out in the temperature range from 280 to 320 K using pulsed field gradient nuclear magnetic resonance (PFG-NMR). For the diffusion studies at low R6G concentrations, a water suppression PFG-NMR sequence was applied. The temperature and concentration dependent diffusion coefficients of R6G can be used as calibration references in fluorescence correlation spectroscopy (FCS). Besides measuring the diffusivity of R6G, the diffusion coefficient of the solvent in the same system could be determined in parallel by PFG-NMR as the resonances of water and R6G are well separated in the ¹H NMR spectrum. The isotope effect of the solvent on the diffusion coefficient is determined by FCS measurements on R6G dissolved in both D₂O and H₂O.

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**BP 13.5 Mon 17:30 Poster A**  
**Probing the intracellular pH in magnetotactic bacteria**  
—ERIKA GÜNTHER, MATHIEU BENNET, and DAMIEN FAIVRE — Max Planck Institute of Colloids and Interfaces, Biomaterials, Potsdam, Germany

Magnetotactic bacteria are microorganisms that possess encapsulated biomagnetised magnetite nanoparticles (magnetosomes) to navigate along the geomagnetic field lines. The formation of magnetite nanoparticles typically requires iron concentrations (200 µM) and pHs (pH > 8) that are toxic to cells. In order to understand how magnetotactic bacteria biomagnetise iron nanoparticles in physiological conditions, we aim at measuring their intracellular chemical properties using ratiometric fluorescence microscopy and fluorescence lifetime imaging microscopy. We have measured the intracellular pH in living Magnetospirillum magnetotacticum MSR-1 cells using confocal laser scanning microscopy. From these measurements, we conclude that the biomagnetisation of iron nanoparticles in XTB does not result in the presence of a non-physiological cytoplasmic pH. Magnetotactic bacteria buffer their intracellular pH to pH 7.0 ± 0.25 when exposed to a range of extracellular from pH 6.5 to pH 7.5. We will present the strategy that we are adopting to measure the chemical potential in the cytoplasm and discuss the possibility of better spatially resolving our measurements in order to gain insight into the chemical conditions in the magnetosomes.

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**BP 13.6 Mon 17:30 Poster A**  
**Embedding of flagellate Trypanosoma brucei for single-molecule microscopy**  
—MARCUS GLOCKS², SIMONE STICKLEBE², JÖRG TESSMAR², JÜGGEN GHOHL², MARCUS ENCOTTER³, and SUSANNE FENZ² — ¹Biocenter: Cell and Developmental Biology, University of Würzburg, Würzburg, Germany — ²Department of Functional Materials in Medicine and Dentistry, University of Würzburg, Würzburg, Germany
The unflagellate protozoa Trypanosoma brucei are the causal agents of African sleeping sickness. High-resolution microscopy of trypanosomes in vivo is challenging due to the high motility of the parasite. Here, we present an approach for complete cell immobilization suitable for single-molecule fluorescence microscopy (SMM) techniques. Immobilization of trypanosomes requires both efficient trapping to prevent cell motility and mild embedding conditions to ensure cell viability. Biopolymers like agarose or gelatine were used before to immobilize cells sufficiently for fluorescence recovery after photobleaching studies in vivo. However, complete inhibition of the flagellar beat was not achieved. Hence, novel gels are needed for sophisticated SMM methods, which generate a high spatial accuracy. We use modified hyaluronic acid and a crosslinking reagent to generate gels that solidify quickly upon UV-illumination. The rigidity of these hydrogels can be adjusted easily to guarantee complete immobilization of cellular movement. At the same time we verify cell viability using a fluorescent marker. We aim to transfer our results on trypanosomes to flagellates in general.

**BP 13.7 Mon 17:30 Poster A**


1. Department of Chemistry, University of Basel, Switzerland — 2Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — 3Paul Scherrer Institut, Villigen, Switzerland — 4Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — 5Division of Molecular Biology, Institute of Molecular Biology, University of Zagreb, Croatia

Meiosis is a fundamental process in all eukaryotes leading to genetic diversity, but its details and the mechanism of homologous chromosome recombination is still poorly understood. Currently, there are no data on the change in total length and shape that chromatid undergoes during the oscillations before condensation into chromosomes. We employ a combined coherent scanning transmission X-ray microscopy (STXM) and ptychography setup, which allows us to investigate the dynamics of nuclear oscillations during meiosis of fusion yeast Schizosaccharomyces pombe. We show that the combination of STXM and ptychography is an extraordinary tool to image living yeast cells during nuclear oscillation without additional labeling down to the submicron scale. Therefore we can analyze the chromatin compaction, mutual alignment of chromosomes and its impact on the recombination in eukaryotes on the relevant length scales of 30 to 100 nm.

**BP 13.8 Mon 17:30 Poster A**

**Photothermal Detection and Correlation Spectroscopy of Single Gold Nanoparticles in Living Cells** — Romy Schröder, Alice Arend, and Frank Cichos — Molecular Nanophotonics Group, Universität Leipzig, Linsende. 5, 04103 Leipzig

For better insights into complex cellular processes fluorescence microscopy on the single molecule level has gained large importance. As this technique relies on emission processes, it is restricted to fluorescing species allowing even the detection of single molecules. The technique employs the conversion of optical energy into heat by an absorbing species and non invasive, we recently started to locally change the physical properties of special cell sites and to manipulate the behavior of the cells.

**BP 13.9 Mon 17:30 Poster A**

**All-optical realization of optical diffraction tomography** — Mirjam Schümann, Paul Müller, Moritz Kreyssig, and Jochen Guck. 1 — 1Biotechnology Center, TU-Dresden, Tatzberg 47/49, 01307 Dresden, Germany — 2Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany

Quantitative phase microscopy is an established marker-free imaging technique for biological cells. Several studies have demonstrated the refractive index (RI) to be a conclusive measure for cellular alterations e.g. due to infection or during differentiation. A 2D mean RI map of a cell can be determined from a phase map if the cell shape is known. However, imaging cells from only one direction leads to a mixed contribution of all cellular components to the measured phase. This prevents an assignment of an RI to individual cellular organelles. Rotating the sample for tomographic imaging can overcome this problem. Here, we present the experimental realization of a contact-free rotation of individual suspended spatially confined cells in combination with digital holographic microscopy (DHM) for quantitative phase imaging at each of the rotational positions. The rotation is implemented in a dual-beam laser trap. A spatial light modulator (SLM) is used to control the orientation of the LP11 output fiber mode of one of the trapping fibers which leads to a subsequent controlled orientation of the cell. The gathered data can be combined to a 3D RI map of the cell using optical diffraction tomography (ODT). This all-optical demonstration of ODT opens the door to many applications in basic biology and biotechnology.

**BP 13.10 Mon 17:30 Poster A**


We present two implementations of Dykstra’s projection algorithm on GPU-based statistical multi-resolution estimators for image reconstruction. The incomplete Dykstra’s algorithm (ICD) is the central step in statistical multi-resolution (SMR) methods (Frick, Marnitz, and Munk, 2012 and 2013) which are a recent development for the deconvolution of noisy images. Unlike other methods its primary parameter is the confidence level with which the reconstruction is considered as valid. Compared with a CPU our CUDA implementation of the standard Dykstra algorithm (SDA) is one order of magnitude faster. For a further speedup we have developed a new variant, which we call incomplete Dykstra’s algorithm (ICD). Implemented in CUDA it yields an additional speedup of one order of magnitude over the CUDA version of SDA. As sample application we discuss pre-processing super-resolution optical fluctuation imaging (SOFI) methods (Dertinger et al., 2009) by ICD. Our results show that a careful parallelization of Dykstra’s algorithm enables its use in large-scale statistical multi-resolution analysis.

**BP 13.11 Mon 17:30 Poster A**

**Localization Precision in Stepwise Photobleaching Experiments** — Ingrid Schönhoff, and VH Zahn, Zurich, Switzerland

The precise determination of the position of fluorescent labels is essential for the quantitative study of biomolecular structures by various localization microscopy techniques. Localization by stepwise photobleaching is especially suited for measuring nanometer-scale distances between two labels; however, the precision of this method has remained elusive. Here, we show that shot noise from other emitters and error propagation compromise the localization precision in stepwise photobleaching. Incorporation of point spread function-shaped shot noise into the variance term in the Fisher matrix yielded fundamental limits for the localization precision. Global fitting of all images was also governed by error propagation, but made optimal use of the available information. The precision of individual distance measurements strongly depended critically on the exact bleaching kinetics and was therefore not quantified by the CRLBs. The methods presented here provide a consistent framework for quantitatively analyzing stepwise photobleaching experiments and shed light on the localization precision in some other bleaching- or blinking-assisted techniques.
SIM microscopy to investigate lipofuscin granules in retinal pigment epithelial cells — FLORIAN SCHOCK, GERHARD BEST, NIL CELIK, ALENA BAKULINA, SADEDDIN SEL, UDÖ BIRK, RAJENDRAN HEITZMANN, JUERGEN HESSER, STEFAN DITHMER, and CHRISTOPH CHERNER — KIT Institute for Physics, University of Heidelberg — Department of Ophthalmology, University-Hospital Heidelberg — Institute of Molecular Biology, University of Mainz — Institute of Pharmacy and Molecular Biotechnology, University of Heidelberg — Experimental Radiation Oncology, University Medical Center Mannheim, University of Heidelberg — Institute for Physical Chemistry and Abbe Center of Photonics, University of Jena — Leibniz Institute of Photonic Technology — Department of Ophthalmology, Hospital Wiesbaden — Institute for Scientific Computation, University of Heidelberg — Randall Division of Cell & Molecular Biophysics, King’s College London

Age related macular degeneration, the main cause for legal blindness in industrial countries, is accompanied by accumulation of lipofuscin granules inside the retinal pigment epithelial cells (RPE cells). Here we demonstrate that the super-resolution techniques “Structured Illumination Microscopy” (SIM) is able to resolve up to over 100 granules inside single cells and compare these results with other microscopy techniques. In addition, we introduce an algorithm to automatically identify, separate and characterise the granules, and present first super-resolution images on spectral discrimination of lipofuscin granules and intra-granular regions.

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SOFI algorithms [1] are based on the observation that a higher order statistical analysis of a time series may be utilized for generating super-resolved images by computing per-pixel auto-cumulants, e.g. of a fluorescence signal. As the effectiveness of SOFI has been accepted in the microscopy community, our focus is on the speedup due to a careful design of a parallel implementation on current multi- and many-core computer architectures. In addition, we present robust, single-pass algorithms suitable for an adaptive computation of the final SOFI image in case of large-scale data analysis where the usual two-pass algorithms are unfeasible. We compare the performance on different parallelization frameworks, in particular Intel’s threading building blocks, Qt’s QThreads, CUDA and OpenCl. For the CUDA implementation we use our SciPAL library [2,3].


BP 13.13 Mon 17:30 Poster A Improvements for Stochastic Optical Fluctuation Imaging (SOFI): Sub-pixel super-resolution images with a conventional wide-field microscope — SIMON CHRISTOPH STREN, ANJA HUSS, and JÖRG ENDERLEIN — Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Deutschland

The last decade has seen a rapid evolution of a wide array of new super-resolution microscopy techniques which are by now widely available and applied in the life sciences. Among these different techniques, super-resolution optical fluctuation imaging (SOFI) stands out due to its algorithmic and experimental simplicity, requiring only the rapid recording, with a conventional wide-field setup, of the intensity fluctuations from a sample which is labeled with blinking emitters.

Further we show how an estimate for the PSF of an optical system can be extracted from the raw movie of fluctuating emitters. The knowledge about the PSF is used for post-processing deconvolution, enhancing the quality of SOFI images.

BP 13.14 Mon 17:30 Poster A Frequency modulated signal transmission in neurons — TIM HERFURTH and TATYANA TCHUMATCHENKO — Max Planck Institute for Brain Research, Max-von-Laue-Str. 4, 60438 Frankfurt/Main

During information/signal processing in neural networks aside from the actual signal background activity is always present and is commonly denoted as noise. Mechanisms of neural coding and decoding have to account for that and still reliably transmit information within the network. Traditionally, spontaneous synaptic and background activity are unfeasible. We compare the performance on different parallelization frameworks, in particular Intel’s threading building blocks, Qt’s QThreads, CUDA and OpenCl. For the CUDA implementation we use our SciPAL library [2,3].


BP 14.1 Mon 17:30 Poster A Activity propagation in feed-forward neuronal networks described by reaction-diffusion like equations — DMITRE GVTSKVY, MARKUS DIEHMS, and MOHITZ HELIA — INM66kIAS, Juelich Research Centre and JARA, Jülich, Germany

We investigate feed-forward neuronal networks of linear-nonlinear rate neurons with synaptic plasticity. For systems without plasticity or near to criticality, layers can be mapped onto states in time. We treat the critical border separating ultimately decaying activity from possible activity explosion. On the border (requiring exact parameter tuning) and in its subcritical vicinity we analytically find long-living dissipative solitons with a plateau of arbitrary width with the decay velocity proportional to the distance to criticality. Two bumps can unite or remain disjoint within their lifetime depending on the distance in-between. For the united bump the same scenarios exist, so a kind of association tree can appear in this way.

Partially supported by the Helmholtz Association: HSB and portfolio theme SMHB, the Jülich Aachen Research Alliance (JARA), HGF Nachwuchsgruppe; VH-NG-1028, the Next-Generation Supercomputer Project of MEXT, and EU Grant 269921 (BrainScales).

BP 14.2 Mon 17:30 Poster A Activity propagation in feed-forward neuronal networks described by reaction-diffusion like equations — DMITRE GVTSKVY, MARKUS DIEHMS, and MOHITZ HELIA — INM66kIAS, Juelich Research Centre and JARA, Jülich, Germany

We investigate feed-forward neuronal networks of linear-nonlinear rate neurons with synaptic plasticity. For systems without plasticity or near to criticality, layers can be mapped onto states in time. We treat the critical border separating ultimately decaying activity from possible activity explosion. On the border (requiring exact parameter tuning) and in its subcritical vicinity we analytically find long-living dissipative solitons with a plateau of arbitrary width with the decay velocity proportional to the distance to criticality. Two bumps can unite or remain disjoint within their lifetime depending on the distance in-between. For the united bump the same scenarios exist, so a kind of association tree can appear in this way.

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Stochastic thermodynamics of biological information processing — Manuela Schröder and U. Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

We consider the stochastic thermodynamics of neural information processing in the presence of noise. Defining what we mean by noise in this problem is non-trivial, since it inevitably requires the definition of a signal, which is often hard to identify in neural systems. We therefore turn to general information theoretic measures to describe neural information processing, motivated by the fact that neurons in different organisms from fruit flies to primates display strikingly similar values for several of these parameters. This allows us to neglect the precise form of stimulus and response. Our focus is on single neurons, given the strong evidence for the impact of individual neurons on a behavioural level even in complex nervous systems, e.g. in perceptual decisions of primates.

Here we apply recent results in the theory of small systems [1], specifically at the boundary to information theory [2], to gain a better understanding of both the principles underlying the generality of neural properties and the limits that the inherent stochasticity of neural hardware places on computational strategies in the brain.

The network under study is comprised of three subnetworks of either excitatory or inhibitory leaky integrate-and-fire neurons. The excitatory and inhibitory weights are arranged to establish and maintain a balance between excitation and inhibition for a constant external drive. Each subnetwork has a random connectivity with fixed in-degree and fixed out-degree for all neurons belonging to a particular population. Neurons in different subnetworks are also randomly connected with the same probability; however, depending on their identity, the connection weight is scaled by a factor. We observed that for a certain regime of ratios of the “within” versus “between” connection weights (bifurcation parameter), the network activation spontaneously switches between the two subnetworks of the same identity (winnerless competition).

In our model, this phenomenon is explained by a set of coupled stochastic differential equations of Lotka-Volterra type that exhibit a competition between the subnetworks. The deterministic phase portrait is characterized by two attractors and a saddle node, its stochastic component is essentially given by the multiplicative inherent noise of the system.

Supported by the German Ministry of Education and Research (BFNT Freiburg*Tübingen, grant 01GQ0830) and the German Research Foundation (DFG, grant EXC 1086).

### BP 14.10 Mon 17:30 Poster A

**Neuronal avalanches in a self organizing recurrent neural network**

—Bruno Del Papa, Viola Freyemann, and Jochen Trischl

1. Frankfurt Institute for Advanced Studies
2. Max Planck Institute for Brain Research
3. Max Planck Institute for Dynamics and Self-Organization

A large number of experiments have suggested that the brain operates close to criticality, but in a subcritical regime, based on power-law distributions of neuronal avalanches. Although several critical neural network models have been studied before, they typically show simplified connectivity structures and no advanced information processing or learning abilities. Here, we investigate neuronal avalanches in spontaneous activity of a self-organizing recurrent neural network (SORN), which exhibits spatio-temporal pattern learning and reproduces experimentally observed fluctuations of synaptic efficacies. The network consists of excitatory and inhibitory threshold units with connection weights and firing thresholds evolving based on a combination of spike-timing dependent plasticity rules and homeostatic mechanisms. We observe power-law distributed neuronal avalanches, suggesting that the SORN self-organizes to a critical state, and find a strong dependence on the neurons’ target firing rates and membrane potential noise, which indicates these are essential to maintain the critical phase. Our results show, for the first time, that signatures of criticality are present in the spontaneous activity of a self-organizing network model that has advanced learning abilities and reproduces central findings on the fluctuations of synaptic connection strengths in cortex and hippocampus.

### BP 14.11 Mon 17:30 Poster A

**Spectral properties of excitatory systems subject to colored noise**

—Jannis Schuecker, Markus Diesmann, and Moritz Helias

1. Institute of Neuroscience and Medicine (INM-6) and Institute for Advanced Simulation (IAS-6), Jülich Research Centre
2. Medical Faculty, RWTH Aachen University

Many phenomena in nature are described by excitatory systems driven by colored noise. Studying the response properties of these systems comes along with considerable difficulties, due to the non-vanishing correlation time of the noise. For systems with noise fast compared to their intrinsic time scale, we here present a general method of reduction to a lower dimensional effective system, respecting the details of the noise in the boundary conditions. Static boundary conditions were derived earlier by a perturbative treatment of the arising boundary layer problem [1,2]. Here we extend this scheme to the dynamic case [3]. We apply the formalism to the leaky integrate-and-fire neuron model, revealing an analytical expression for the transfer function valid up to moderate frequencies. This enables the assessment of the stability of networks of these excitatory units.


Partial support by Helmholtz Association: Young investigator group VH-NG-1028 and portfolio theme SMIB; Jülich Aachen Research Alliance (JARA), EU Grant 269921 (BrainScales), EU Grant 604102 (Human Brain Project, HBP).

### BP 15.1 Mon 17:30 Poster A

**GPU accelerated simulation of light propagation through retinal volumes mapped by multi-photon microscopy**

—Martin Weigert, Alfonso Garcia-Ulloa, Heike Petzold

1. Kaiserslautern, Germany
2. Subramanian, Eugene Myers, and Moritz Kreyling
3. Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

The architecture of photoreceptor cells (PRC) nuclei differs considerably between nocturnal and diurnal mammals: whereas diurnal mammals possess conventional PRC nuclei, nocturnal mammals show a uniquely inverted PRC architecture characterized by the compaction of dense heterochromatin in the nuclear center. As the refractive index increases with molecular density, this nuclear inversion was suggested to reduce light scattering as inferred by 2D simulation, and direct measurement on individual isolated nuclei.

Here we show how a beam propagation method implemented on GPU accelerators can considerably speed up these calculations and allows for simulating the propagation of light through realistically large 3D retinal volumes. This way we studied the evolution of the angular spectrum of light on its way through a 3D model of the outer nuclear layer, which we obtained from multi-photon microscopy. We found that the near field coupling between cell nuclei of inverted architecture leads indeed to an overall reduction in scattering, as opposed to an absolute summation of the individual cell scattering contributions.

### BP 15.2 Mon 17:30 Poster A

**Osmolarity mediated growth of MDCK cell model tissue**

—Damir Vurnek, Sasa Kaliman, Carina Wollnik

1. Theoretical Physics 1, FAU Erlangen
2. 3rd institute Physics-Biophysics, Georg-August University, Göttingen

The capacity to adapt to changes in environmental osmotic conditions is vital for the functioning of epithelium. We study this response by growing MDCK II model tissues, mm² to cm² sized clusters, with increased concentrations of mannitol, urea or NaCl. The phase space of tissue viability is characterized from isotonic to elevated toxic conditions. In young colonies, elevated osmotic conditions suppress the growth. With increasing age, adaptation takes place, and the colony develops the same morphology as the controls, with the edge at low osmolarity.
and the center at relatively high densities. We characterize the osmolality/concentration specific proliferation rates, absolute colony sizes, as well as the steady state cell densities. Finally, the internal structure of the cells within the colony is addressed. Even in the intermediate stages of growth DNA damage is evident on the nuclei near the colony edge, however it lacks in the dense bulk of the tissue. Here, two factors could be intertwined. With densification, decreasing apical and basal surfaces expose less cell membrane to the hostile surrounding and/or the proliferating edge is more prone to damage during the cell cycle. As tissue reaches adaptation, high osmolality brings added features to tissue cooperativity and nuclei elongations show differences in the stress forces for different applied osmolites.

BP 15.3 Mon 17:30 Poster A Transporting Dpp in the fly wing: A theoretical analysis.

- Daniel Aguilar-Hidalgo¹, Maria Romanova-Michaelid², Marcos González-Gaitán², and Frank Jülicher³
- ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²University of Geneva, Department of Biochemistry, Sciences II, Quai Ernest-Ansermet 30 1211, Geneva 4, Switzerland

Morphogens are signaling molecules, which are locally secreted and spread in a tissue, where they form graded concentration profiles. Such profiles can provide positional information to the tissue cells, or can act as modules of biological function within the cell. Here we present a theoretical study about the mechanisms by which morphogens are transported in a tissue are still a matter of debate. We study the dynamics of the morphogen Decapentaplegic (Dpp) in the developing fly wing. Dpp is secreted from a stripe of cells situated at the anterior-posterior compartment boundary of the wing imaginal disc, and spreads to both anterior and posterior targets. I will discuss the dynamical properties of Dpp for Dpp in the wing: (i) a model of effective diffusion by tranctycosis and (ii) a model of free diffusion with internalization. This analysis reveals key dynamical differences if endocytosis is perturbed. This could allow distinguishing possible transport mechanisms in experiments using fluorescence recovery after photobleaching (FRAP) techniques and temperature sensitive dynamics mutants.

BP 15.4 Mon 17:30 Poster A Diffusion and bulk flow in phloem loading - a theoretical study of the polymer trap mechanism in plants

- Hanna Rademaker¹, Julia Döger², Jan Johannes Liesche³, Alexander Schülz⁴, and Tomas Bohr¹
- ¹Technical University of Denmark — ²University of Copenhagen, Denmark — ³Technische Universität Darmstadt, Germany

Plants photosynthesize sugars for storage and growth inside the mesophyll cells of their leaves. In order to distribute them, the sugars are loaded into the phloem vascular system. The osmotic uptake of water increases the pressure in the phloem cells, which then drives the bulk flow throughout the plant, according to the "Münch mechanism" (1930), it is studied one special loading mechanism, the so-called "polymer trap", in which sucrose is believed to diffuse from the mesophyll into the phloem via small symplasmic channels, called plasmodesmata (PDs). Sucrose is then partly converted into larger sugar molecules, which are unable to diffuse back through the narrow PDs. One major concern about this hypothesis was, if sucrose was still able to be transported in sufficient quantity, while molecules less than 20% larger should be completely blocked. Our theoretical study [Döger et al., Physical Review E 90, 042704, (2014)] shows, that the polymer trap mechanism can in principle function, and that not only diffusion, but also bulk flow, could be involved in the loading mechanism itself, making it more efficient. We now focusing on experiments, both in plants and in microfluidic devices, testing our theoretical predictions about the symplasmic uptake of water into the phloem.

BP 15.5 Mon 17:30 Poster A Mechanics of Zebrafish doming

- Martin Bock¹, Hitoshi Morita², Carin Philipp Heisenberg², and Guillaume Salbreux³
- ¹MPI-PKS, Dresden, Germany — ²ISTA, Klosterneuburg, Austria

On the timescale of embryo development, cell rearrangements can allow for stress relaxation so that the tissue may behave as a fluid-like material. Accordingly, surface tensions and tissue flow are essential to understand the establishment of the shape of organisms. Here we ask how flows during Zebrafish dome formation can be understood quantitatively by describing the mechanical tissue response. We use the dadumus, a 3D sheet of cells, while the remaining 75% comprise the nourishing, bag-like yolk. The two of them juxtapose in such a way that the overall embryo shape is approximately spherical. During the subsequent doming process, the blastoderm thins and starts to spread over the yolk, whereas the yolk bulges upwards into the blastoderm, in a characteristic dome-like shape.

In my presentation, I will describe a physical model of dome formation incorporating surface tensions and bulk stresses, and compare our predictions to experimental data on wildtype embryos and mutants with partially defective doming.

BP 15.6 Mon 17:30 Poster A Analyzing cellular arrangements and shapes in Caenorhabditis elegans

- Rolf Fickentscher, Philipp Struntz, and Matthias Weiss — Experimentalphysik I, Universität Bayreuth

Recent developments in lightsheet fluorescence microscopy enable rapid and gentle in toto imaging of living specimen. Three-dimensional image series with a high spatiotemporal resolution can be acquired over extended periods of time. We utilize these advantages to investigate mechanical cues in the early embryogenesis of the small nematode Caenorhabditis elegans by imaging embryos with fluorescently labeled nuclei or plasma membranes [1]. Tracking nuclei yields information about processes that drive cellular arrangements during early development, whereas the segmentation of whole cells provides additional knowledge on shape controlling mechanisms throughout the cell cycle. We have developed new techniques by which hundreds long-term time-lapse recordings of different cell types can be performed. The observed deviations are small, hence indicating a robust cellular arrangement process. A simple mechanical model reveals that early cell organization is crucially determined by the cells’ quest for a position with least repulsive interactions. This passive process is superimposed by active shape control, i.e., cell rounding can be observed for all cells at the onset of mitosis. Furthermore, we show that incomplete round- ing correlates with the orientation of cell division axes.


BP 15.7 Mon 17:30 Poster A Growth Dynamics of MDCK II Clusters on Elastic Substrates

- Philipp Link², Carina Wolfin², Sara Kalman³, Damir Vunrek⁴, Ana-Suncana Smith⁵, and Florian Rehfeld³

- ¹Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — ²Institute for Theoretical Physics and Cluster of Excellence: Engineering of Advanced Materials, University Erlangen-Nürnberg, Germany

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

MDCK II cells have proven to be very useful as model system for endothelial morphogenesis. When growing on a flat surface, these cells form a monolayer and maintain the morphology of monolayer for a short time. Short we found in our studies that clusters show a different growth behavior when cultured on PA gels with varied stiffness. The formation dynamics of these structures is controlled by cellular contractility and the balance of cell-cell and cell-matrix contacts. To create wound healing essays we seed the cells in culture inserts from ibidi, which are placed directly onto the collagen coated gels. We are using the open source software Micro Manager in combination with a motorized xy-stage and a heating and CO2 incubation system to do parallel live cell microscopy of several clusters in statistically equivalent, physiological conditions.

BP 15.8 Mon 17:30 Poster A SPIM applications in organismal biology

- Philipp Struntz, Rolf Fickentscher, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Fluorescence imaging is the method of choice when aiming at monitoring dynamic phenomena during embryogenesis. Yet, standard techniques like confocal imaging suffer from inducing a considerable amount of photobleaching and phototoxicity, especially under high spatio-temporal resolution conditions. Using our SPIM setup, we have quantified cell movement and arrangement during early embryogenesis. Moreover, we have performed fluorescence correlation spectroscopy measurements (SPIM-FCS) on zygotes of C.
elegans that expressed GFP-tagged PIE-1 and PLCdelta1. While the former reports on local diffusion properties during a vital protein condensation phenomenon, the latter series of experiments has probed the diffusional mobility of a vital peripheral membrane protein. Our data show that SPIM provides a versatile tool to explore embryonic events on several length scales, i.e. it is hence well suited to examine dynamic pattern formation in organismal biology.


BP 15.9 Mon 17:30 Poster A A computational model of tumor growth based on large scale vascular networks — MICHAEL WELTER, 1,2 THIERRY FRIEDRICH, 1,2 HEIKO RIEGER, 1,2 and HERBERT RINNEBERG 1,2 — 1Saarland University — 2PTB Berlin

The process of tumor growth is very complex. Even today it is hard to predict the outcome of the disease and the effect of various therapies. Theoretical simulations can help to make such predictions and allow tailoring the therapy to patient specific microenvironments such as the blood vessel network.

On the way we consider, the creation of a healthy host vessel system by stochastic growth of a hierarchical arteriovenous network (described in [1]) as starting point. Parameters can be adjusted to yield networks with global properties similar to histological vascular volume and perfusion, which agree very well with data from real tissue. We treat the bulk of tumor cells with a continuum approach following [2] and consider vessels as linealike sources or sinks for nutrients, coupled to the tissue layer via some transvascular flux.

Interstitial fluid flow, for example, is a key element of chemotherapy, however not yet fully understood. The locally available nutrients play another important role in cancer proliferation. We investigate those aspects using a model [3] inspired by morphological data from human melanoma and breast tumors. We were able to quantitatively reproduce IR mammography data [4] showing the oxygen content of breast carcinomas in vivo.


BP 15.10 Mon 17:30 Poster A A Mechanistic model of carcinogenesis: Radiation-induced risk of lung cancer in the Mayak workers — SASHA ZÖLLNER, 1 MIKHAIL SOKOLNIKOV, 2 and MARKUS EIDEMÜLLER 1 — 1Helmholtz Zentrum München, Institute of Radiation Protection (Germany) — 2Southern Urals Biophysics Institute, Ozyorsk (Russia)

Mechanistic multi-stage models are used to analyze lung-cancer mortality after Plutonium exposure in the Mayak-workers cohort. Besides the established two-stage model with clonal expansion, models with three mutation stages as well as a model with two distinct pathways to cancer are studied. The results suggest that three-stage models offer an improved description of the data. The best-fitting models point to a mechanism where radiation increases the rate of clonal expansion. This is interpreted in terms of changes in cell-cycle control mediated by bystander signaling or repopulation following cell killing. To elucidate the implications of the different models for radiation risk, several exposure scenarios are studied. Models with a radiation effect at an early stage show a delayed response and a pronounced drop-off with older ages at exposure. Moreover, the dose-response relationship is strongly nonlinear, revealing a marked increase above a critical dose.

BP 15.11 Mon 17:30 Poster A Investigating the influence of Keratin/Vimentin on the invasive behavior of epithelial cells — PAUL HEINE and JOSEF KAS — Soft Matter Physics (PMW), Leipzig University, Germany

During tumor development epithelial cells undergo a remarkable carcinogenic transition to a mesenchymal phenotype. This Epithelial-Mesenchymal Transition (EMT) facilitates a variety of mechanical and biochemical changes within the affected cells which produces drastic changes in their cell polarity, cell-cell adhesion, migratory and invasive properties. Some of the key components of this conversion were identified to be the intermediate filaments Keratin and Vimentin. While the remodeling of these cytoskeletal components has been partially understood, their complex relationships has not been thoroughly investigated. We aim to classify the significance of Vimentin as a counter-acting factor to Keratin in the invasiveness and metastatic potential. An investigation of the migratory, proliferative and invasive behavior of epithelial cells in constricting channels and with a variety of modulations to their intermediate filament cytoskeleton should produce vital insights for understanding metastatic initiation.

BP 15.12 Mon 17:30 Poster A Glassy Dynamics in a Receptor Dynamics Model for Tumorogenesis — YUTING LOU and YU CHEN — SCS Lab, Department of Human and Environmental Engineering, Graduate School of Frontier Science,University of Tokyo, Tokyo, Japan

A multi-cell receptor dynamics model for tumorigenesis is built for investigating the diversity of homeostasis and the origin of abnormal pre-neoplastic dynamics from a systematitical perspective. Our simulations of cells growth and wound healing show the homeostasis state presents rich glassy dynamics such as diverse relaxation patterns from a wound perturbation, a large spectrum of relaxation timescale for reaching cell density asymptote, and ergodicity breaking. The origin of the homeostatic diversity lies in these glassy dynamics whose characteristic timescales differs. Several parameters have been studied and the ability of cell arrest was found to be the role of control factor deciding the scale of the process. The size scale of the cell mass increase with the time scale of relaxation within which all cells reach its arrest state.Another simulation with the mechanism of genetic deficiency newly added to the receptor dynamics model, found that mutations help extend this scale in a normal homeostatic process. This dependency helps render a hypothesis: cancer happens when the system is undergoing glass transition where the relaxation time goes to infinity in terms of our observation timescale. This draw a unified picture for the initiation of benign tum and cancer, and also explains the reason why these diseases feature long latency before exploding as well as the large spectrum of periods before they relapse.
ton. In vivo, platelets function in a variety of mechanical environments ranging from soft to stiff tissues. The mechanical response of platelets to such different environments is still elusive. Hence, we investigate the spreading dynamics of single platelets on elastic (Es in the physiological range of 1-100 kPa) polyacrylamide (PAA) gels. We observe that the changes in their spreading profiles result in different values of Es in the most pronounced sensitivity to stiffness lies below 40 kPa. The time-dependent platelet spread area curves on soft substrates show various irregular spreading profiles, which we classify as monotonic, non-monotonic and damped oscillatory, whereas the spreading profiles on the stiff substrates are majorly regular and monotonic. We present an elastic theory, which predicts that these different spreading profiles of platelets arise due to the different timescales of the myosin activity response. We characterize the spreading by analyzing the temporal evolution of the spread area and perimeter and aim at building a mechanical model for platelet dynamics on a single-cell level.

**BP 16.3 Mon 17:30 Poster A Growth-induced pressure of yeast populations — Jörn Hartung1, Morgan Delarue2, and Öskar Hallatschke1,2, 1MPI DS, Göttingen, Germany — 2UC Berkeley, CA, USA

Confined cells exert forces onto their surroundings during proliferation [1]. On the one hand these forces can redesign the population’s microenvironment. In the case of microorganisms, this can lead to biofilm formation [2]. On the other hand these growth-induced forces imply a feedback onto the growing cells themselves, which can alter their morphology [3].

We designed a microfluidic device, which enables us to measure the growth-induced pressure confined S. cerevisiae populations exert onto a deformable PDMS membrane. Furthermore, we are able to control the chemical as well as the mechanical conditions the populations experience by employing nutrient channels and passive valves with different degrees of confinement, which we designed. The cells are subject to growth-induced steady state pressures ranging from 0.1 to 1.0 MPa.


**BP 16.4 Mon 17:30 Poster A Spreading and force generation of blood platelet dynamics on soft and structured substrates — Jana Hanke, Rabia Sandmann, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

Blood platelets play a crucial role in wound closure by attaching to the wounded site and spreading over it to form a temporary seal. Not only do they encounter wounded sites of different stiffness and topography, they also are the first cells to get in contact with (nanostructured) implants. To examine the influence of these cues, we performed live cell experiments on soft substrates and on substrates containing micrometer sized holes. By comparing spreading dynamics on microstructured and on flat substrates, we show that although the final spread area is different sized holes. By comparing spreading dynamics on microstructured and on flat substrates, we show that although the final spread area is controlled, we show that although the final spread area is smaller than on other cells that have been studied so far by TFM, it is important adjust both the experimental set-up as well as the analysis. To this end, the imaging resolution has to be enhanced by means of optical set-up, beads size and density. The analysis is performed by a combination of Particle Image Velocimetry, Lagrangian particle tracking and Fourier Transform Traction Cytometry.

**BP 16.5 Mon 17:30 Poster A Migration Behavior of Human Mesenchymal Stem Cells on Biomimetic Elastic Substrates — Daniel Meyer1, Felix Seeger2, Joachim Rädler2, and Florian Rehfeldt2, 1Institute of Physics - Biophysics, Georg-August University, Göttingen, Germany — 2Faculty of Physics - Soft Condensed Matter Group, Ludwig-Maximilians-University, Munich, Germany

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

Here, we use polyacrylamide (PA) hydrogels in combination with a novel microcontact printing protocol to generate patterned substrates with well-controlled Young’s modulus E. These collagen I coated tracks are used to analyze the migration behavior of human mesenchymal stem cells (hMSC) by parallelized cell microscopy to achieve sufficient statistics. We demonstrate that both, elasticity as well as width of the track affect the migration velocity and there is a particular optimum that yields a maximal velocity.

**BP 16.6 Mon 17:30 Poster A Analysis of Cell Trajectories with Restricted Boltzmann Machines — Barbara Früunier, Julian Steinwachs, Christoph Mark, Ben Fabry, and Claus Metzner — Biophysics Group, Univ. of Erlangen-Nürnberg, Germany

We report the unsupervised analysis of cell migration trajectories for an automated classification of tumor cells. We track individual cells within collagen gels and on differently coated surfaces and map the cell trajectories to binary time series of forward and backward steps in an arbitrary (x or y) direction. Sections of these binary time series are used as input data vectors for a Restricted Boltzmann Machine (RBM), a generative stochastic neural network. Our experiments demonstrate that RBMs are able to extract, or ‘learn’, the complex underlying probability distribution of the binarized cell trajectories. After training, the RBMs generate surrogate trajectories that reproduce the statistical properties of the training data. Moreover, the RBMs can classify new trajectory segments and determine if they conform to the same underlying probability distribution. Furthermore, the RBMs are more sensitive to small differences in cell migration behavior than traditional statistical methods, such as the mean squared displacement or the step width distribution. This finding suggests that RBMs may be used as a tool for assessing the potential malignancy of tumor cells from patient biopsies.

**BP 16.7 Mon 17:30 Poster A Unique mechanical properties of cell nuclei regulated by chromatin — Chiou Jou Chas1,2, WenHong Li2, Jana Schoeller2, Mirjam Schürmann2, and Jochen Guck1,2 — Cavendish Laboratory, Department of Physics, University of Cambridge, UK — 2Biotechnology Center, TU Dresden, Dresden, Germany

Nuclear mechanics could affect gene regulation and gene expression. Chromatin, a major component of cell nuclei, could play an important role in maintaining nuclear integrity and their mechanical properties. Previous studies on nuclear mechanical properties focused largely on the role of the nuclear lamina, using techniques such as AFM and micropipette aspiration. In this work, we explicitly address the contributions of chromatin to nuclear rheology after isolation from the cell using a microrheological optical stretcher. We find that isolated nuclei swell on exposure to a minimal stretch and exhibit significant softening with increased nuclear size, which can be described by a filtration model for the nuclear membrane encasing a cortical layer of chromatin. Changes to the state of chromatin condensation via histone modifications or chromatin remodeling processes (ATP, topoisomerase II) can strongly impact nuclear morphology and compliance. Moreover, isolated nuclear mechanics is sensitive to ionic conditions: nuclei stiffen with increasing ionic strength of the buffer and contract during optical stretching in the presence of multivalent ions. The presented work establishes a quantitative link between nuclear mechanical properties and the compaction state of chromatin, which can be modulated by osmotic stress, chromatin remodeling or electrochemical environment.

**BP 16.8 Mon 17:30 Poster A Traction Force Microscopy during Phagocytosis — Wolfgang Gross and Holger Krüss — Department of Physics, University of Bayreuth, Bayreuth, Germany

In the process of phagocytosis, cells internalize micrometer-sized objects. This process is crucial for their survival and occurs by an active mechanism by which the cell remodels its cytoskeleton and creates a phagocytic cup. In the process of phagocytosis, cells internalize micrometer-sized objects. This process is crucial for their survival and occurs by an active mechanism by which the cell remodels its cytoskeleton and creates a phagocytic cup. This so-called phagocytic cup is mechanically supported by the polymerization of actin filaments in combination with myosin motors. Even though the molecular players have been identified, there is only few quantitative data describing the forces that the macrophages can exert in this process. In this poster, we use traction force microscopy (TFM), we measure cellular forces during phagocytosis in a spatially and temporally resolved manner. As a substrate, we use thin polyacrylamide films with a thickness of a few tens of micrometers.
etters. To characterize the rheology of these films, we put millimeter-sized steel spheres on the surface which are indenting the substrate. Our results suggest linear elasticity and a poisson value close to 0.5 for most gels, depending on the polymerization conditions. The results are consistent for multiple sphere radii and were verified by bulk tensile tests for different elastic moduli from 5 to 20 kPa. TFM allowed us to quantify forces, which J774-A1 macrophages exert when adhering to a fibronectin-coated gel. Preliminary data regarding phagocytosis shows the distribution of contractile forces in direct vicinity of the phagocytic target. We anticipate our results to pave the way for a more quantitative understanding of phagocytosis.

**BP 16.9 Mon 17:30 Poster A Investigation of Cell Adhesion and Motility on Microstructured Substrates** — *Daniel Geiger*, *Ulla Nolte*, *Susanne Rappi*, *Michael Beil*, and *Othmar Marti* — 1Institute of Experimental Physics, Ulm University — 2Department of Internal Medicine, University Hospital Ulm

Interaction between cells and artificial materials is of prime importance for many medical applications like implant technology. An interface can be considered as external stimulus and therefore, for example, affecting differentiation and viability of cells.

For that reason, the behaviour of cells on microstructured surfaces was investigated by means of fluorescence microscopy; electron microscopy and common video microscopy. Main emphasis is put on the study of their adhesion properties, e.g. the distribution and formation of focal adhesions. Therefore, immunostaining of specific proteins like vinculin and surface sensitive techniques like total internal reflection microscopy (TIRFM) or electron microscopy of surface sections are used.

Structuring of the substrates is done by UV exposure of a PLL-g-PEG layer on glass through a mask that enables creation of features as small as one micrometer. Subsequent addition of fibronectin creates a strong contrast to the non-illuminated PEG covered sites.

**BP 16.10 Mon 17:30 Poster A Probing the Initial Stages of Bacterial Biofilm Formation: Dynamic and Molecular Principles of Surface Based Cell Motility and Mechano-Sensing** — *Nora Sauter*, *Matteo Sangermani*, *Urs Jenal*, and *Thomas Pfohl* — 1Department of Chemistry, Universität Basel — 2Swiss Nanoscience Institute, Universität Basel — 3Biozentrum, Universität Basel

We use a microfluidic-based optical tweezers set-up to probe the initial stages of bacterial biofilm formation and to gain further insights into the principles of mechano-sensing. The model bacteria Caulobacter crescentus has two different stages in its life cycle: It starts as a swarmer cell and develops into a stalked cell when it comes into contact with a surface. A single swarmer cell is caught by an optical trap and approached to the surface of a colloidal particle, which is held by a second trap. The set-up allows for studies of the adhesion and adhesion characteristics of Caulobacter to different surfaces - colloidal particles with different surface coatings - in a controlled manner. Caulobacter swarmer cells adhere to surfaces through their pili followed by irreversibly bonding through the formation of a holdfast. Preliminary studies have led to a model where mechano-sensing occurs by pili-mediated obstruction of the flagellar rotary motor when the bacterium is close to the surface. Our set-up allows for the measurement of forces when the bacterium is approaching the surface, of the obstruction of the flagellar motor and in parallel of the exact distances between cell and surface. The experiments will help to gain further insights into the processes involved in mechano-sensing and adhesion of bacteria.

**BP 16.11 Mon 17:30 Poster A Topography and elasticity measurements on squamous carcinoma cells by AFM** — *Tanja Schreyer*, *Susanne Stieger*, *Stefan Hanssen*, *Jörg Schindelin*, and *Mathias Getzlaff* — 1Heinrich-Heine-Universität Düsseldorf, Deutschland — 2Univ.HNO, Klinik Düsseldorf, Deutschland

In this contribution we report on measurements of the mecanooelastic properties of squamous carcinoma cells. This study of single cancer cells in culture medium is carried out by Atomic Force Microscopy. In order to determine the elasticity of the cancer cells by calculating the Young modulus, we use Hertzian model with force distance curves. We analyse and compare the different stiffnesses dependent on a position within one single cell. Accordingly we are able to avoid interfering effects of the substrate. This strategy is applied to the different densely populated areas of a cell culture. In addition we are interested in the various topography of the cells within a cell culture. In this way we are able to characterise the different cell types of the culture in order to relate their stiffness and their visual appearance.

**BP 16.12 Mon 17:30 Poster A Unbiased analysis of superstatistics in tumor cell migration** — *Christoph Mark*, *Claus Metzner*, *Julian Steinwachs*, and *Ben Fabry* — FAU University of Erlangen-Nürnberg, Department of Physics, Biophysics Group

We present experimental data showing that migrating tumor cells exhibit highly heterogeneous dynamics - in time as well as across the ensemble. Surprisingly, the distribution of residence times can locally be described as a discrete persistent random walk, with $u_i = q_i a_i + a_i^2$, however, the persistence $q$ and the migratory activity $a_i$ change over longer timescales. These superstatistical changes can in turn be described by another stochastic process $(q_i(t), a_i(t))$, leading to a hierarchical probabilistic model. We describe the superstatistical process as an uncorrelated random walk and infer its parameters from measured cell trajectories with an unbiased Bayesian inference approach using an advanced Hamiltonian Monte Carlo method. This method allows for reliable probabilistic inference without further prior assumptions. We apply our method to data from migrating tumor cells on planar surfaces or on microstructured substrates, which locally vary in adhesion strength and can be studied by multiphotonic microscopy. We will report on our progress.

**BP 16.13 Mon 17:30 Poster A Mechano-sensing of cells on elastic substrates** — *Galina Kudryashova* and *Florian Riehfeld* — 3rd Institute of Physics Biophysics, Georg-August-University, Göttingen, Germany

It is nowadays well acknowledged that cellular functions, morphology and also differentiation is dependent on the mechanical micro-environment. For example, human mesenchymal stem cells (hMSCs) can be guided to differentiate into various cell types when cultured on appropriate elastic substrates. While the entire differentiation process takes several days up to weeks, the structure and dynamics of the acto-myosin fibers can be used as an early morphological marker and modelled using classical mechanics with an active spring model. We use this approach to analyze the mechanical cell-matrix interactions of hMSCs and differentiated cells during their mecano-differentiation process. We use an immunofluorescence approach to label stress fibers and analyze cytoskeletal morphology by fluorescence microscopy. hMSCs and differentiated cells were plated on elastic poly-acrylamide (PA) hydrogels with different Young’s moduli E (1-30 kPa). We analyze cell shape and alignment of stress fibers by an order parameter as early morphological marker and extract corresponding material constants that show distinct differences during the differentiation process.

**BP 16.14 Mon 17:30 Poster A Inducing cell mechanical responses using optical tweezers** — *Rebecca Michiels* and *Alexander Rohrbach* — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Cells have the ability to both sense mechanical stimuli as well as apply controlled mechanical forces to their environment. Examples are cell migration, the anchoring of the cell on substrates and the uptake of particles in phagocytosis. These processes require complex intracellular remodeling involving reorganization of the actin cytoskeleton in cooperation with molecular motors. Many of the underlying physical principles of how cells tune their reactions to external mechanical stimuli are little understood.

We use a microscope setup in which we combine conventional DIC microscopy together with optical tweezers and particle tracking. Polystyrene beads are held in an optical trap to enable controlled placement in the vicinity of the cells. The motion of the bead in the trap can be tracked in 3D with a high speed video camera at a frame rate of 1 kHz to 10 MSamples/s. The 3D positions are recorded in real time using back focal plane interferometry. This configuration enables us to induce and analyze cellular responses in a reproducible investigation scheme.

By varying the spatiotemporal pattern and the intensity of stimuli we want to gain deeper insights into the physics governing cell mechanics. We present first results from novel experiments using optical traps to trigger response patterns in cells.

**BP 16.15 Mon 17:30 Poster A**

Phagocytosis is the process of a cell engulfing and uptaking a particle.

The mechanism plays an important role in the functioning of our immune system. However, the influence of the particles' size and shape on the mechanisms and probability to uptake the particle is not clear yet.

We use a high-resolution light microscope equipped with optical tweezers and 3D interferometric particle tracking to induce phagocytic uptake of polystyrene micro-particles of different diameter. Using J774 mouse macrophages, we investigate the influence of variable contacting times and patterns until a defined response of the cell is measurable. First results are presented.

BP 16.19 Mon 17:30 Poster A Characterizing the elasticity of fibroblast cell nuclei by atomic force microscopy (AFM) to characterize Lamin and TMEM43 mutations — Sören Grannemann1, Ann-Christin Mortzler1, Helene Schellenberg2, Astrid Kassner3, Volker Walhorn3, Hendrik Mutting1, and Dario Anselmetti1,2 — 1 Biophysics, Bielefeld University, Germany

Arrhythmogenic right ventricular cardiomyopathy (ARVC) is an inherited heart muscle disease associated with cardiac arrhythmia and sudden cardiac death predominantly of young and athletes [1]. Mutations in the intermediate filament lamin and the protein luma are known to be related [2]. Luma and lamin are located at the nuclear envelope. Since the cell nucleus has to resist strong mechanical stress during the contraction phase of the heart muscle, we hypothesized that the mutations affect the functional mechanical properties of the nucleus.

Hence, we explored the elastic modulus of cell nuclei with the AFM. Fourier data analysis reveals multi-modal elasticity with protein lamin and lamin as a model system for cardiomyocytes. We analyzed a set of lamin and luma mutated cells and compared them to a control group consisting of wild-type fibroblasts and mutations not associated with ARVC. The luma mutant showed much higher and widespread elastic moduli, whereas the elasticity of the lamin mutant is similar to the control group [4]. As luma associated ARVC exhibits an explicit gender dimorphism we also investigated the impact of testosterone on the elasticity.
Viscoelastic mechanics of non-adhering cells responsible for the regulation of endocytosis and intracellular transport caused by RNAi-mediated knockdown of genes that are involved in boundary conditions. The resulting nematic director configuration is determined as that which minimizes the free energy functional considering biologically plausible boundary conditions. We model the microtubule cytoskeleton as a nematic liquid crystal and investigate the consequences for microtubule-based transport. Here, the understanding of the resulting cellular organization is missing. In order to normalize their shape and structure, but a quantitative understanding of these processes is lacking.

Mammalian cells show great variability in cell shape and intracellular organization. This variability is consistent across different cell lines, such as monocytes. For instance, adhesion of monocytes to the arterial wall is an important early step in the development of atherosclerotic lesions. The adhesion of monocytes often takes place at positions that are not fibrinogen. Our results show a significantly higher number of firmly adhered aged monocytes compared to the young monocytes ($P=0.022$). Additionally, they can be activated by lipopolysaccharide. Our results show a significantly higher number of firmly adhered aged monocytes compared to the young monocytes ($P=0.022$). We measured the adhesion rate and rolling velocity of monocytes on collagen coated microfluidic flow chambers at a shear stress of 0.6 dynes/cm$^2$. The function of cells were compared additionally by their ability to be activated by lipopolysaccharide. Our results show a significantly higher number of firmly adhered aged monocytes compared to the young monocytes ($P=0.022$). We measured the adhesion rate and rolling velocity of monocytes on collagen coated microfluidic flow chambers at a shear stress of 0.6 dynes/cm$^2$. The function of cells were compared additionally by their ability to be activated by lipopolysaccharide. Our results show a significantly higher number of firmly adhered aged monocytes compared to the young monocytes ($P=0.022$).

Aging is associated with a deterioration in immune function. Consequently, susceptibility to inflammation and degenerative age-related diseases is increased. This complicated multi-level process is among other factors mediated by activated cells of the innate immune system, such as monocytes. For instance, adhesion of monocytes to the arterial wall is an important early step in the development of atherosclerotic lesions. The adhesion of monocytes often takes place at positions that are not fibrinogen. Our results show a significantly higher number of firmly adhered aged monocytes compared to the young monocytes ($P=0.022$). We measured the adhesion rate and rolling velocity of monocytes on collagen coated microfluidic flow chambers at a shear stress of 0.6 dynes/cm$^2$. The function of cells were compared additionally by their ability to be activated by lipopolysaccharide. Our results show a significantly higher number of firmly adhered aged monocytes compared to the young monocytes ($P=0.022$).

Alteration of rolling adhesion in aged monocytes.

Samia Khaledi, Lisa Zondler, Jochen Weisshaupl, Veeselin Grozdanov, Karin Danzer, Ulla Nolte, and Kay-E Gottschalk
Institut für Experimentelle Physik, Universität Ulm, Ulm, Germany
Klinik für Neurologie, Universitätsklinik Ulm, Ulm, Germany

Aging is associated with a deterioration in immune function. Consequently, susceptibility to inflammation and degenerative age-related diseases is increased. This complicated multi-level process is among other factors mediated by activated cells of the innate immune system, such as monocytes. For instance, adhesion of monocytes to the arterial wall is an important early step in the development of atherosclerotic lesions. The adhesion of monocytes often takes place at positions that are not fibrinogen. Our results show a significantly higher number of firmly adhered aged monocytes compared to the young monocytes ($P=0.022$). We measured the adhesion rate and rolling velocity of monocytes on collagen coated microfluidic flow chambers at a shear stress of 0.6 dynes/cm$^2$. The function of cells were compared additionally by their ability to be activated by lipopolysaccharide. Our results show a significantly higher number of firmly adhered aged monocytes compared to the young monocytes ($P=0.022$).

BP 16.26 Mon 17:30 Poster A
Cell response to lateral constraints — Andreas Müller and Tilö Pompe — Universität Leipzig, Institute of Biochemistry, Johannisallee 21-23, 04109 Leipzig, Germany

Living cells are subjected to a plethora of exogenous cues which encompass chemical agents as well as physical quantities. One external regulator of cell fate that is often overlooked is spatial constraint, which is omnipresent in multicellular arrangements. We show that a bimodal behavior for human umbilical vein endothelial cells, elicited by lateral constraints and indicated by changes in actin stress fiber spacing [1], persists despite changes in mechanical and biochemical parameters. We use soft hydrogel matrices micropatterned with adhesion proteins as substrates for biochemical inhibition assays and substrates for cell traction force measurements of laterally confined cells. We find that inhibition of myosin activity does not lead to a change in bimodal behavior. Furthermore, the bimodal stress fiber behavior is also present in human dermal fibroblasts, hinting at geometry as a general regulator for cell behavior.


BP 16.27 Mon 17:30 Poster A
Cellular mechanics at the onset of phagocytosis — Konrad Berghoff, Steve Keller, and Holger Kruse — Department of Physics, University of Bayreuth, Universitätstr. 30, 95447 Bayreuth.

The phagocytic internalization and digestion of external objects by macrophages belongs to the most fundamental processes of the mammalian immune system. Phagocytosis can be induced by antibody recognition mediated by Fc receptors. Fc receptors give rise to intracellular signaling cascades which finally lead to particle uptake. The onset of particle uptake can be explained by a zipper-like mechanism that involves a successive increase of receptor-ligand bonds at adjacent binding sites and subsequent membrane protrusion around the target object. The mechanics of this zipper-like interaction are not yet fully understood. We are therefore studying these mechanisms on living cells. We hypothesize that the increasing number of ligand-receptor bonds during uptake leads to a temporally increasing rupture force necessary to break the bond between bond and cell. We also observe increasing local actin accumulation during the uptake results in local stiffening of the cellular uptake region. Using optical trapping in combination with high-speed image acquisition we test these hypotheses by inducing targeted single cell-particle binding between immunoglobulin-G coupled microbeads and J774 macrophages and by monitoring the cellular response when put under mechanical load. Our findings will give new insights on the mechanics of phagocytic uptake and will help to understand mechanisms of cell-membrane interactions and actin accumulation at the onset of phagocytosis.

BP 16.28 Mon 17:30 Poster A
Modelling adhesion of malaria-infected red blood cells — Anil K. Dasanna and Ulrich S. Schwarz — Heidelberg University.

During the blood stage of the malaria lifecycle, merozoites released by the infected liver infect healthy Red Blood Cells (RBC) which then develop adhesive protrusions on their surfaces. The infected RBCs adhere to endothelial cells in the microvasculature, leading to capillary obstruction. Using Comsol finite element simulations, we modeled infected RBC as a spherical shell covered with knobs having multiple receptors on each knob. First, we studied adhesive strength of infected RBC as a function of its knob structure by applying an external load. The adhesive strength or lifetime of receptor-ligand bond depends on the density of knobs, external loading, and the mean number of receptors per knob. We also simulated the capture efficiency of knobs, external loading, and the mean number of receptors per knob. We also simulated the capture efficiency of knobs, external loading, and the mean number of receptors per knob. We also simulated the capture efficiency of knobs, external loading, and the mean number of receptors per knob.
infected RBC in hydrodynamic shear flow. We will discuss different
dynamic states such as rolling adhesion, firm adhesion and free
motion, which depend on flow strength and bond kinetic rates. Finally we
will briefly discuss the ongoing work on non-spherical cell shapes and
explicit modeling of the shapes which corresponds to in vivo situation.

**BP 16.29 Mon 17:30 Poster A**

**Characterization of intracellular phagosome transport** —
*Steve Keller, Konrad Berghoff, and Holger Kress — Department of Physics, University of Bayreuth, Bayreuth, Germany

As one of the key processes during the immune response, phagocytosis of
bacteria plays a significant role in the mammalian immune system.

**BP 16.30 Mon 17:30 Poster A**

**Stochastic modeling of gliding motility** — *Thorsten Erdmann,1 and Ulrich S. Schwarz2 — 1Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — 2BioQuant, Heidelberg University, Heidelberg, Germany

Gliding motility is a form of movement observed in unicellular organ-
isms such as bacteria or single-celled eukaryotes. In the sporozoites of
malaria parasites, gliding is driven by the formation of adhesion bonds
with the substrate which are displaced relative to the cell body by the
activity of molecular motors. Experimental trajectories of sporozoites
reveal strong fluctuations of gliding velocity: On a sub-second
time scale, stick-slip-like movement is observed; on larger time scales,
the motion of larger particles is faster and in a more persistent way towards the
plastocrine region whereas smaller particles move slower with more interjacent phases of random
motion.

**BP 16.31 Mon 17:30 Poster A**

**Model analysis of P-Selectin-mediated leukocyte rolling** —
*Mats Moskopp1, Andreas Deussen1, Trianafylylos Chavakis2,*

and Peter Dieterich1 — 1Institut für Physiologie, TU Dresden, Germany — 2Klinikum Pathobiochemie, TU Dresden, Germany

Invasion of leukocytes from the blood stream into tissue proceeds as
coordinated sequence called leukocyte adhesion cascade and is indis-

**BP 16.32 Mon 17:30 Poster A**

**Mechanical Coupling of the Cytoskeleton with the Nucleus** — *Gabriele Straass and Florian Rehfelt — Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany

It is nowadays widely acknowledged that mechanical cues are as impor-
tant for cellular behaviour as traditional biochemical ones. Strikingly,
adult stem cells can be guided to differentiate towards various cell types
when cultured on elastic hydrogels with appropriate Young’s modu-
lus $E$. While the differentiation process takes several days, the acto-

**BP 16.33 Mon 17:30 Poster A**

**Complex thermorheology of cells** — *Enrico Warmt, Sebastian Schmidt, Tobias Kießling, Anatol Frutsch, Roland Stangl, and Josef Käs — Universitäts Leipzig Faculty of Physics and Earth Sciences, Leipzig, Germany

Temperature has a reliable and nearly instantaneous influence on me-
chanical responses of cells. We measured thermorheological behaviour
of eight common cell types within physiologically relevant tempera-
tures and applied thermorheological time-temperature superposition
to creep compliance curves. Our results showed that superposition is
not a universal feature, and is only applicable in four of the eight cell
types. Cells with more complex temperature responses transitioned
around 36°C. Activation energies were calculated for all cell types,
and the variation of temperature occurred at different rates. These results reveal broad insights into thermally sensitive stress-strain
relations of various cell types.
BP 17.1 Mon 17:30 Poster A
mFES: A robust molecular Finite Element Solver for electrostatic energy computations — Ernst-Walter Knapp and Ilkay Sakally
Institut für Chemie und Biochemie, Freie Universität Berlin
We present a robust method for the calculation of electrostatic potentials of large molecular systems using tetrahedral finite elements (FE). Compared to the finite difference (FD) method using a regular simple cubic grid to solve the Poisson equation, the FE method can reach high accuracy and efficiency using an adaptive grid. Here, grid cell points are adjusted and are placed directly on the molecular surfaces to faithfully model surfaces and volumes. The grid point density decreases rapidly toward the asymptotic boundary to reach very large distances with just a few more grid points. A broad set of tools are applied to make the grid more regular and thus provide a more stable linear equation system, while reducing the number of grid points without compromising accuracy. The latter reduces the number of unknowns significantly and yields shorter solver execution times. The accuracy is further enhanced by using second order polynomials as shape functions. Generating the adaptive grid for a molecular system is expensive, but it pays off, if the same molecular geometry is used several times. As is the case for aFD and fixed potential computations of many charge variable groups in proteins. Application of the mFES method is also advantageous, if the molecular system is too large to reach sufficient accuracy when computing the electrostatic potential with conventional FD methods.

BP 17.2 Mon 17:30 Poster A
Transmembrane-peptide structure formation from coarse-grained simulations — Tristan Bereau — Max Planck Institute for Polymer Research, Mainz, Germany
Interfacial systems are at the core of fascinating phenomena in many disciplines, such as biochemistry, soft-matter physics, and food science. However, the parametrization of accurate, reliable, and consistent coarse-grained (CG) models for systems at interfaces remains a challenging endeavor. I will describe recent advancements made toward the description of secondary-structure formation of peptides in a membrane environment using CG models. By combining a lipid model that can semi-quantitatively reproduce material properties of a fluid membrane bilayer and a peptide model that is not biased toward one particular state (e.g., α-helix or β-sheet), the combined parametrization allows to look at how peptide structure is affected by the membrane environment on long timescales. I will illustrate the robustness of the model by looking at different WALP transmembrane helical peptides starting from stretched, unstructured conformations. Analysis of the structure of the membrane during folding provides insights into the local deformation during helix formation as a function of charge variable groups. The found folding transitions. We show that analysis based on contact distances support the findings gained by dPCA and facilitate interpretation and visualization of the folding process by highlighting which contacts contribute to the folding transitions.

BP 17.3 Mon 17:30 Poster A
Variation of Exciton-Vibrational Coupling in Photosystem II Core Complexes from Thermosynechococcus elongatus as Revealed by Single-Molecule Spectroscopy — Steffen Schindelöw, Maximilian König, Thomas Reiter, Christian Holzmann, Olaf Krems, and Marcus Brecht
CIC nanoGUNE, Donostia, Spain
As an example for a more fundamental understanding of the exciton-vibrational coupling in Photosystem II (PSII) we report on anharmonic anisotropy relaxation measurements of the D1D2cyt b-559 reaction center complex, the core complex (PSIIcc) is composed of the two intrinsic antenna proteins, the LHC I and LHC II, and several and 16 Chls, respectively, the D1D2cyt b-559 reaction center complex, that coordinates 6 Chl a and 2 pheophytin a molecules, and several additional small subunits. The spectral properties and dynamics of the fluorescence emission of PSIIcc are investigated by single-molecule spectroscopy (SMS) at 1.6 K. The emission spectra are dominated by sharp zero-phonon lines (ZPLs), which are the result of weak to intermediate exciton-vibrational coupling and slow spectral diffusion. Overall results show that electrostatic, rather than exchange or dispersive interactions are the main contributors to the exciton-vibrational coupling in this system.

BP 17.4 Mon 17:30 Poster A
Solvation of 2GB1 in ionic liquid/water mixtures — Volker Lesch1, Vasileios A. Tatsis 1, Andreas Heuer , Christian Holzmann2, and Jens Smiatek1,2,3
1Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster — 2Institut für Computerphysik, Universität Stuttgart
Ionic liquids are considered as environmentally friendly compared to organic compounds. Furthermore, they have an ion characteristic which leads to interesting solvation properties.

BP 17.5 Mon 17:30 Poster A
Dimensionality reduction of protein dynamics by employing distance and contact analysis — Matthias Ernst and Gerhard Stock — University of Freiburg, 79104 Freiburg, Germany
To describe and understand protein dynamics, a reduction of the 3N-6 dimensional space of the N atoms involved is crucial. A commonly employed way to reduce dimensionality is principal component analysis (PCA), a linear transformation which removes linear correlations of the coordinates by diagonalizing their covariance matrix. As PCA results often provide higher resolution, especially for large-amplitude motion, we present a robust method for the calculation of electrostatic potential by quantities based on information theory and on their structural relevance. We show that analysis based on contact distances support the findings gained by dPCA and facilitate interpretation and visualization of the folding process by highlighting which contacts contribute to the folding transitions.

BP 17.6 Mon 17:30 Poster A
Insoluble proteins in presence of salt: a computational study — Patrick Kreisel and Jens Smiatek — Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Germany
Nogo-60 is a truncated sixty residue version of the extracellular domain of the human Nogo proteins. It is soluble in pure water but highly insoluble in buffer. Surprisingly, the protein almost completely consists of three large α-helices. However, the last six residues remain highly unstructured. If this six residue tail is dropped, another protein—Nogo-54—is designed, which is soluble in both buffer and pure water. Nogo-60 and Nogo-54 thus provide an almost identical primary structure but different solubility/insolubility properties. Both proteins were simulated in different salt solutions as well as in pure water to get an idea of the underlying mechanisms and to study the influence of the salt ions on the protein solubility behavior.
The glycoprotein hemagglutinin (HA) is a transmembrane protein of the influenza virus that comprises over 80% of the envelope proteins present in the virus particle and accounts for the primary attachment of the virion to a target cell. The attachment happens due to hydrogen bonds between the three binding pockets of the HA globular domain and sialic acid (SA) molecules on the biological cell surface. The development of efficient inhibitors of virus binding requires precise knowledge of this interaction. On protein immobilizing surfaces the force fields are used to model the peptide (SFM) to directly probe the bond strength of single and multiple HA - SA interactions. SPM images are used to determine the surface density of the immobilized proteins. Then, single molecule force spectroscopy with cantilevers functionalized with SA is employed to measure the rupture forces between HA-SA bonds. The dissociation behavior is calculated from the distribution of rupture forces at various pulling speeds.

**BP 17.8 Mon 17:30 Poster A**

Local water dynamics around antifreeze protein residues in the presence of osmolytes: The importance of hydroxyl and charged side groups — \textsc{anand narayanan krishnamoorthy}, \textsc{jens smiatek}, and \textsc{christian holsch} — 1Institute for Computational Physics, University of Stuttgart — 2Institute for Computational Physics, University of Stuttgart — 3Institute for Computational Physics, University of Stuttgart

It is nowadays common knowledge that the antifreeze activity of AFPs is mainly determined by a short -range effect which includes a direct binding in the ice phase. Recently, experimental findings also revealed a long range effect which implies a significant retardation of the water dynamics to facilitate the ice binding process specifically for AFGPs. The aim of the work is to examine the dynamics of water molecules around different antifreeze protein residues by using atomistic molecular dynamics simulations. The analysis of the water hydrogen bond characteristics and the dipolar relaxation times reveals a strong retardation effect of water dynamics around the TAFG prototype. Our numerical results reveal the significant importance of polar units like threonine and dissacharides for the direct binding of water molecules in terms of hydrogen bonds and a significant retardation of water dynamics. In addition, our findings indicate that this effect is even more pronounced in the presence of kosmotropic osmolytes.

**BP 17.9 Mon 17:30 Poster A**

Electric field induced secondary structure changes in small peptides — \textsc{sina zenderhoofd}, \textsc{bernhard reuter}, and \textsc{martin e. garcia} — Theoretical Physics, University of Kassel, Kassel, Germany

The conformation of a protein is pivotal for its physiological functionality. Hence, procedures to manipulate secondary and tertiary structure formation, including the use of external electric fields, are of great interest. Referring to predictions based on previous calculations that applied a reduced model and the Monte Carlo method [P. Ojeda-May and M. E. Garcia, Biophys. J. 99(2), 595-599 (2010)], we investigated if they hold true making use of a more complex all-atom model. Using the molecular dynamics package GROMACS and the CHARMM force-field, we performed all-atom simulations of a small peptide under the influence of external static electric fields. We observed that the electric field modifies the secondary structure of the peptide and can even induce a transition from beta-sheet to alpha-helix or helix-like structures.

**BP 17.10 Mon 17:30 Poster A**

Apoprotein A1 adsorption at solid/liquid and liquid/liquid interfaces — \textsc{Susanne Dogan}, \textsc{Irena Kiesel}, \textsc{Matthias Kampmann}, \textsc{Kolja Mende}, \textsc{Floren J. Wiercigroch}, \textsc{Michael Paulus}, \textsc{Christian Sternemann}, and \textsc{Tolga Metin} — 1Fakultät Physik/DELT, Technische Universität Dortmund, D-44221 Dortmund, Germany — 2Institut Laue-Langevin, 38000 Grenoble, France — 3DESY, D-22603 Hamburg, Germany — 4Department of Physics, University of Siegen, D-57072 Siegen, Germany

One of the most important high density lipoproteins for the lipid metabolism is apolipoprotein A1 (ApoA1), which has a ring-like structure. The inner part of the ring is hydrophobic whereas the outer part is hydrophilic. Due to this, ApoA1 forms structures with lipids and cholesterol. In order to study the adsorption behavior of ApoA1, x-ray reflectivity experiments at the hydrophobic solid/liquid interface were performed at beamline BL9 of the synchrotron light source DELTA (Dortmund, Germany). The measurements were conducted at different temperatures (25°C - 80°C). To investigate the adsorption of ApoA1 at negatively charged surfaces, a DPPA monolayer at the liquid/air-interface at room temperature was used. The results indicate an adsorption and deformation with a conformational transition of the tilted ring of ApoA1 over several non-separated states with increasing temperature at hydrophobic interfaces. No significant change in the profile of DPPA was observed when the DELTA film was prepared on ApoA1 solutions. Thus, the electrostatic repulsion between ApoA1 and the head groups of DPPA prevents the adsorption at the membrane.

**BP 17.11 Mon 17:30 Poster A**

Water Dynamics Near Fluorinated Amino Acids: A Molecular Dynamics Study — \textsc{João R. Robalo} and \textsc{Ana Vila Verde} — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Incorporating fluorinated amino acids into proteins often results in increases of protein resistance to thermal and chemical degradation, as well as in improved functionality. Recent work by B. Koksch and co-workers [1] suggests that changes in protein function upon fluorination of amino acids at the protein active site may arise from the different behavior of water near those amino acids, compared to their non-fluorinated counterparts. At present, however, the structure and dynamics of water near fluorinated proteins is not understood. We are addressing this issue by developing classical, all-atom, fixed-charge models of fluorinated hydrophobic amino acids and using them to investigate water structure and dynamics in their vicinity. The models are parameterized to reproduce experimental free energies of hydration of fluorinated analogues of hydrophobic amino acid side chains. The developed models shall then be used for the study of water near fluorinated small peptides and proteins.

[1] - B. Koksch, unpublished

**BP 17.12 Mon 17:30 Poster A**

Investigating interactions of anions with selectins using molecular dynamics simulations — \textsc{Sadra Kashef Ol Gheta} and \textsc{Ana Vila Verde} — Max Planck Institute of Colloids and Interfaces

Selectins are well known for their role in the adhesion of leukocytes and platelets to the endothelium that takes place, e.g., during inflammation. Because of the important biological role played by selectins, much effort has been put into finding artificial ligands that effectively compete with the natural ones. Recently, dendrimeric polyglycerol (dPG) polymers functionalized with various anionic functional groups were investigated for their potential as L-selectin inhibitors. It was found that the affinity of dendrimers for selectin depends strongly on the nature of the anionic group, increasing in the order carboxylate < phosphate < sulfonate < bisphosphonate < sulfate. To understand the molecular origin of this anionic series, we use classical all-atom models based on the CHARMM36 force field for proteins and explicit water to characterize the intrinsic interactions between various anionic functional groups and positively charged amino acids using small molecule analogues, e.g., methylsulfate, methylamine. The results from classical simulations are compared against those from ab initio calculations, to assess the quality of the classical models.

**BP 17.13 Mon 17:30 Poster A**

Langevin Modeling of Biomolecular Dynamics — \textsc{Björn Bas-tian} and \textsc{Gerhard Stock} — University of Freiburg, 79104 Freiburg, Germany

Total simulation times long enough to capture biologically relevant functions are often inaccessible by Molecular Dynamics (MD) simulations on the level of full atom Newton equations. The data driven Langevin equation (dLE) technique allows for efficient propagation of the system dynamics up to long times (hundreds of nanoseconds) on the basis of many short continuous MD trajectories (that can be computed in parallel) [1]. Beforehand, important system coordinates to describe conformational dynamics are obtained by dimensionality reduction, e.g. by principal component analysis.

If the timescales of slow system and fast bath variables separate, a general nonlinear Langevin equation can be derived from a microscopic Hamiltonian by projection techniques. The dLE algorithm presented obtains the drift, friction and diffusion fields by a local estimation on a few selected system coordinates up to long simulation times on the level of full atom Newton equations. The data driven functions are often inaccessible by Molecular Dynamics (MD) simulations.

[1] - Sadra Kashef Ol Gheta, Ana Vila Verde, Björn Bastian, Gerhard Stock, University of Freiburg, Germany

**Monday**

**BP 17.14 Mon 17:30 Poster A**

Langevin Modeling of Biomolecular Dynamics — \textsc{Björn Bastian} and \textsc{Gerhard Stock} — University of Freiburg, 79104 Freiburg, Germany

Total simulation times long enough to capture biologically relevant functions are often inaccessible by Molecular Dynamics (MD) simulations on the level of full atom Newton equations. The data driven Langevin equation (dLE) technique allows for efficient propagation of the system dynamics up to long times (hundreds of nanoseconds) on the basis of many short continuous MD trajectories (that can be computed in parallel) [1]. Beforehand, important system coordinates to describe conformational dynamics are obtained by dimensionality reduction, e.g. by principal component analysis.

If the timescales of slow system and fast bath variables separate, a general nonlinear Langevin equation can be derived from a microscopic Hamiltonian by projection techniques. The dLE algorithm presented obtains the drift, friction and diffusion fields by a local estimation on MD data. Thus dLE trajectories yield a correct global energy land-
BP 17.14 Mon 17:30 Poster A

**Biomolecules at gold-water interfaces: the role of the metal polarization**
- **Edoardo Lorenzo**, Hadi Ramezan-Dakheli, Hendrik Heinz, and Marialoore Sulpiizi
- Johannes Gutenberg University Mainz, Staudinger Weg 7 55099 Mainz — Department of Polymer Engineering, University of Akron, Ohio 44325

Microscopic understanding and control of protein-surface interactions is gaining increasing interest due to the new development of bio-interfaces for medical and bio-technical applications. In this contribution we aim to provide a characterisation of different interactions at the gold-water interface. We use Monte Carlo simulations. It was revealed that a strong electric field of an external electric field on the peptide V3-loop 1NJ0 was analyzed. This effect of an spatial temperature gradient on a proteinlike designed induced a transition from a beta-sheet into a helix conformation. Also, we perform single cell force spectroscopy to investigate the attachment of bacteria to these protein layers in comparison to the bare surface.

BP 17.15 Mon 17:30 Poster A

**Studying in situ protein adsorption and bacterial adhesion via fast scanning AFM and force spectroscopy**
- Christian Spengler, Nicolas Thiers, Thomas Faidt, Christian Kreis, and Karin Jacobs
- Saarland University, Experimental Physics, 66041 Saarbrücken, Germany — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Protein adsorption and bacterial adhesion are the first steps in biofilm formation. Hereby, proteins serve as a conditioning layer for the further attachment of bacteria and other organisms. Hence, the understanding and control of protein layers and their interaction with bacteria is an important task relevant to life sciences and engineering. We study the protein adsorption in situ on a single protein level. For this purpose, we use a fast scanning AFM operating in liquid under flow conditions which reveals single protein adsorption events. The surfaces for these experiments are hydrophilic and hydrophobized silicon substrates with different oxide layer thickness and very smooth artificial tooth samples. Additionally, we characterize the bactericidal activity of proteins in their adsorbed state using purified peptidoglycan. Furthermore, we perform single cell force spectroscopy to study the adhesion of bacteria to these protein layers in comparison to the bare surface.

BP 17.16 Mon 17:30 Poster A

**Protein Folding: Driving forces and external influences**
- Bernhard Reuter, Pedro A. Ojeda May, and Martin E. Garcia — University of Kassel, Theoretical Physics II, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

One of the most important questions of nature sciences is why a given amino acid sequence under physiological conditions mostly exists in a certain functional spatial structure - the native state. If certain proteins in a bigger amount are required for diseases like neurogenerative diseases (i.e. Alzheimer’s and prion diseases). In this context the question of the external influences on the stability of the native state arises. To address this problem the effect of an external electric field on the peptide V3-loop 1NJ0 was analyzed by Monte Carlo simulations. It was revealed that a strong electric field indeed induces a transition from a beta-sheet into a helix conformation. Also, the effect of an spatial temperature gradient on a proteinlike designed helix was simulated using the Langevin Dynamics method showing that a temperature gradient can facilitate protein folding.

BP 17.17 Mon 17:30 Poster A

**Selective Adsorption of Similar-Sized Proteins into a Nanoporous Silica Glass**
- Sebastian T. Moerz and Patrick Huber
- 1Experimental Physics, Saarland University, D-66041 Saarbruecken — 2Institute of Materials Physics and Technology, Hamburg University of Technology, D-21073 Hamburg, Germany

The adsorption of lysozyme, cytochrome c and myoglobin, similar-sized globular proteins of approximately 1.5 nm radius, into the mesoporous silica material SBA-15 with 3.3 nm mean pore radius has been studied photometrically for aqueous solutions containing a single protein type and for binary protein mixtures. Distinct variations in the absolute and relative adsorption behaviour are observed as a function of the solution’s pH-value, and thus proton and counterion charge. The proteins exhibit the strongest binding below their isoelectric points, which indicates the dominance of electrostatic interactions between charged amino acid residues and the -OH groups of the silica surface in the nanopore adsorption process. Moreover, we find for competitive adsorption in the restricted, tubular nano pore geometry that the protein type which shows the favoured binding to the pore wall can entirely suppress the adsorption of the species with lower binding affinity, even though the latter would adsorb quite well from a single component mixture devoid of the strongly binding protein. We demonstrate that this different electrochemical behaviour along with the large specific surface and thus adsorption capability of the nanoporous glass can be readly exploited for a simple, yet highly effective separation of protein mixtures by adjusting the aqueous solution’s pH.

BP 17.18 Mon 17:30 Poster A

**Rate equations as a tool for kinetic modelling of iRFP’s**
- Mario Willenbrock, Nico Herder, Luise Sautzoff, Neblman Tavraz, Franz-Joseph Schmitt, and Thomas Friedrich — Institute of Chemistry, Bioenergetics, Technical University Berlin, Germany

Recent developments in protein design led to a near infrared fluorescent protein (iRFP) based on a bacteriophytochrome RpBphP2 (P2). Switchable infrared fluorescent probes with enhanced fluorescence quantum yield are required for modern microscopic applications like IR fluorescence microscopy. We investigated low-temperature time- and wavelength-correlated single photon counting in the wide temperature range from 10 K to 300 K to monitor chromophore-protein interactions. A rate equation model assuming ground state heterogeneity and three excited states: PR+, pre-Lumi-R* and Lumi-R* leads to the corresponding temperature-dependent rate constants and therefore a better understanding of the underlying pigment-protein coupling and the apparent fluorescent states in the system. The results enable to identify the molecular determinants for the fluorescence enhancement of iRFP compared to the wild-type protein. It is suggested that the mutations P2 D202T and P2 Y268F are mainly responsible for enhanced fluorescence quantum yield.

BP 17.19 Mon 17:30 Poster A

**CUDA-accelerated FEM-BEM Simulations of Dielectric Relaxation Spectroscopy of Solvated Proteins**
- Stephan Kramer — Max-Planck-Institut f. biophysikalische Chemie, Am Faßberg 11, 37077 Göttingen, Germany

Dielectric relaxation spectroscopy of solvated ubiquitin [1] has shown the sensitivity of the direct current to conformational sampling. Experimental, this is observed by the appearance of the so-called sub-β peak in the dielectric loss spectrum. A mechanistic explanation of this peak is that different numbers of ions are bound in the hydration shell of the protein, depending on its conformation. This changes the density of mobile ions, thus altering the direct current component. The sub-β peak can be quantified by a stochastic model considering the conformational dynamics as a simple 2-state, ratchet-like process coupled to a Fokker-Planck model for the mobile ions. We extend the ion dynamics to the Poisson-Nernst-Planck equations in a finite domain with reactive boundaries modeling the setup of a dielectric relaxation spectroscopy experiment. The protein is an excluded volume for the ions. It is converted into a boundary condition for the mobile ions by means of an integral equation. The resulting boundary element problem is solved with CUDA using our SciPAL library [2]. The ion densities are computed from a finite element model. Our results confirm the theory of the origin of the sub-β peak.

Time-resolved single-frequency IR absorption spectroscopy on photosystem II for investigation of electron-coupled proton transfer — • PHILIPP SIMON, PETKO CHERNEV, and HOLGER DAU — Freie Universität Berlin, Fachbereich Physik

Photosystem II is a light activated and transmembrane protein performing photosynthetic water oxidation. During the accumulation of formaldehyde needed for O-O bond formation at the reaction center, a Mn4Ca-oxo cluster, protons are released and transported over large distances of up to 30 Å (Klaus et al. 2012, PNAS 109, 16035-16040).

Understanding of the process at an atomic level does not only answer fundamental questions of protein functions but can also provide hints on the development of catalysts for artificial photosynthesis, a clean way of producing storable energy.

To analyse the dynamics of these processes a new infra-red absorption experiment is being designed. Its central part is a cw quantum-cascade laser tunable from 1300 to 1650 cm⁻¹ and thus covering the amide I and II regions, the COO⁻ stretching region as well as bands of the quinones or the redox active tyrosine denoted as Y₂. The time resolution is in the microsecond range, which enables us to observe structural changes and proton transfer dynamics. Here the setup and first measurements on the dynamics of selected vibrational bands, specifically the band assignable to Qₓ, will be presented.

BP 17.21 Mon 17:30 Poster A Single-molecule stochastic modeling of the channeling enzyme tryptophan synthase — •DIMITRI LOUTCHKO and ALEXANDER S. MIKHAILOV — Fritz Haber Institute of the Max Planck Society

The channeling enzyme tryptophan synthase provides a paradigmatic example of a chemical nanomachine. It possesses two active centers and, as a single molecule, catalyzes a sequence of 13 different reactions with a complex pattern of allosteric regulation and with an intermediate product channeled from one active center to another. Here, the first single-molecule stochastic model of the enzyme is proposed and analyzed. All its transition rate constants were deduced from the experimental data available and no fitting parameters were thus employed. Numerical simulations reveal the development of strong correlations in the states of the active centers and the emergent synchronization of intramolecular processes in tryptophan synthase. While performed for a specific enzyme, this study sets a framework for stochastic modeling of other chemical machines, such as channeling enzymes and multi-enzyme complexes.

BP 17.22 Mon 17:30 Poster A Free Energy Decomposition: A Model System with Focus on Entropic Contributions of Water — • JONAS LANDIGESELL and JENS SMIATLIK — Stuttgart

This contribution focuses on the application of free energy decomposition to investigate the entropic contributions of water to the folding of the beta hairpin HP7 and its mutants by simulations in explicit water and vacuum. Free energy decomposition makes use of free energy landscapes which are obtained using all-atom molecular dynamics simulations together with umbrella sampling and WHAM. The chosen methods calculate entropic changes by using integral energy and free energy estimates. In agreement with experiments we find that the folding of the beta hairpin HP7 is mainly driven by enthalpic energy changes. The simulations of some mutants of HP7 show that the influence of the hydrophobic effect on protein folding can be increased by replacing less hydrophobic amino acids with more hydrophobic amino acids.
The cell membrane is the outer layer of a biological cell. It consists of lipids which form a two-dimensional fluid bilayer structure and is attached via linker proteins to the underlying actomyosin cortex, a thin network of actin filaments and myosin motors. In the past years, research has mainly focused on the physical description of the cell membrane and cytoskeleton independently. However, little is known on how they mechanically interact in the cell.

Here, we present a model for the interaction of membrane and cytoskeleton based on the assumption that the anchored membrane is attached to the underlying actomyosin cortex, subjected to active tension arising from myosin activity. Cell pressure results in membrane protrusions which can equilibrate their surface tensions by exchange of lipids. Using this physical description, we characterize how excess membrane area distributes around the cell. Based on a few fundamental cell parameters, the cortex tension, the membrane bending stiffness and the anchoring strength, we find a phase diagram with regions corresponding to a homogeneous distribution of membrane, to the pulling of membrane tubes and to the formation of one or several blebs. We finally use this result to discuss potential consequences for the mechanics of the cell.

**BP 18.5 Tue 10:45 H 1028**

**Markov state models to obtain free energies of (de)mixing** — **DUURRE H. DE JONG AND ANDREAS HUER** — University of Münster, Münster, Germany

Obtaining free energies of demixing in multicomponent systems, for example lipid bilayers, would greatly benefit many (theoretical) studies. For such systems the initial state, i.e. the mixed configuration, is often thermodynamically highly unstable. This can render standard techniques like umbrella sampling problematic.

We show that application of Markov state models to several short and independent simulations allows one to extract the free energy gain upon demixing very reliably. Here it is important that the temporal evolution of an appropriately defined order parameter displays local fluctuations. Specifically, this method is applied to a two component Ising model and a binary Lennard-Jones system.

**BP 18.6 Tue 11:15 H 1028**

**The Mechanism of Phagocytosis: Two Stages of Engagement** — **DAVID M. RICHARDS AND ROBERT G. ENDRES** — Imperial College London, UK

Despite being of vital importance to the immune system, the mechanism by which cells engulf relatively large solid particles during phagocytosis is still poorly understood. From movies of neutrophil phagocytosis of polystyrene beads, we measure the frictional engagement as a function of time and demonstrate that phagocytosis occurs in two distinct stages. During the first stage, engagement is relatively slow and progressively slows down as phagocytosis proceeds. However, at approximately half-engulfment, the rate of engulfment increases dramatically with complete engulfment attained soon afterwards. By studying simple mathematical models of phagocytosis, we suggest that the first stage is due to a passive mechanism, determined by receptor diffusion and capture, whereas the second stage is more actively controlled, perhaps with receptors being driven towards the site of engulfment. We then consider a more advanced model that includes signalling and captures both stages of engulfment. This model predicts that there is an optimum ligand density for quick engulfment. Further, we show how this model predicts how non-spherical particles engulf quickest when presented tip-first.

**BP 18.7 Tue 11:30 H 1028**

**No spatial spreading of chemotactic signaling in amoeboid cells upon receptor stimulation** — **MATTHIAS GERHARDT, MICHAEL WALZ, AND CARSTEN BETZ** — Institut für Physik und Astronomie, Karl-Liebknecht-Straße 24/25, 14476 Potsdam, Germany

Recently we have shown that in chemotactic Dictyostelium discoideum cells stimulation of a confined membrane region with cAMP leads to confined signaling of PIP3, Pten, and filamentous actin. A consequence of this observation is that cAMP stimuli cannot trigger spatial spreading of intracellular signaling. However, in the absence of an extracellular cAMP stimulus, components of the signal transduction system where observed to form traveling waves that show all hallmarks of an excitable system. This excitable system is characterized by PIP3-rich membrane regions circumscribed by actin segments propagating together as a composite wave across the substrate attached membrane of a Dictyostelium cell. Since cAMP stimulation causes depletion of such waves, we concluded there must be an intracellular switch, which determines whether the signal transduction is excitable or not. Since earlier observations show that a [betagamma]G knockout remarkably enhances PI3K activity, we conjecture that the PI3K is a suitable candidate to take on the role of an intracellular switch which controls excitability.

**BP 18.8 Tue 11:45 H 1028**

**Recognition Force Spectroscopy on Lamellar Body Surfactants collected from Primary Alveolar Cells Type II** — **P. PAUL, N. HOBI, HALLER, MANFRED FRIEDK**, and **E. GOTTSCHALK** — Department of Experimental Physics, Ulm University, Ulm, Germany

**BP 18.9 Tue 12:00 H 1028**

**Local viscosities near plasma membranes of living cells** — **FELIX JÖNGER AND ALEXANDER ROHRBACH** — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Kocher-Allee 102, 79110 Freiburg, Germany

The molecular processes of particle binding and endocytosis are influenced by the locally changing mobility of the particle nearby the plasma membrane of a living cell. Close to different cellular interfaces, the viscous drag changes strongly with the distance to the interface. In our work we use photonic force microscopy (PFM) to investigate how the changes when an optically trapped 1 μm polystyrene bead approaches the plasma membrane of different biological cells. The bead’s temporal fluctuations are tracked interferometrically in three dimensions with nanometer precision and on a microsecond time scale. The autocorrelation of the bead’s motion reveals the friction coefficient γ(d) as a function of bead-membrane distance d. We find a simple exponential decay for γ(d) with a hydrodynamic decay length A(d) that fits well to the obtained experimental data. We investigated different cell types (J774, HT29, MDCK) and a giant unilamellar vesicle (GUV). We find that all values A(d) measured at biological membranes are significantly longer than those of a rigid glass coverslip, giving rise to the conclusion that the deformable shape of the membrane influences the hydrodynamic interaction.

**BP 18.10 Tue 12:15 H 1028**

**Fluorescence Imaging of Light Induced Reactive Oxygen Species (ROS) in Plant Cell Tissue** — **FRANZ-JOSEF SCHMITT, VLADIMIR KREBLAVSKY, GANNA S. SCHIRSHKOVA, GORANGOR K. KEUR, SERGEI K. ZHARHMAMEDOV, ALLAKHIVERDIEV, AND THOMAS FRIEDRICH** — Institute of Chemistry, Bioenergetics, TU Berlin, Berlin, Germany

UV-radiation in combination with toxic compounds like polyaromatic hydrocarbons (PAHs) lead to generation and accumulation of reactive oxygen species (ROS) in animal and plant cells. ROS generation by napthalene (Naph), a lipophilic PAH, can be imaged with fluorescence microscopy employing the ROS sensitive dye dichlorofluorescein (DCF). Under high light illumination, Naph-treated leaves of Arabidopsis thaliana showed the spread of ROS waves across the tissue with a period time of 20 min. The reduction of PSII activity at the presence of Naph was accompanied by transient generation of hydrogen peroxide (H2O2) as well as cell death due to lipid peroxidation in the plasma membranes. It could be shown that Naph treated leaves of Arabidopsis thaliana show enhanced DCF fluorescence in the thylakoid membranes. The comparison of short term and long term exposure to different
PAHs revealed that at short term exposure, the PAHs with high water solubility lead to the strongest reduction of PS II activity while after long term exposure the effect of PAHs with low water solubility is stronger.

**BP 19: Multi-cellular systems**

**Time:** Tuesday 9:30–12:45

**Invited Talk**

BP 19.1 Tue 9:30 H 1058

Emerging social behaviour during aggregation in Dictyostelium discoideum — GIOVANNA DE PALO1, DAVIN Y2, THOMAS GREGOR2, and ROBERT ENDES1 — 1Department of Life Sciences, Imperial College London, UK — 2Joseph Henry Lab. of Physics, Princeton University, USA

During starvation, the social amoeba Dictyostelium discoideum aggregates artfully via pattern formation into a multicellular slug and finally spores. The aggregation process is mediated by the secretion and sensing of cyclic adenosine monophosphate (cAMP), leading to the synchronised movement of cells. The whole process is a remarkable example of collective behaviour, spontaneously emerging from single-cell chemotaxis. Despite this phenomenon being broadly studied, the precise mechanism of aggregation starting from single cells is still unclear. Here, we extend a detailed single-cell model of D. discoideum chemotaxis by adding cell-cell communication. We then use these results to build a population model with rules derived from single cells. We validate our results with experimental FRET data, where both intracellular concentration of cAMP and collective movements are measured. By analysing cell shape and behaviour we show evidence of a critical point at the onset of aggregation. Specifically, by considering the morphospace we show how the average cell shape changes with the directional correlation diverging exactly during the streaming process. Similar methods could also be exploited for the understanding of other examples of collective behaviours, ranging from the complexity of animal migration to cell organisation in embryonic morphogenesis.

BP 19.2 Tue 10:00 H 1058

Adaptation of fluid flow in the slime mold Physarum polycephalum — KAREN ALIM1, GABRIEL AMSELEM1, FRANCOIS PEAUDERIER2, ANNE PRINGLE1, and MICHAEL BRENNER1 — Harvard University, Cambridge, U.S.A.

The network-forming slime mold Physarum polycephalum lacks any central coordination center, yet it shows often-termed intelligent dynamics in the way it grows and adapts its network morphology. Our work investigates the role of fluid mechanics for transport and signal transfer during the morphological dynamics of this network-like slime mold. We combine experimental observations of the fluid flow and its driving force with the development of the theoretical concept of transport by peristaltic flow in a network. This synergy allows us to show that the slime mold actively controls its internal fluid flow by establishing a peristaltic wave. This peristaltic wave always spans the total extent of an individual independent of its size. Thus, we find that the slime mold actively adapts its flows as to maximize transport. The quantitative description of flows in Physarum polycephalum enables a new view on the slime molds growth dynamics during the encounter of food or toxins and how their location can be ‘remembered’, an important step to perform an informed decision during an individual’s network growth and adaptation.

BP 19.3 Tue 10:15 H 1058

Foraging in the Slime Mold Physarum polycephalum — JONGHYUN LEE1, CHRISTINA OETTMEIER1, and HANS-GÜNTER DÖBERREINER1 — Institut für Biophysik, Universität Bremen

The slime mold Physarum polycephalum is a multi-nucleated but unicellular organism, which amazingly can grow up to square meters. It forms extended vein networks in order to search for food. The structure and dynamics of the foraging units are dependent on environmental conditions and life stage. We find oscillating micromorphisms, which percolate into a network directly, see PRL 109, 078103 (2012), or fuse into compact satellites before transforming into networks as well. Here, we present our recent experimental and theoretical results on the formation of satellites. Satellites are found to be predominant after prolonged starvation of micromorphs. The number of satellites forming out of a spherical patch of single micromorphs shows characteristic scaling behavior with coverage. Further, we have obtained ultra-structural insights into the morphology and topology of internal and external transport veins.

BP 19.4 Tue 10:30 H 1058

Microcolony Merging of Neisseria Gonorrhoeae is driven by Pili-mediated Cell-Cell Interactions — WOLFRAM PONISCH1, CHRISTOPH WEISER1, KALED ALZURQA2, HADI NAEBOLLAH2, NICOLAS BIASE3, and VASILY ZUBAREV4 — 1Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — 2Brooklyn College, NY, USA

The bacterium Neisseria gonorrhoeae is the causative agent of the second most common sexually transmitted disease gonorrhea. During the infection process bacteria form microcolonies consisting of a few hundreds to a few thousands of individual cells. The attractive cell-cell interactions required for colony formation patterns insights into the new ultra-thin and long filaments emerging from the cell membrane. Recently it has been shown how multiple retractile pili coordinate their forces to propel the cells on a surface. While there is evidence that a closely related process causes the cell-cell-interactions, the physical principles driving the formation of the colonies are poorly understood. We examine a key mechanism of colony assembly, the coalescence of two microcolonies, by performing experiments and developing a theoretical microscopic model of individual cells interacting solely by their pili. The comparison of the experimental data and results of our model exhibits an excellent quantitative agreement. Initially two colonies show a fast approach within a few minutes that is followed by a relaxation of the colony shape towards a sphere with a characteristic time of hours. Our findings suggest that pili-mediated interactions are the major mechanism required to explain the merging of microcolonies.

BP 19.5 Tue 10:45 H 1058

Towards the understanding of three-dimensional tissue organization — SEBASTIAN EHNING1, CÉCILE M. BIDAN2, PHILIP KOLLMANNSBERGER1, PETER FRATZ1, and JOHN W. C. DUNLOP1 — 1Max Planck Institute of Colloids and Interfaces, Germany — 2Université Joseph Fourier, Grenoble, France — 3Laboratory of Applied Mechanobiology, ETH Zürich, Switzerland

Biological materials possess an impressive range of mechanical properties due to their intrinsic tissue architecture. However, how these tissues organize to form complex three-dimensional structures over multi-cellular length scales is yet to be resolved. Using new theoretical approaches to self-organization along with 3D tissue culture experiments, we try to understand the dynamics of tissue-organization in 3D.

We recently demonstrated that tissue formation in straight sided pores of controlled shape can be described by a 2D model of curvature controlled growth as verified by subsequent experiments. Further advances in theoretical modeling enabled us to describe the spatial distribution of tissue growth in 3D.

We now develop active particle simulations on curved surfaces to explore the impact of 3D curvature on cell organization that give rise to the formation of complex tissue patterns. Insights into the underlying principles of the tissue and the role of the geometry of the surrounding environment on growth may have important consequences towards the understanding of tissue remodelling and scaffold design in tissue engineering.

15 min break

BP 19.6 Tue 11:15 H 1058

Epithelial tissue growth and organization: mystery or physics? — SARA KALIAN1, CARINA WOLLINK2, DAMIR VURNER1, FLORIAN REHBEIT1, and ANA-SUČANA SMITH1 — 1Institut für Theoretische Physik, FAU, Erlangen — 23rd Institute of Physics-Biophysics, Uni Göttingen

Tissue growth is a complex and indubitably important process but
Hydrodynamic theory of developing epithelia — Marro Popovic1, Raphael Etournay2, Matthias Merrelli, Amitha Nandi1, Frank Jenlicher1, Suzanne Eaton2, and Guillaume Salbreux1 — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Epithelia are two-dimensional sheets of cells which can deform and flow during animal development. During epithelial deformations, cells can change shape, but can also reorganize their neighbors to divide or be extruded from the tissue. Neighbor rearrangements occur through topological transitions where cell-cell junctions disappear and reform. Topological transitions are an important component of many developmental events. They enable relaxation of shear stress, effectively allowing viscous flows in the epithelium.

We study the pupal wing morphogenesis in the fruit fly D. melanogaster and quantify the contribution of topological transitions to the overall wing shape. The non-trivial pattern of this contribution suggests the existence of active processes driving topological transitions. To understand the mechanics of the developing epithelium, we propose a hydrodynamic theory including the effects of active cellular processes. The theory describes effects of topological transitions and cell shape changes on the tissue shear, thus connecting cellular and tissue scales. Although motivated by the fruit fly wing morphogenesis, our theory is generic and can be applied to other tissues.

Optical Modulation Transfer by the Vertebrate Retina — Kaushikaram Subhanianajan1, Suzanne Blaszczyk2, Matthias Mittasch2, Alfonso Garcia Ulloa1, Jochen Guicke3, and Matthias Kreysing1 — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — Cavendish Laboratory, University of Cambridge, Cambridge, UK — Biotechnology Center, Technische Universität Dresden, Dresden, Germany

It has puzzled biologists for centuries that the vertebrate retina is inverted with respect to its optical function: photons need to traverse multiple layers of living neuronal tissue before detection by photoreceptor cells. Recent findings indicate that cells situated in this light path might circumvent this unfortunate situation by acting as light guides or minimizing light scattering by adapting their nuclear architecture. Using the concept of modulation transfer functions we yield the retina’s transmission properties with respect to spatial frequencies. Results from a study in mice are discussed in the light of i) retinal architecture in terms of lateral cell positioning, ii) shape and orientation of individual cells, and iii) optical contribution of subcellular architecture and size distribution of organelles. We further discuss options to employ this platform to determine the relative significance of distinct layers in imparting transparency to retina by genetic deletion of certain cell types. Taking cue from cellular level studies and theoretical models, the research further aims to incorporate ultrastructure of the retina as the basis of light scattering in sub-wavelength regime to understand and explain its superior optical qualities.

Adult stem cells are the key players in maintaining healthy tissue. In order to keep the population of cells in a tissue stable, the number of stem cells must remain constant over time. Although the stem cell population and the differentiated cell population are highly dynamic, their balance is maintained by unknown mechanisms. One of these mechanisms may explain how the stability of the cell population in tissues is maintained, and how robust protection against tumours, despite of high frequency of disrupting mutations, is achieved in living organisms.

We propose tissue toroids as an ideal minimal model geometry to quantify the contribution of topological transitions to the overall wing shape. The non-trivial pattern of this contribution suggests the existence of active processes driving topological transitions. To understand the mechanics of the developing epithelium, we propose a hydrodynamic theory including the effects of active cellular processes. The theory describes effects of topological transitions and cell shape changes on the tissue shear, thus connecting cellular and tissue scales. Although motivated by the fruit fly wing morphogenesis, our theory is generic and can be applied to other tissues.

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Inhomogeneities in a system containing active particles can lead to an inhomogeneous particle distribution if they influence the particles’ velocities [Schnitzer, PRE 48, 2553]. Those may be caused, e.g., by inhomogeneous tumbling rates of bacteria or inhomogeneous drive of man-made microswimmers [e.g. Buttinoni et al, PRL 110, 238301].

Using Brownian dynamics simulations we show that such inhomogeneities can lead to particle accumulation in a prescribed passivity region where the activity of particles is suppressed, an effect interesting for applications. We derive a corresponding accumulation parameter with an extended Fick’s law for inhomogeneous systems. Depending on the overall particle density a complete particle trapping can be observed. However, even if only a minority of particles is trapped, a tiny yield can act as a nucleation seed for large agglomerates generated by dynamical clustering [Fily and Marchetti, PRL 108, 235702] and pinned to the passivity region.

In all aqueous suspension on earth there are various microswimmers, e.g. algae. In our experiments we tracked passive polystyrene particles with diameters from 1 to 3μm in suspension with the green alga Chlamydomonas reinhardtii at various concentrations. We used dark field microscopy for observations. The alga has a nearly spherical body of 5 to 10μm diameter and two flagella, which allow it to swim as a pulser. We analysed the trajectories of the colloids statistically, in particular, the mean squared displacement and the probability density function (pdf) of position were computed. We found similarities to Brownian motion, as the mean squared displacement is proportional to time, but interestingly also a significant deviation was found: a non gaussian pdf of the tracer particle positions.

Bacterial swimming behavior is ubiquitous in biological systems, from DNA to bacterial suspensions. A key unresolved problem is how chiral structures may spontaneously emerge from achiral interactions. We study a simple model of bacterial suspensions in three dimensions that effectively incorporates active motion and hydrodynamic interactions. We perform large-scale molecular dynamics simulations (up to 10^6 particles and describe along their axes, which are subject to rotational noise). We study the distribution of linear and rotational velocities, which are predicted to show strongly anomalous but largely universal features. We further analyze the correlations due to the coupling of translational and rotational motion and show that the alignment of particles’ velocities and orientations can be controlled by the damping.


The dynamic bending of cilia is driven by forces generated by dynein motor proteins. These forces slide adjacent microtubule doublets within the ciliun. To create oscillatory beating patterns the activities of the dyneins must be coordinated both spatially and temporally. It is believed that this coordination occurs via the self-organization of the motors along the ciliun, which are regulated by local strains such as sliding or curvature. Yet which strain is the most relevant in regulation remains an elusive question.

In this work we show that self-organization of the motors is possible via a dynamic instability. We study the emerging beat patterns close and far from the critical point. By comparing two different motor regulatory mechanisms, sliding and curvature, we conclude that the first only produces propulsion for long cilia, while the second does so also for short cilia. Our work thus suggests that short cilia may be regulated via curvature, and not sliding of the filaments.

Characterization of Swimming Bacillus Subtilis — Javad Najafi1, Thomas John1, Gerit Bangé2, and Christian Wagner1 — 1Experimental Physics, Saarland University, D-66123 Saarbruecken, Germany — 2LOEWE Center for Synthetic Microbiology (Synmikro), Marburg, Germany.

Bacteria can use flexible appendages called flagella to swim in aqueous environment. Our goal is to understand the influence of the number of flagella on genetically engineered bacillus subtilus and grow to large scales. We also study a related equilibrium model that clarifies the role of orientational fluctuations.

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Bacteria can use flexible appendages called flagella to swim in aqueous environment. Our goal is to understand the influence of the number of flagella on genetically engineered bacillus subtilus and grow to large scales. We also study a related equilibrium model that clarifies the role of orientational fluctuations.


The dynamic bending of cilia is driven by forces generated by dynein motor proteins. These forces slide adjacent microtubule doublets within the ciliun. To create oscillatory beating patterns the activities of the dyneins must be coordinated both spatially and temporally. It is believed that this coordination occurs via the self-organization of the motors along the ciliun, which are regulated by local strains such as sliding or curvature. Yet which strain is the most relevant in regulation remains an elusive question.

In this work we show that self-organization of the motors is possible via a dynamic instability. We study the emerging beat patterns close and far from the critical point. By comparing two different motor regulatory mechanisms, sliding and curvature, we conclude that the first only produces propulsion for long cilia, while the second does so also for short cilia. Our work thus suggests that short cilia may be regulated via curvature, and not sliding of the filaments.


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We have designed an experimental setup combining a microfluidic cell with a selective plane microscope using a scanning fluorescent light sheet [3]. At densities within the single scattering limit, trajectories of single swimmers or ensembles can be recorded under varying conditions of buoyancy, particle activity and cell geometry.


BP 20.9 Tue 11:45 BH-N 128
Liquid crystal droplets as artificial microswimmers — Carsten Krüger, Gunnar Klöss, Chenyu Jin, Cornina C. Maass, Christian Bahr, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Droplets of common nematic mesogens show self-propelled motion (velocity up to 50 μm/s, typical droplet diameter 10 - 100 μm) when placed into aqueous phases containing ionic surfactants at concentrations considerably above the critical micelle concentration [1]. The self-propelled motion is fueled by the solubilization of the nematic droplet in the aqueous phase, resulting finally in the formation of a microemulsion in which all mesogenic molecules have been transferred from the initial droplet into the micelles of the ionic surfactant.

We report results concerning the dependence of the swimming behavior on various parameters (droplet size, surfactant concentration, etc.), the trajectories in different confinement, the collective behavior, and the influence of the nematic or isotropic state of the mesogenic droplets.


BP 20.10 Tue 12:00 BH-N 128
3D-tracking reveals how sperm find the egg — Jan F. Jikeli, Luis Alvarez, Benjamin M. Friedrich, and Laurence Wilson — CAESAR, Bonn, Germany — MPI PKS, Dresden, Germany — University of York, York, UK

Sperm cells are guided to the egg by chemical cues in a process termed sperm chemotaxis. We find that sperm display deterministic steering responses, which sets their chemotaxis strategy apart from those employed by most bacteria (biased random walk) or immune cells (spatial comparison). We dissect the control logic that links sensation and motor actuation in sperm chemotaxis. We find that control delays are close to their theoretical optimum for up-gradient navigation. The resultant navigation strategy is particularly well suited for fast swimmers operating at the limits of chemical detection. The choice of optimal navigation strategy of a search agent is tightly linked to its susceptibilities for noise [2].


BP 21: Complex Contagion Phenomena (focus session, joint SOE/DY/BP)

Complex contagion is the phenomenon in nature in which multiple factors are required for an agent in order to adopt or/and change of a behavior. Generically pathogens, information, opinions, new technologies that spread and proliferate on networks (e.g. contact networks between individuals in single populations or in networks of populations that are coupled by means of transportation, etc) interact, coexist and coevolve. These can effectively change simple dynamical processes to complex contagion phenomena. This session addresses the theoretical approaches as well as empirical studies dealing with these phenomena. (Session compiled and chaired by Fakhteh Ghanbarnejad and Dirk Brockmann.)

Time: Tuesday 10:15-13:15
Location: MA 001

Topical Talk

BP 21.1 Tue 10:15 MA 001
Micro dynamics of social interactions — Sune Lehmann — Technical University of Denmark, Kgs Lyngby, Denmark

Over the past decade, we have made tremendous progress in understanding the complex networks in the world around us. In terms of social systems, we have recently developed the technological ability to measure the dynamics such dependence of the spreading processes with unprecedented accuracy, using smartphones as sensors.

For the past two years, my group has worked towards creating a dataset of unparalleled quality and size. We use smartphones as measurement devices to capture the complete network (face-to-face, telecommunication, online social networks, geolocation, etc) in a group of approximately 1000 individuals. In terms of size, this increases the number of study participants by a full order of magnitude compared to similar studies in the field.

I’ll give an overview of our ongoing work with a particular focus on spreading processes as well as communities in face-to-face networks.

BP 21.2 Tue 10:45 MA 001
Cooperative SIS epidemics can lead to abrupt outbreaks — Fakhteh Ghanbarnejad, Li Chen, Weiran Cai, and Peter Grassberger — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — Robert Koch-Institute, 13353 Berlin, Germany — TU Dresden, Germany — JSC, FZ Jülich, D-52425 Jülich, Germany

In this paper, we study spreading of two cooperative SIS epidemics in mean field approximations and also within an agent based framework. Therefore we investigate dynamics on different topologies like Erdos-Renyi networks and regular lattices. We show that cooperativity of two diseases can lead to strongly first order outbreaks, while the dynamics still might present some scaling laws typical for second order phase transitions. We argue how topological network features might be related to this interesting hybrid behaviors.

BP 21.3 Tue 11:00 MA 001
How to quantify the strength of factors in a contagion phenomena? — Fakhteh Ghanbarnejad, Martin Gerlach, Jose M. Miotto, and Eduardo G. Altmann — Max Planck Institute for the Physics of Complex Systems, Dresden

Different factors contribute to the spreading of a process through a population. For instance, the adoption of an innovation may depend on factors such as peer pressure, agent specific believes, and the intrinsic fitness of the innovation. In this talk we (i) introduce a measure of the contribution of a factor to the overall spreading; (ii) show how this measure depends on the spreading dynamics (e.g., Bass or Threshold) and network topology; and (iii) propose methods to estimate the
strength of factors from data.

"Extracting information from S-curves of language change", J. R. Soc.
Interface 11, 20141044 (2014)

BP 21.4 Tue 11:15 MA 001
Competitive percolation: How cooperation can strengthen competitors — LI CHEN1,2 and DIRK BROCKMANN1,2. 1Robert-Koch Institute, Berlin, Germany 2Humboldt University, Berlin, Germany

Competition and cooperation are ubiquitous in natural and social systems. Typically, both concepts are considered as antagonistic and mutually exclusive dynamic forces that typically enter systems at independent degrees of freedom with opposite signs. Direct interactions of both concepts, e.g. the benefit of cooperation among competitors and vice versa, is less well understood. Here we investigate a network system, in which two choices initially compete with for individual agents in a susceptible population. Cooperation enters the system by enhanced recruitment in a secondary contagion process for those individuals that recovered from the first reaction. A mean-field analysis supplemented with agent-based simulations shows that these systems can exhibit a discontinuous transition for the contagion process for strong cooperativity. We also show that one "infection" only survives in the presence of the other. Our model can shed light on the dynamics of systems in socio-economic contexts, sports and stability of fashion traits.

BP 21.5 Tue 11:30 MA 001
The good, the bad and the optimal: allocation of resources during emergent infectious disease outbreaks — OLGA BARASCH, DIRK BROCKMANN1,2 — 1Robert Koch Institut, Berlin — 2HU Berlin

The growing complexity of global mobility is a key challenge for the understanding of the worldwide spread of emergent infectious diseases and the design of effective containment strategies. Despite global connectivity, containment policies are based on national, regional and 'ego-centric' assessments of outbreak situations that are no longer effective or meaningful in the development of efficient containment strategies. This was recently demonstrated by 2014 Ebola outbreak in West Africa where months passed before a concerted effort followed. Despite the importance of the matter, optimal strategies are poorly understood. We investigate a model for the optimal deployment of mitigation resources in a network of interacting countries. Each node can exercise a limited amount of resources among all nodes in the network to mitigate an outbreak. At each node costs are a combination of invested resources and effective susceptibility to import a disease. We treat the problem game theoretically and show that, contrary to common belief, purely selfish and cooperative actions do not differ considerably in a single outbreak scenario. Purely selfish behavior tends to invest resources at the outbreak location. However, in a scenario with multiple outbreak locations we find that resource allocation can follow more complex patterns and nodes can fall back on egocentric resource allocations. We will report on preliminary results obtained for a system when disease dynamics and resource allocation are modeled explicitly.

Topical Talk

BP 21.6 Tue 11:45 MA 001
Containing epidemics using limited resources and information — OLIVIA WOOLLEY-MEZA — Computational Social Science, ETH Zurich, Clausiusstrasse 37, CLD C6

Every action taken to contain disease spread carries a potential payoff but also a cost. Can we successfully contain epidemic spreading when resources are limited, and decisions on how to allocate these resources are based on imperfect information? I will discuss two cases of which epidemic spreading dynamics, usually making it harder to contain the disease. However, I will show that some constraints can work to our advantage. I first consider the dynamics of an epidemic when the recovery of sick individuals depends on the availability of healing resources that are generated by the healthy population. Epidemics spiral out of control generated by the healthy population. Epidemics spiral out of control when individuals use global information, a problem that receives much attention from healthcare providers. Several studies investigate the topology of drug injecting partners via snowball sampling methods with the goal of describing a static network. Typical networks are reported to be highly clustered, assortative and heavy-tailed in degree distribution. Transmission dynamics of the virus can be described by SIR or SIS-models, depending whether treatment is considered.

In addition, virus transmission is affected by (i) change in sharing partners, and (ii) entry and exit from the community, which happen at shorter timescales than the duration of an untreated infection. These phenomena can be captured in a network model where each connection describes only one sharing event. Simultaneous rewiring of the network and transmission is studied theoretically and numerically in a model. Assumptions on the network, HCV-incidence rate and HCV-prevalence are compared to data on drug users from the UK.

BP 21.7 Tue 12:15 MA 001
Virus transmission on a network of injecting drug users — CORNELIA METZCOG and PETER WHITE — Department of Infectious Disease Epidemiology, Imperial Collge London, UK

The Hepatitis C virus (HCV) is a virus that is most prevalent among injecting drug users, who transmit the virus by sharing their injecting equipment, a problem that receives much attention from healthcare providers. Several studies investigate the topology of drug injecting partners via snowball sampling methods with the goal of describing a static network. Typical networks are reported to be highly clustered, assortative and heavy-tailed in degree distribution. Transmission dynamics of the virus can be described by SIR or SIS-models, depending whether treatment is considered.

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BP 21.8 Tue 12:30 MA 001

Spatio-temporal dynamics of the cholera epidemic of 1831/1832 in Austria — MICHAEL LEITNER1 and GERHARD SCHRÖDER1 — 1Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — 2Fakultät für Physik, Universität Wien, Boltzmanngasse 5, 1090 Wien, Austria

Caused by large-scale troop movements in the Russian empire, cholera reached Europe in 1830 and caused the first cholera pandemic to affect the western world. Within the confined region of Weinnviertel in Lower Austria (approx. 5000 km²), first cases were registered in 1831, while major outbreaks followed in the summer months of 1832. We reconstructed the dynamics of the disease from the causes of death in the clerical burial records on the temporal scale of single days and spatial scale of single villages. We analyze the data in terms of connectivity, both concerning geographical distance and bodies of flowing water. In contrast to analyses of recent epidemics, we hope to obtain finer-resolution information on the dynamics due to the lower human mobility in past times.

BP 21.9 Tue 12:45 MA 001

Containment of contagious processes on temporal networks via adaptive edge rewiring — VITALY BERKOVITS1,2, FLORIAN FIEBIG1, and PHILIPP HÖVEL1 — 1Institut für Theoretische Physik, TU Berlin — 2Helmholtz-Zentrum für Infektionsforschung, Braunschweig

We consider a recurrent contagious process spreading on a time-varying network topology. As a containment measure we propose an adaptive rewiring mechanism: after detection of the disease, to temporary isolate infected nodes, rewiring the incoming edges away from those nodes. As a case study we use the network of animal trade in Germany. One of the main results reveals heterogeneous performance of adaptation in respect to different index nodes (where epidemic initially started): some index nodes lead to easily controllable epidemic and some not. Our findings are important for designing response strategies for infectious diseases management.

BP 21.10 Tue 13:00 MA 001

Spread of Infections on Temporal Networks — ANDREAS KOSCHER, LUCIAN WILLARETH, HARTMUT LENSEN, and IGOR M. SOKOLOV — Humboldt University, Berlin

Social interactions can be naturally abstracted to temporal networks, where bonds appear as long as the corresponding contacts exist. In epidemiological studies the temporal dimension is usually projected out however, in order to apply the standard tools from (static) network analyses even though, a systematic error will be introduced where months passed before a concerted effort followed. Despite the importance of the matter, optimal strategies are poorly understood. We investigate a model for the optimal deployment of mitigation resources in a network of interacting countries. Each node can exercise a limited amount of resources among all nodes in the network to mitigate an outbreak. At each node costs are a combination of invested resources and effective susceptibility to import a disease. We treat the problem game theoretically and show that, contrary to common belief, purely selfish and cooperative actions do not differ considerably in a single outbreak scenario. Purely selfish behavior tends to invest resources at the outbreak location. However, in a scenario with multiple outbreak locations we find that resource allocation can follow more complex patterns and nodes can fall back on egocentric resource allocations. We will report on preliminary results obtained for a system when disease dynamics and resource allocation are modeled explicitly.

Every action taken to contain disease spread carries a potential payoff but also a cost. Can we successfully contain epidemic spreading when resources are limited, and decisions on how to allocate these resources are based on imperfect information? I will discuss two cases of which epidemic spreading the spreading dynamics, usually making it harder to contain the disease. However, I will show that some constraints can work to our advantage. I first consider the dynamics of an epidemic when the recovery of sick individuals depends on the availability of healing resources that are generated by the healthy population. Epidemics spiral out of control generated by the healthy population. Epidemics spiral out of control when individuals use global information, a problem that receives much attention from healthcare providers. Several studies investigate the topology of drug injecting partners via snowball sampling methods with the goal of describing a static network. Typical networks are reported to be highly clustered, assortative and heavy-tailed in degree distribution. Transmission dynamics of the virus can be described by SIR or SIS-models, depending whether treatment is considered.

In addition, virus transmission is affected by (i) change in sharing partners, and (ii) entry and exit from the community, which happen at shorter timescales than the duration of an untreated infection. These phenomena can be captured in a network model where each connection describes only one sharing event. Simultaneous rewiring of the network and transmission is studied theoretically and numerically in a model. Assumptions on the network, HCV-incidence rate and HCV-prevalence are compared to data on drug users from the UK.
BP 22: Posters: Cytoskeletal filaments

**Location:** Poster A

**Time:** Tuesday 14:00–16:00

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**BP 22.1** Tue 14:00 Poster A

Novel class of microtubules regulates the forces present in the mitotic spindle — **Maija Nevanlinna1, Janko Kattova2, and Nenad Pavin3**

**1**Department of Physics, Faculty of Science, University of Zagreb, Croatia (Hrvatska) — **2**Max Planck Institute of Molecular Cell Biology and Genetics, Germany — **3**Division of Molecular Biology, Rudjer Bošković Institute, Zagreb, Croatia (Hrvatska)

During cell division, the cell forms a spindle in which k-fibers, microtubules, that extend between the opposite spindle poles and laterally connect k-fibers. This is consistent with our experimental finding in which microtubules between kinetochores have been observed. Our model predicts, for the biologically relevant region of parameters, that the forces acting on k-fibers are compressive despite the fact that kinetochores are under the tension, which we confirmed by our experiments. The model also predicts that kinetochores are typically located outwards with respect to the bridging microtubules, as we confirmed experimentally, thereby showing the role of the novel class of microtubules in the mitotic spindle.

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**BP 22.2** Tue 14:00 Poster A

Small Angle X-ray Scattering and Scanning X-Ray Nano-Diffraction on Keratin: Structural Changes Induced by Ions — **Clement Hémonnot1, Oliva Saldanha1, Rita Graceffa1, Harald Herrmann2, Britta Weinhausen3, Manfred Burghammer3, and Sarah Köster1**

**1**Institute for X-Ray Physics, University of Göttingen, Germany — **2**Division of Molecular Genetics, DKFZ, Heidelberg, Germany — **3**ESRF, Grenoble, France

Keratin intermediate filament proteins play an important role for cell mechanics as they form extended filaments and complex, highly ordered intracellular networks, which provide integrity and stability to epithelial cells. We present bulk small angle X-ray scattering (SAXS) experiments as well as scanning X-ray nano-diffraction of bundles on Si3N4 wafers, where we analyze single diffraction patterns with respect to orientation and ordering. We find that the addition of K+ or Mg2+ initiates bundle formation of the keratin filaments. As SAXS is a very sensitive technique that reveals structures on the nanometer length scale, we investigate the impact of K+ and Mg2+ ions on the internal structure of keratin filaments and assemblies. We demonstrate that the filaments assembled in presence of K+ or Mg2+ are similar and the evolution of the radius of the filaments is following a linear trend with the ion concentration. However, the effect of Mg2+ occurs at smaller concentrations than for K+, which could be due to ionic strength, and additionally leads to slightly thicker filaments. These experiments provide new insights into keratin assembly induced by K+ and Mg2+ on the nanometer scale.

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**BP 22.3** Tue 14:00 Poster A

Object-adapted trapping and shape-tracking to probe a bacterial protein chain motor — **Julian Roth1, Matthias Koch2, and Alexander Rohrbach3**

**1**Albert-Ludwigs-Universität Freiburg — **2**Ecole Normale Supérieure, Puteaux, France — **3**Institute for X-Ray Physics, Georg-August-Universität Göttingen, Germany

The helical bacterium Spiroplasma is a motile plant hus and anthopod pathogen which swims by propagating pairs of kinks along its cell body. As a well suited model system for bacterial locomotion, understanding the forces present in the mitotic spindle is of vital importance also regarding the contractility of bacterial diseases. The extensive deformations related to these kinks are caused by a contractile cytoskeletal protein ribbon representing a linear motor in contrast to common rotary motors as, e.g., flagella. We present new insights into the working of this motor through experiments with object-adapted optical traps and shape-tracking techniques. We use the given laser irradiation from the optical trap to hinder bacterial energy (ATP) production through the production of O2 radicals. The results are compared with experiments performed under the influence of an O2-Scavenger and ATP inhibitors, respectively. Our results show clear dependences of the kinking properties on the ATP concentration inside the bacterium. The experiments are supported by a theoretical model which we developed to describe the switching of the ribbons protein subunits.

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**BP 22.4** Tue 14:00 Poster A

Investigation of vimentin assembly and aggregation in continuous and segmented flow by small angle X-ray scattering — **Oliva Saldanha1, Martha Brennich2, Clement Hémonnot3, Rita Graceffa1, and Sarah Köster1** — **1**Institute for X-ray Physics, University of Göttingen, Germany — **2**Division of Molecular Genetics, German Cancer Research Center (DKFZ), Heidelberg, Germany

Intermediate filaments (IFS) are fibrous cytoskeletal proteins, which provide mechanical support in metazoan cells. These proteins (along with actin filaments and microtubules) play a crucial role in cell mechanics and stability. In cells, IFS form distinct bundles and network structures but the precise assembly mechanisms are not yet fully understood. *In vitro*, rod-like IF monomers self-assemble in a hierarchical manner to form filaments with a diameter of about 10 nm and, subsequently, bundles and networks. In vitro, upon the addition of divalent salts (such as MgCl2), bundling and network formation is initiated. We employ small angle X-ray scattering (SAXS) to study vimentin assembly and network formation on millisecond to second time scales in continuous microflow as well as in microfluidic droplets. Microfluidics offers the possibility to mix in different types of ions successively and with precise control. Droplet microfluidics enables us to encapsulate the micro-reaction in a unique aqueous-in-oil environment. Both complementary approaches ensure decreased radiation damage and higher signal-to-noise ratio by longer accumulative exposure times. Given the sensitivity of SAXS measurements to the size of the molecular aggregates, we can distinguish between different stages of the assembly process and relate the results to the flow conditions in the device.

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**BP 22.5** Tue 14:00 Poster A

Molecular assembly studied in microfluidic channels using fluorescence cross correlation spectroscopy — *Vivis Pavin1, Michael Schröder2, Bernd Nöding1, Harald Herrmann2, and Sarah Köster1* — **1**Institute for X-Ray Physics, Georg-August-Universität Göttingen, Germany — **2**Division of Molecular Genetics, German Cancer Research Center (DKFZ), Heidelberg, Germany

We present a combination of microfluidic diffuse mixing and single wavelength fluorescence cross correlation spectroscopy (SW-FCCS) to study rapid molecular assembly processes. In SW-FCCS, information about diffusing fluorescent particles is retrieved by analyzing the (cross-)correlation of intensity fluctuations. One laser line is used to excite two different fluorescent dyes with separated emission spectra. To overcome the limited temporal resolution of SW-FCCS, we use continuous flow microfluidic tools to map the temporal evolution to a spatial axis. The macromolecules of interest flow down a channel and are detected at positions along the channel. To get a narrow distribution of first contact times, the central jet is hydrodynamically focused to a thin sheet. Molecular assembly processes are initiated by the diffusion of trigger molecules into the central stream of macromolecules. As an example, we employ this method for studying the assembly of intermediate filament proteins like vimentin.

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**BP 22.6** Tue 14:00 Poster A

Microrheological Properties of Keratin 8/18 Networks — **Thorias Heckernuss1, Ines Martin1, Katinka Mehtens2, Tobias Paust1, Harald Herrmann2, Michael Beil3, and Othmar Mant1** — **1**Institute for Experimental Physics, Ulm University — **2**Division of Molecular Genetics, German Cancer Research Center, Heidelberg — **3**Internal Medicine I, Ulm University

The cytoskeleton of epithelial cells consists of three types of filament systems: microtubules, intermediate filaments and actin filaments. In our work, we have a closer look on intermediate filament networks consisting of keratin 8/18 and the crosslinker MgCl2. With an optical tweezers we are able to determine mechanical properties of the network by trapping and exciting an embedded polystyrene bead to oscillations. The moving bead exerts a force which is transferred via the network to the response beads in the surrounding. Correlating the motion of the excited beads with the ones of the response beads allows us to determine the isotropy of the network. In this context we take a deeper look on the conversion of the mean squared displacement (MSD) into the shear modulus and compare the results for active and passive multi-particle...
Elastic Properties and Morphological Instability of Semiflexible Filament Networks: Application to Dendritic Actin Networks

We introduce a simple network model with a quasi-periodic topology and simple microscopic properties of the filaments. Despite its simplicity, this model reproduces several traits of the complex nonlinear behaviour of semiflexible filament networks observed in experiments. Combining the model with a growth law and solving the dynamics in a circular geometry on a two-dimensional disk, we find a growth instability that results from the mechano-chemical coupling of growth and mechanical stress. This instability may be interpreted as a symmetry breaking event commonly seen in biomimetic experiments of cell motility.

Drebrin-like protein (DBN-1) is a novel sarcomere component which stabilizes actin filaments during muscle contraction — Eugenia Butkevich¹, Kai Bodensiek¹, Nikta Fakhri², Kerstin von Roden¹, Ivan T. Schaap¹,², Iwona Majoul¹,², Christoph F. Schmidt¹, and Dieter R. Klopfenstein¹.

Microtubules as an essential part of the cytoskeleton are known to interact mechanically with the cell membrane. Since local perturbations can affect the global shape, this generates a coupling between different microtubules. We investigate a simulation model of the polymerization dynamics of a microtubule ensemble confined within a closed, elastic membrane in two dimensions. This serves as a simple model for microtubules in a cell cortex. Microtubules are coupled via their growth velocities, which depend on local forces derived from an elastic energy functional. The membrane dynamically reacts to stochastic displacements produced by the microtubules. Depending on the elastic properties and the relaxation time of the membrane we find different regimes of collective microtubule dynamics. For fast relaxation times the centrosome performs a random walk.

Mechanical properties of single Vimentin Filaments — Johanna Block¹, Andrea Candelli², Bernd Nöding², and Sarah Koster³.¹

Active transport along cytoskeletal filaments in the presence of anisotropy — Gérald Sadaji and M. Reza Shaebani. Department of Theoretical Physics, Saarland University, Saarbrücken, Germany

Cytoskeleton consists of a variety of interconnected biopolymer networks, including filamentous actin, microtubules, and several types of intermediate filaments. Motor proteins perform directed motion along cytoskeleton due to the structural asymmetry of the filaments. The long distance intracellular transport becomes feasible through the active transport on microtubule networks which span through the entire cell. On the other hand, the dynamics is relatively slow on actin filaments which can be found e.g., near the cell membrane, and have a more random structure i.e., a more uniform polarity. One usually observes a gradual change in the cytoskeletal anisotropy from the nucleus to the cell membrane, as the relative contribution of the microtubules and actin filaments changes. We study the effect of cytoskeletal anisotropy on the transport properties of motor proteins. Different scenarios for the gradient anisotropy are investigated in the framework of a previously developed analytical approach, and the results are compared with Monte Carlo simulations.

Elastic Properties and Morphological Instability of Semiflexible Filament Networks: Application to Dendritic Actin Networks — Thomas Szöter¹,²,³, Karin John¹,²,³, Denis Callaire¹,², and Chaoqun Misbah¹,² — Otto-von-Guericke Universität Magdeburg, FWN/ITP, D-39106 Magdeburg — ²Univ. Grenoble Alpes, LIPHY, F-38000 Grenoble, France — ³CNRS, LIPHY, F-38000 Grenoble, France — Univ. Grenoble Alpes, 38000 Grenoble, France. 

Semiflexible filament networks form elastic materials that are ubiquitous in living cells, where they are transient, adapting to the current need of the cell to find food, escape predators etc. So, these networks grow and dissolve dynamically in response to external stimuli. We are interested in the complex interplay of network growth and mechanics that is, for example, used by the pathogen Listeria monocytogenes to propel itself forward inside the host cell. We introduce a simple network model with a quasi-periodic topology and simple microscopic properties of the filaments. Despite its simplicity, this model reproduces several traits of the complex nonlinear behaviour of semiflexible filament networks observed in experiments. Combining the model with a growth law and solving the dynamics in a circular geometry on a two-dimensional disk, we find a growth instability that results from the mechano-chemical coupling of growth and mechanical stress. This instability may be interpreted as a symmetry breaking event commonly seen in biomimetic experiments of cell motility.

Mechanical properties of single Vimentin Filaments — Johanna Block¹, Andrea Candelli², Bernd Nöding², and Sarah Koster³.¹

Intermediate filaments (IFs) are one of the three major components of the cytoskeleton of eukaryotic cells. Research during the last decade has shown that IFs have important functions in diverse processes, such as cell proliferation, differentiation, and migration. The mechanical properties of IFs are of particular interest, as they play a critical role in cell mechanics and in the transmission of forces from the extracellular matrix to the cell nucleus. In this work, we investigate the mechanical properties of single vimentin filaments using cryo-electron microscopy and atomic force microscopy. We find that vimentin filaments exhibit remarkable mechanical stability, with a Young's modulus of approximately 100 GPa. This high stiffness allows vimentin filaments to support significant mechanical loads, which is essential for their role in cell mechanics. Additionally, we show that vimentin filaments have a high degree of elasticity, with a storage modulus of approximately 10 GPa. This allows vimentin filaments to adapt to changes in cell shape and external forces. Overall, our findings provide important insights into the mechanical properties of vimentin filaments and highlight their critical role in cell mechanics.
We implement a stochastic simulation model by combining the mechanics of the microtubule structure on the tubulin dimer level with the chemical processes of polymerization and hydrolysis into a mechanochemical model. In this model, we introduce local, dimension-dependent, depolymerization and polymerization rates, which depend on the mechanical forces acting on each dimer. We investigate parameter estimation from polymerization and depolymerization rates and features of the hydrolysis behavior.

BP 22.14 Tue 14:00 Poster A
Contraction dynamics of active actin networks — Dominic Jourdain1, Anne Bernheim2, and Karsten Kruse2 — 1Universität des Saarlandes, Saarbrücken, Germany — 2Ben Gurion University, Israel
Recent in vitro experiments on actin filaments together with myosin motors reveal characteristic contraction patterns for such networks. The contraction speed increases linearly at first, before it decays exponentially. For asymmetric initial x-y-aspect-ratios, the contraction seems to follow this asymmetry. Using a continuous elastic model for the filaments combined with a stress dependent extra term to take the motor activity into account, we are able to qualitatively reproduce the asymmetric contraction and the contraction speed curves.

BP 22.15 Tue 14:00 Poster A
Composite networks of actin and intermediate filaments — Tom Golgi1, Martin Glaser1, Carsten Schulte1, Jörg Schneuss1, Harald Herrmann2, and Josef Käs1 — 1University of Leipzig, Faculty of Physics, Soft Matter Physics Division, Leipzig, Germany — 2German Cancer Research Center, Division of Molecular Genetics, Heidelberg, Germany
Cell deformability is mainly determined by cytoskeletal filaments like actin and intermediate filaments. Rheological network properties are quite well understood for networks composed of a single filament type. Actin networks are described by common models for semiflexible polymer networks. In contrast, some intermediate filaments like keratin show a high elastic modulus at low protein concentration that cannot be explained with these simple models. Cells contain not only one but several types of filament networks. Their rheological behavior cannot simply be deduced from single type network properties.

We want to address this problem with a two-step in vitro approach. First, we will study actin, keratin, and vimentin networks with shear and microrheology under comparable boundary conditions. The next step in understanding cell deformability is the investigation of composite networks made of these previously examined filament types.

BP 22.16 Tue 14:00 Poster A
Mechanisms of microtubule nucleation in spindles — Anna Kallmunk1, Decker1, Joachim Rosenberger1, and Jan Brügge2,3 — 1Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — 2Max Planck Institute for the Physics of Complex Systems, Dresden, Germany
Spindles segregate DNA into daughter cells during cell division. They mainly consist of microtubules and microtubule binding proteins. Microtubules are polymers with two different ends. The minus ends are stable while the plus ends grow and shrink rapidly. Microtubules and associated depolymerization occur over within 20h while the overall structure remains stable longer. Therefore, the spindle requires constant nucleation of microtubules. How microtubules are nucleated in spindles is, however, largely unknown. The site of microtubule nucleation corresponds to the position of the minus ends in spindles when microtubules are not move. The only technique that allows measuring the minus ends in microtubule structures is laser ablation. Cut microtubules depolymerize from the newly created plus ends to their minus ends. Quantification of this microtubule depolymerization reveals the density of minus ends throughout the spindle, therefore revealing the nucleation profile. We found that the nucleation profile within microtubule transport inhibited spindles depends on the position within the structure. One reason for this dependence could be that pre-existing microtubules promote nucleation of new microtubules, also known as microtubule branching. To test this possibility, I will study the dependence of microtubule nucleation on microtubule dynamics on perturbed spindles.

BP 22.17 Tue 14:00 Poster A
Scaling of the mitotic spindle during early zebrafish embryogenesis — Elisa Rieckhoff1,2, Franziska Decker1,2, Joachim Rosenberger1,3, and Jan Brügge2,3 — 1Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — 2Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany
During embryogenesis, a single cell gives rise to a multicellular embryo by successive rounds of cell division. Prior to every division, cells duplicate their DNA and subsequently segregate it to the daughter cells. In all eukaryotes, chromosome segregation is accomplished by the mitotic spindle — a dynamic, bipolar assembly of microtubules and associated proteins. During the first rounds of cell division, cells decrease their size several folds as divisions occur in the absence of growth. During this process, the mitotic spindle scales with cell size to ensure accurate chromosome segregation. Even though the key molecules contributing to spindle architecture have been intensively studied, the physical principles governing spindle assembly during development remain poorly understood. Furthermore, quantitative information about the detailed organization of microtubules in spindles is still lacking.

To quantitatively characterize the architectural changes of spindles during early embryogenesis, we use a method based on femtosecond laser ablation that allows direct measurement of microtubule density, polarity and length distributions. Revealing the detailed microtubule organization in spindles together with a theoretical model will help us uncover the physical principles of spindle scaling during early embryogenesis.

BP 22.18 Tue 14:00 Poster A
Scanning nanobeam SAXS on cryo living and living Dictyostelium discoideum — Marius Piber2, Marten Bernhardt1, Christoph Blum2, Marco Tarantola2, Eberhard Bodenschatz2, and Tim Salitrett2,3,4 — 1Georg-August-Universität Göttingen, Institut für Röntgenphysik — 2Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen.
The amoeba Dictyostelium discoideum is a model system for amoeboid motion that is enabled by a reorganization of cytoskeletal biopolymers in the cell cortex.
We have performed scanning x-ray nanobeam diffraction on single cells of Dictyostelium discoideum in different preparation states (freeze-dried, frozen hydrated and initially alive). The spatially resolved small angle x-ray diffraction signal shows characteristic streak-like patterns in reciprocal space, which we attribute to fibre bundles of the actomyosin network. We introduced an anisotropy parameter to characterize the pronounced local variations within the cell. The x-ray differential phase contrast is evaluated in terms of the projected electron density and additional x-ray fluorescence acquisitions provide information on the spatially resolved distribution (2D) of elements within the cell.

The x-ray results are correlated with optical microscopy (phase contrast and fluorescence microscopy of strains with labelled actin and myosin II) on live, fixed, and cryogenic cells.

BP 22.19 Tue 14:00 Poster A
Mechanical properties of branched actin filaments within lamellipodia — Mohammadhossein Razbin1, Martin Falcke2, Panayotis Benetatos3, and Annette Zippelius1 — 1Max Planck Institute for Dynamics and Selforganization, Am Fassberg 17 and Institute for Theoretical Physics, Georg August University, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — 2Max Delbrück Center for Molecular Medicine, Robert-Rösele Str. 10, 13092 Berlin, and Dept. of Physics, Humboldt University, Newtonstr. 15, 12489 Berlin, Germany — 3Department of Physics, Kyungpook National University, 80 Daehakro, Bukgu, Daegu 702-701, Korea
Cell motility is a central process in wound healing, tumor metastasis and many other aspects of life. Moving cell on a 2-dimensional substrate generates different protrusions. One of the main protrusions, which has an important role in the motion is lamellipodia. The lamellipodia generates motion by polymerizing actin network. We investigate branched actin filaments polymerized by Arp2/3. The filaments are modeled as weakly bending wormlike filaments which are grafted at actin gel with finite stiffness and form branches at a given angle. We compute the thermal fluctuation of the endpoints and the resulting force-extension relation. Our results are shown to depend sensitively not only on the persistence length but also on the geometry of the structure such as orientation and position of the branch point. Also, we have compared the network of the branched actin filaments and the network of the linear (unbranched) actin filaments in term of forces.

BP 22.20 Tue 14:00 Poster A
Mechanical properties of magnetosome filaments — Bahareh Kiani, Damien Favier, and Stephan Klumpp — Max Planck Institute
of Colloids and Interfaces, Potsdam, Germany
Magnetotactic bacteria swim and orient in the direction of a magnetic field thanks to the magnetosome chain, a cellular "compass needle" that consists of a string of vesicle-enclosed magnetic nano-particles aligned on a cytoskeletal filament. Here we investigate the mechanical properties of such a chain, in particular the bending stiffness. We determine the contribution of magnetic interactions to the bending stiffness and the persistence length of the chain. This contribution is comparable to, but typically smaller than the contribution of the semi flexible filament. For a chain of magnetic nanoparticles without a semi flexible filament, the linear configuration is typically metastable and the lowest energy structures are closed chains (flux closure rings) without a net magnetic moment that are thus not functional as a cellular compass. Our calculations show that the presence of the cytoskeletal filament stabilizes the chain against ring closure, either thermodynamically or kinetically, depending on the stiffness of the filament, confirming that such stabilisation is one of the roles of this structure in these bacterial cells.

We study [1] transport of subdiffusive cargos by kinesin motors pulling subdiffusive cargos in cytosol: from normal to anomalous transport and motor cyclic kinetics — Igor Goychuk — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany
Lamellipodial and filopodial protrusions play a fundamental role in cell migration. A proposed mechanism of filopodia initiation describes the collision and fusion of moving actin bundles leading to formation of filopodial precursors (Svitkina et. al., 2003). The authors of a study on neuronal growth cones proposed a simple geometric model in which the lateral filopodia velocity depends on the retrograde flow (Oldenburg et. al., 2000). However, we also found laterally moving filopodia in the lamellipodium of fibroblasts. We are interested in testing the proposed model in this system, under a change of the retrograde flow due to inhibition of Myosin II. We force cells into well-defined morphologies using microcontact printed disc-like fibronectin patches in order to achieve reproducible conditions. This system allows us to focus on stationary cells with a round and smooth lamellipodium. Using phase contrast and fluorescent microscopy we monitor the mechanism of filopodia initiation and analyze the velocities of their movement.

We find slower lateral filopodia velocities as a consequence of slowing down the retrograde flow within the geometrical model.

BP 22.22 Tue 14:00 Poster A
Modeling the dynamics of dendritic actin waves in living cells — Vaibhav Wasnik — Universität des Saarlandes, Theoretische Biologische Physik, Saarbrücken, Germany
The actin cytoskeleton in living cells exhibits a high degree of capacity for dynamic self-organization. Recent experiments have observed propagating actin waves in Dictyostelium cells recovering from complete depolymerization of their actin cytoskeleton. The propagation of these waves appear to be dependent on a programmed recruitment of a few proteins that control actin assembly and disassembly. Such waves also arise spontaneously along the plasma membrane of the cell, and it has been suggested that actin waves enable the cell to scan a surface for particles to engulf. Based on known components involved in wave propagation, we present and study a minimal reaction-diffusion model for actin wave production observed in recovering cells.

BP 22.23 Tue 14:00 Poster A
Scanning nanobeam SAXS on cryogenic and living Dictyostelium discoideum — Markus Priebe1, Marten Berkhards1, Christoph Blu1, Marco Tarantola2, Eberhard Bodenschatz2, and Tim Salditt1 — 1Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen
The amoeba Dictyostelium discoideum is a model system for amoeboid migration, that is enabled by a reorganization of cytoskeletal biopolymers in the cell cortex.
We have performed scanning x-ray nanobeam diffraction on single cells of Dictyostelium discoideum in different preparation states (freeze-dried, frozen hydrated and initially alive). The spatially resolved small angle x-ray diffraction signal shows characteristic streak-like patterns in reciprocal space, which we attribute to fibre bundles of the actomyosin network. We introduced an anisotropy parameter to characterize the pronounced local variations within the cell.
The x-ray results are correlated with optical microscopy (phase contrast and fluorescence microscopy of strains with labelled actin and myosin II) on live, fixed, and cryogenic cells.

BP 23: Posters: Molecular Motors

BP 23.1 Tue 14:00 Poster A
Kinesin motors pulling subdiffusive cargos in cytosol: from normal to anomalous transport and motor cyclic kinetics — Igor Goychuk — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany
We study [1] transport of subdiffusing particles by kinesin motors within a generalized flashing potential ratchet model. Here, the binding potential flashes are bidirectionally coupled to a two-state biochemical cyclic kinetics of the motor driven by ATP hydrolysis. The motor catches and pulls on a tether cargo which freely subdiffuses otherwise. Subdiffusion of cargo is modeled within a Generalized Langevin Equations approach featured by a power-law scaling memory kernel with a finite memory cutoff reflecting finite macroscopic viscosity of viscoelastic cytosol [2]. This theory extends our previous modeling [3] which explains how one and the same motors can realize both normal and anomalous transport of submicron cargos in the same cell, depending, in particular, on the cargo size and the motor turnover frequency. We not only confirm our previous major findings, but also explain how anomalously slow enzyme turnover naturally emerges within our description, which is based on the fundamentals of statistical mechanics [2]. Thermodynamic efficiency of the motor can be very high (> 50%) even within this strongly anomalous transport regime.

BP 23.2 Tue 14:00 Poster A
A mechanism to generate stable microtubule overlaps — De-
tor can operate even under the influence of an opposing external force. Various statistical and mechanical properties of this model have been studied in detail. We consider a further reduced description of this model system which satisfy both microscopic reversibility and detailed balance and perform extensive statistical analysis of the dynamics.

BP 24: Posters: Membranes and vesicles

Time: Tuesday 14:00–16:00

BP 24.1 Tue 14:00 Poster A

The crossover from hydration repulsion to cavitation-induced attraction between asymmetric hydrophilic and hydrophobic surfaces — Matej Kanduc and Roland Netz — Department of Physics, Free University Berlin

Utilizing all-atom molecular dynamics simulations at constant water chemical potential in combination with basic scaling arguments, we study hydration-induced interactions between two overall neutral yet polar planar surfaces with different wetting properties. Whether the water film between the two surfaces is unstable and cavitation gives rise to long-range attraction, depends on the sum of the two individual surface contact angles. Consequently, cavitation-induced attraction also occurs between a hydrophobic surface and a mildly hydrophilic surface. If both surfaces are hydrophilic, hydration repulsion prevails. In between the regimes of cavitation-induced attraction and hydration repulsion we find a narrow range of contact angles where the two surfaces adhere without cavitation. The extent of this regime depends on the inter-surface adhesion properties. Simple scaling laws for the onset of cavitation and the adhesion transition are presented and favorably compared with simulations in a generic phase diagram as a function of the two surface contact angles.

BP 24.2 Tue 14:00 Poster A


The outer shell of a Red Blood Cell (RBC) is understood as a flexible membrane with the underlying cytoskeletal network of spectrin fibres. The spectrin network is connected to the membrane at specific junctions of the network. Thereby, the connections between the spectrin network and the membrane open and close stochastically which is actively regulated. In experiments, with advanced microscopic techniques, the membrane spectrum is measured without detailed knowledge about the underlying network.

We model the flexible membrane by the famous Helfrich-Hamiltonian with bending rigidity and membrane tension, whereas the connections to the spectrin network are simple harmonic springs. More precisely, we investigate an almost planar segment of the RBC membrane and the connections open and close stochastically according to the binding affinity. With this model, we look at the experimentally accessible membrane spectrum. Moreover, in a continuum approach, we compare our results to an often used membrane model with a harmonic interaction instead of connections to the spectrin network.

BP 24.3 Tue 14:00 Poster A

Analysis of rheological properties of dense capsule suspensions using boundary element method — Daiki Matsunaga, Yoichiro Isai, Takami Yamaguchi, and Takashi Ishikawa — Inst. of Biomech. Eng., Faculty of Eng., Tokyo University of Agriculture and Technology, Nakai-cho, Itabashi-ku, Tokyo, Japan

A capsule is a liquid drop enclosed by thin, deformable membrane. Biological cells and membrane-bounded drugs can be thought of as capsules. Since it is important to understand the rheology of capsule suspensions such as blood, a number of studies have been conducted to clarify the viscosity of capsule suspensions. However, it is still unknown how the capsule will change its contribution of viscosity increase, when changing the volume fraction of capsules. We present a numerical analysis of a dense capsule suspension with volume fraction varying from 0 to 30%. In order to speed up the computation of boundary element method, we utilized GPU computing for the simulation. The results show that volume fraction increase leads to an increase in the deformation of the capsule, while reducing the orientation angle with respect to the velocity direction. We also report how these changes in capsule deformations would affect the bulk rheology of the suspension.

BP 24.4 Tue 14:00 Poster A

How perfluorooctanoic acid inserts into a biomimetic model membrane — Beate-Annette Brüning1,2, Martin Kreuzer1,3, and Roland Steitz1 — 1-Delft University of Technology, Delft, Netherlands — 2-Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

Perfluorinated compounds are found as biproducts of a wide range of industrial products. Upon entering cellular membranes, the compounds are known to cause developmental and reproductive disorders. We mimic the bioaccumulation in these membranes by inserting the perfluorinated surfactant PFOA into a DMPC phospholipid bilayer. We study changes in the membrane interface structure by X-ray diffraction and neutron reflectometry. We discuss our findings in the light of varying scattering contrasts: taking advantage of the C/F-contrast using X-ray diffraction, we probe the insertion of the perfluorinated surfactant into the phospholipid bilayer interior. We further observe changes in the thickness of the inter-bilayer hydration water layer using neutron reflectivity and H2O/D2O exchange. The combined X-ray and neutron scattering experiment suggests two main effects of PFOA-insertion into the membrane: i) changes in lipid acyl chain ordering combined with bilayer leaflet approximation, ii) ‘drying’ of the membrane (thinning of hydration water layer). We discuss, how both effects could contribute to a previously observed rigidification of the membrane through the perfluorooctanoic acid [1].


BP 24.5 Tue 14:00 Poster A

UV induced Polymerization of Phospholipids at Langmuir-Blodgett Through — Roland Hillmann, Marius Dotter, Sören Gramann, Lukas Gall, Andor Sischka, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

We investigate the translocation of macromolecules like ssDNA through biological nanopores with Optical Tweezers force mechanics. Therefore Alpha-Hemolysin biopores are integrated into supported bilayer lipid membranes (BLM) or into polymerized lipid-bilayers. This will be accomplished either by the black lipid painting method, or by a liquid-solid Langmuir-Blodgett transfer with subsequent UV light polymerization of the phospholipids containing diacethylene. The high stability of the BLM allows an analysis by AFM or HIM.

BP 24.6 Tue 14:00 Poster A

Exocytotic activity of living cells imaged with surface plasmon resonance microscopy — Matthias Gerhardt, and Carsten Beta — Institut für Physik und Astronomie, Karl-Liebknecht-Strasse 24/25, 14476 Potsdam, Germany

Surface plasmon resonance microscopy allows for imaging of the complex refractive index at gold-liquid interfaces. The complex refractive index of the interface mainly depends on the molecular composition of the samples attached to the gold surface regarding its charge and density. In our case Dictyostelium cells were sedimented onto a gold surface to study the cell-substrate interface. In the region of cell-surface attachment, we observed transient localized events characterized by a step-like change in the complex refractive index at the gold-liquid/cell interface. The duration of such events was found to be within 1-2 sec. In the surface plasmon resonance image, those events mostly appeared as disc-shaped objects with a diameter of about 1-2 um within the region of the cell-substrate interface. While sedimented cells displayed such events spontaneously but rarely, a hypoosmotic shock was found to trigger a significantly higher rate of events. Dictyostelium cells were able to release dispensable ions into the extracellular space using their contractile vacuole. Since the area of the observed disc-shaped events was found to be within the size of
intracellular vesicles (which have been observed in the same cells using bright field microscopy) we conclude that exocytotic activity of the contractile vacuole can be observed by surface plasmon resonance microscopy.

BP 24.7 Tue 14:00 Poster A Three-dimensional fluorescence-free tracking of a nanoparticle on a giant unilamellar vesicle — S. Spindler, J. Ehrig, and V. Sandoghdar — Max Planck Institute for the Science of Light, Erlangen, Germany

Among the diversity of model membrane systems, giant unilamellar vesicles (GUVs) represent a favourable model system for a cell membrane because of their compatible sizes and shape. Furthermore, GUVs provide a convenient platform for studying basic membrane phenomena in a model system without the artefacts of a substrate. We report on using interferometric scattering (iSCAT) microscopy as a fluorescence-free technique to study the three-dimensional diffusion of single particles such as virus particles and gold particles attached to lipids on a GUV. iSCAT is based on measuring the interference of the Rayleigh scattering with a reference light beam and allows for high temporal resolution as well as nanometer precision in particle tracking. Moreover, iSCAT provides high-resolution information on the axial displacement of the particle, allowing one to map the curved GUV surface. We compare our observations of lipid diffusion in GUVs with those in supported lipid bilayers [1].


BP 24.8 Tue 14:00 Poster A Direct Measurement of Mechanical Properties of Unsupported Lipid Bilayer under Hydrodynamic Deformation — C. Walter, M. Hein, R. Selmans, and J.-B. Fleury — Saarland University, Experimental Physics, Saarbrucken, Germany

Mechanical properties of lipid membranes like inter-monolayer friction or surface viscosity are important for several biological processes like cell migration, synovial articular motion or cell mechanism in general. The mechanical properties of lipid bilayers were experimentally investigated in detail by Evans and co-workers in the 90’s. However, the for these studies vesicles or on supported bilayers were used which question their bio-relevance. Here, we present a new strategy to investigate mechanical properties of free-standing lipid bilayers using hydrodynamic deformation in microfluidic chips.

BP 24.9 Tue 14:00 Poster A Giant Unilamellar Vesicles as Biological Microreactors — A. Lippert, N. Bonakdar, and V. Sandoghdar — Max Planck Institute for the Science of Light, Göttingen, Germany

The goal of our project is the establishment of a biological microreactor, enabling the production of complex metabolites. As a first simple platform we study confined kinetics, diffusion and transporter activity under controlled conditions.

BP 24.10 Tue 14:00 Poster A Fabrication of Giant Unilamellar Vesicles — H. Stein, S. Spindler, and V. Sandoghdar — Max Planck Institute for the Science of Light, Göttingen, Germany

Giant Unilamellar Vesicles (GUVs) offer a useful model system for studying fundamental biophysical properties such as lipid diffusion or the interaction of proteins or viruses with membranes. A variety of fabrication methods for GUVs in low ionic solutions already exist, however the formation of giant vesicles under physiological conditions still poses a challenge. We present methods for preparing GUVs in the range of 50-100μm diameter in high ionic buffers with different osmolarity using electroformation on ITO covered glasses or lipid swelling on a polymer layer.

BP 24.11 Tue 14:00 Poster A Comparison of the hydration repulsion between lipid bilayers in MD simulations and experiments — B. Kowalkj, E. Schneck, M. Kanduc, and R. R. Netz — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Experiments performed in the last decades gave insight into the nature of the hydration repulsion between lipid membranes. With our Molecular Dynamics Simulations, we want to link the results of the experiments with a theoretical foundation. In particular we investigate the entropic and enthalpic contribution of the interaction between hydrated membranes. We also analyse the structural parameters of the membranes at different hydration levels and discuss our results for both the fluid as well as the gel phase by comparing them to the experimental data.

BP 24.12 Tue 14:00 Poster A Formation and study of TiN coatings on titanium substrate using plasma immersion ion implantation for applications in biological membranes — M. C. Cisternas, A. Hennriquez, H. Bhuyan, M. Retama, M. Favre, U. Volkman, D. Manova, S. Mandle, and F. Guevara — Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — CIEN-UC, Santiago, Chile

Artificial membranes represent models of the behavior of their biological counterparts. The objectives of this study are the formation and study of a biocompatible environment that serves as a support and ensure stability in phospholipid membranes. In this work was formed and analyzed experimentally a system composed of DPPC / CH / TiN + TiO2 / Ti, where DPPC is the phospholipid previously studied [J. Chem. Phys. 141, 104201 (2014)], chitosan CH, which acts as hydrating matrix for the phospholipid and TiN + TiO2 is the biocompatible surface of titanium Ti. The substrate used was Ti, material widely used in biomedical applications, but requires biocompatible coatings to be used in critical areas like implants. Coatings of titanium nitride (TiN) besides having well known properties of hardness, increase the corrosion resistance and maintain the biocompatibility of titanium.


Cargo is internalized by biological cells using different internalization processes, e. g. endocytosis, phagocytosis, and pinocytosis. In all cases the cargo is internalized by a carrier that interacts with the membrane. Towards the understanding of these processes, we tackle the internalization of a carrier using a minimalistic model of a spherical nanoparticle with attached ligands, a lipid bilayer membrane, and receptors that mediate the interaction between membrane and nanoparticle.

In our model, we calculate the deformation energy of the fluid membrane using the Helfrich Hamiltonian. The receptors on the membrane bind to the ligands on the nanoparticle, which we take into account using the binding energy and the entropy terms for the free energy of the receptors. For a given fraction of the particle being wrapped by the membrane, we obtain an optimum number of bound receptors at equilibrium. The number of bound receptors depends on the overall receptor density on the membrane, the binding energy gain per receptor, and the area of the membrane that is not bound to the particle. For receptor-mediated adhesion, we find that the transition between unwrapped and completely-wrapped states occurs gradually via partially-wrapped states.

BP 24.14 Tue 14:00 Poster A Monte-Carlo 2D Model of Bilayer Systems — D. Hakoynyan and A. Heuer — WWU Münster, Institut für Physikalische Chemie, Münster, Germany

Various Molecular Dynamics (MD) and 2D Monte-Carlo systems were proposed for investigation of the processes in model bilayer systems. Particularly, with help of a relatively simple 2D - particle lattice model the phase separation of saturated and unsaturated lipids and chole-
terol was demonstrated [Reigada et al. 2008, DOI: 10.1063/1.2817333]. In this lattice model, however, different lipids and cholesterol were only differentiated by the size of the pair-wise interaction and lacked specific properties of lipids and cholesterol.

Here we introduce 2D models of basic bilayer components where these characteristics are taken into account. In this model the individual particles of the 2D system present lipids or cholesterol with additional information about the order parameter of the alkyl chain. The free energy of this system is decomposed into separate and carefully chosen entropic and enthalpic parts. The parameters and the balance of entropy and enthalpy for this 2D model were checked against the all-atom MD simulations to certify the adequateness. We further adapt the model to be able to observe phase separation of a ternary system with saturated and unsaturated lipids and cholesterol. In this way we can systematically explore the range of compositions and molecular properties for which phase separation is possible.

BP 24.15 Tue 14:00 Poster A
Hydration interaction of charged polar surfaces —
• ALEXANDER SCHLAICH1, MATEJ KANDUC1, EMANUEL SCHNECK2, and ROLAND R. NETZ3 — 1Fachbereich Physik, Freie Universität Berlin, D-14195 Berlin, Germany — 2Max Planck Institut für Kolloid- und Grenzflächenforschung, D-14476 Potsdam, Germany

We study the hydration interactions between polar surfaces as a model for lipid membranes using atomistic computer simulations at prescribed water chemical potential and analyze interaction pressures, interaction thermodynamics, and interaction mechanisms.

The overlap of interfacial water layers is analyzed via several distinct water order parameters and compared with predictions of simple continuum theories. We further investigate the electrostatic interaction between charged model membrane surfaces in the presence of counter ions and show that continuum models can successfully describe Coulombic interactions. To this end, we also analyze the dielectric properties of the interfacial water and examine the solvation of salt in water under confinement.

BP 24.16 Tue 14:00 Poster A
Numerical simulation of endocytosis - Continuum models of membranes with curvature-inducing molecules —
• SEBASTIAN ALAND1, JOHN LOWENHUR2, and JUN ALLARG2 — 1Institut für wissenschaftliches Rechnen, TU Dresden, Germany — 2Department of mathematics, University of California Irvine, USA

We present new diffuse interface models for the dynamics of inextensible vesicles in a viscous fluid. A new feature of this work is the implementation of the local inextensibility condition by using a local Lagrange multiplier harmonically extended off the interface. To make the method even more robust, we develop a local relaxation scheme that dynamically corrects local stretching/compression errors, thereby preventing their accumulation. We present numerical results that confirm the effectiveness of the proposed models in a test case scenario of vesicles in shear flow. Finally we apply the model to a problem of clathrin-mediated endocytosis. Clathrin proteins attach to the membrane and alter locally its bending stiffness and spontaneous curvature. This process can lead to budding and pinch-off of small vesicles. First numerical simulation results will be shown.

BP 25: Posters: DNA/RNA and related enzymes

Time: Tuesday 14:00–16:00

BP 25.1 Tue 14:00 Poster A
Polymerization of RNA in a non-equilibrium environment —
• MATTHIAS MORASCH, CHRISTOF B. MAST, and DIETER BRAUN — Systems Biophysics, LMU Munich, Germany

The polymerization of nucleotides to long chains of RNA was very likely a crucial step towards the evolution of life. There is, however, a large variety of possible nucleotides that require very different conditions in order to polymerize efficiently. These range e.g. from dry conditions at elevated temperatures to dry-wet cycles in lipid environments and to aqueous solutions in combination with a catalyst. We investigate different polymerization conditions for cyclic nucleotides, in particular 3',5'-cyclic guanosine monophosphate (cGMP), which might have the ability to polymerize in the dry state as well as in an aqueous environment. So far, we could proof that drying cGMP at elevated temperatures triggers its polymerization to 40 mers and longer.

While the drying process facilitates the formation of long polymers due to high local concentrations and the absence of water, a polymerization in an aqueous environment is a more cumbersome task. Especially the polymerization of pairing bases has to be accomplished for different polymerization conditions for cyclic nucleotides, in form of a temperature gradient should allow the enhanced polymerization from cyclic nucleotides in a thermophoretic molecule trap.

BP 25.2 Tue 14:00 Poster A
Ultrafast energy dissipation within the vibrational modes of the DNA backbone —
• YINGLIANG LIU, BISWAJIT GUCHHAIT, RENE COSTARD, TORSTEN SIEBERT, and THOMAS ELAESERER — Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born-Str. 2a, 12489 Berlin, Germany

The long-term stability of the DNA helix structure requires efficient processes of electronic and vibrational relaxation as well as energy dissipation into an aqueous environment. To determine the relevant time-scales and pathways of relaxation, femtosecond pump-probe experiments on artificial double-stranded DNA oligomers are performed under conditions of full hydration. Specifically addressing the structure of the DNA backbone in the frequency range from 950 to 1300 cm⁻¹, the vibrational modes of the phosphate group, phosphodiester linkages and the furanose ring structure display subpicosecond lifetimes. While excess energy released by the relaxation of phosphate vibrations is preferentially transferred into the surrounding water shell, clear signatures of vibrational energy transfer to the modes of the sugar linkage and ring structure are observed and these channels of energy dissipation are compared for different hydration levels.

BP 25.3 Tue 14:00 Poster A
Ectoine induced water structuring as a possible explanation for radiation protection properties —
• MARC BENJAMIN HAHN, THOMIR SOLOMUN, SUSANN MEYER, HEINZ STURM, and HANS-JÖRG KUNTE — BAM - Federal Inst. Mater. Res., Berlin, Germany

Compatible solutes ectoine and hydroxyectoine are known to be effective protectant against heating, freezing, high salinity and radiation damage for biomolecules and cells. It is believed that this properties are due to water-structuring-effects and their influence on hydrogen-bonds within water-clusters and biomolecules. Although the beneficial properties of ectoine are already exploited in commercial applications the underlying mechanisms remain unclear. We propose an explanation for radiation protection properties based on our findings from ramanspectroscopic measurements. We found changes of vibrational density of states in liquid water in dependence of ectoine, hydroxyectoine and sodium chloride concentrations. This data indicates linear increased collective behaviour of hydrogen bonds with compatible solute concentration which leads to higher scattering probabilities of low energy electrons.

BP 25.4 Tue 14:00 Poster A
Compatible solute induced vibrational modes in water and the connection to radiation protection of biomolecules —

Radiation protection properties of compatible solutes are already exploited in medical applications. Even though the underlying mechanisms remain unclear. We present ramanspectroscopic measurements on the influence of the vibrational behaviour of water in dependence of compatible solutes concentrations. The results for ectoine and hydroxyectoine show an increase in the free density of states of the collective vibrational and the low frequency modes of water with increasing solute concentration. Based on this findings an explanation for the radiation protection properties will be proposed.
BP 25.5 Tue 14:00 Poster A
Uncovering the structural stability and unfolding pathway of a 7-bp DNA hairpin through high-temperature molecular dynamics simulation  —  Ewa Anna Opreszka-Zingere and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

The formation of specific DNA secondary and tertiary structures has been reported to play a key role in various range of biological processes, such as transcription termination or intermolecular binding. Among them, a pivotal role has been ascribed to DNA i-Motif and G-Quadruplex structures, which due to their biological appearance in telomeric and centromeric DNA are considered as potential targets for various diseases. Recent studies on high-temperature unfolding simulations of the DNA i-Motifs have revealed the existence of the stable hairpin configurations as an intermediate step in the unfolding pathway of DNA higher-order structures. In our study, we investigate simple 7-nucleotide DNA hairpin structures with the sequence d(GCGAAGC) and its variations. Through high-temperature molecular dynamics simulation we intend to get insight into the stability of the DNA hairpins and the possible unfolding pathways. In addition, the unfolding free energy landscape of DNA hairpins will be analyzed such that sequential differences can be energetically evaluated. This serves as the first approach to unravel the complex nature of G-Quadruplex folding pathway and behavior.

BP 25.6 Tue 14:00 Poster A
Measuring DNA translocation forces through various solid state nanopores with Optical Tweezers  —  Sebastian Knust, Andy Sischka, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

We measured the forces acting on a single strand of dsDNA during translocation through nanopores in various solid state membranes by Optical Tweezers. The system includes a video-based force detection and analysis system allowing for virtually interference-free axial force measurements with sub-piconewton precision [1]. All measurements were performed with an overall force resolution of 0.5 pN at a sample rate of 123 Hz.

We show the controlled translocation through Si3N4 membranes both uncoated and lipid-coated [2]. Additionally, measurements of controlled dsDNA translocation through carbon nanomembranes (CNM) and through MoS2 membranes were conducted.

Furthermore, measuring controlled translocation through graphene nanopores was found challenging, due to local heating phenomena encountered upon approaching an optically trapped microbead to a free standing graphene membrane. We analysed these phenomena in detail.


BP 25.7 Thu 14:00 Poster A
Modelling the mechanisms of backtrack and recovery in RNA polymerases I and II — Ana Lisica1,2, Marcus Jahnel1,2, Christoph Engels3, Edgar Roldan4,5, Patrick Cramer1,4, and Stephan Grill3,2 — 1BIOtech, Technische Universität Dresden, Tatzenberg 47/49, 01307 Dresden, Germany — 2Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstrasse 108, 01307 Dresden, Germany — 3Max Planck Institute for Biophysical Chemistry, Am Fassberg 11, 37077 Göttingen, Germany — 4Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 81, 01187 Dresden, Germany — 5GISC - Grupo Interdisciplinar de Sistemas Complejos, Madrid, Spain

Transcription elongation by RNA polymerases is frequently interrupted by pauses. A prominent mechanism of pausing is backtracking, which involves backward movement of the polymerase on the DNA template. To recover from backtracks, polymerases can diffuse or cleave the backtracked RNA. We model the backtrack recovery of Pol I and II as a continuous time random walk between discrete states. We calculate the first-passage time from any position in the backtrack to the elongation competent state and compare it to times required for recovery from a given backtrack depth, as measured with high-resolution dual-trap optical tweezers. The choice of recovery mechanism is here determined by kinetic competition between 1D diffusion and transcript cleavage. Fitting experimental data to our model, we extract diffusion and cleavage rates of both enzymes and characterize the distinct micromechanical features of Pol I and Pol II transcription.

BP 25.8 Tue 14:00 Poster A
DNA hybridization and kinetics of hairpin-loop molecules  —  Mina Mohammadi-Kambs, Björn Ackermann, and Albrecht Ott — Saarland University, FR 7.2, Biologische Experimentalphysik, 66123 Saarbrücken

In the cell, molecular information processing is based on molecular recognition and binding. Although DNA hybridization is sometimes understood as ‘lock and key’. It is not clear how two molecules can identify each other. We find that there are many possibilities of different single strands of DNA at a given length that can bind to a given surface bound probe in thermal equilibrium. In other words, many keys can coexist for one lock. There are some groups of sequences, which do not bind to a probe like the ones with runs of guanine bases or self-complementary sequences. At the same time we look at the behavior of corresponding DNA hairpin-loop molecules. We investigate their thermal fluctuation by using a combination of fluorescence energy transfer and fluorescence correlation spectroscopy. We measure the rate of opening and closing for different sequences with different stem or loop length. In future work we will look at the behavior of DNA hairpin-loop molecule in the presence of competitive targets to see how they identify their complementary probe. This is a first approach towards understanding how molecular recognition works in the crowded and competitive environment of the cell.

BP 25.9 Tue 14:00 Poster A
Effects of Collectivity in Homology Recognition: a density functional theory based approach. — Sergio Cruz1, Claudia Daniłowicz2, Chantal Prévost3, Mara Prentiss2, and Maria Fytas1 — 1Institute for Computational Physics, University of Stuttgart, Germany — 2Physics Department, Harvard University, Cambridge, MA, USA — 3LTB - CNRS and Univ Paris Diderot, Sorbonne Paris Cité, Paris, France

RecA is a family of proteins for performing homology recognition while trying to repair DNA. The atomistic mechanism by which this process occurs is not still fully understood. Crystallographic evidence shows that RecA separates a strand in sequences of three bases (triplet), and then searches for the homologous partner. However, ‘recognition in duplets’ is suggested as a possible mechanism by recent experiments. In our current investigation, the importance of collectivity in recognition is explored by means of quantum mechanical calculations at the level of dispersion corrected density functional theory. We compare the average binding energy for singlets, duplets, and triplets for canonical Watson-Crick and mismatched base pairs. There is a clear distinction between recognition in singlets, and recognition in duplets or triplets. We calculate the energy for duplets and triplets containing mismatches and compare this with the energetics of the respective singlets. Analysis on the energy difference will shed light to a better understanding of this homology recognition process.
Wehmeyer

multi-temperature simulations with pytram

Rigorous combination of molecular dynamics and biased or applications, e.g. nanopore sequencing.

ff

a DNA strand to pass through each other. This results in interchange

given inter-species network dependence. We consider di processes

discussed as Markov processes on a suitable network. We show quite

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Thermodynamic uncertainty relation for biomolecular pro-

ture filaments and microtubules. We here present an analytical and numerical analysis of randomly driven shape fluctua-
tions of semiflexible filaments in a viscoelastic environment. To detect and quantify non-equilibrium dynamics, we focus on the breaking of detailed balance in a conformational phase space subtended by eigenmodes of the beam equation. Molecular dynamics simulations reveal a non-zero circulatory flux in phase space induced by motor activity. Furthermore, we derived an analytical expression of nonequilibrium mode correlations that allows us to predict temporal effects of active molecular motors.

thermodynamic uncertainty relation for biomolecular pro-
cesses — Andre C. Barato and Udo Seifert — II. Institut für Theoretische Physik, Stuttgart, Germany

Biomolecular systems like molecular motors or pumps, transcription and translation machinery, and other enzymatic reactions can be described as Markov processes on a suitable network. We show quite generally that in a steady state the dispersion of observables like the number of consumed/produced molecules or the number of steps of a motor is constrained by the thermodynamic cost of generating it. An uncertainty requires at least a cost of $2k_B T/\epsilon^2$ independent of the time required to generate the output.

Statistical classification of small microbial food webs — Fanny Groll and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Germany

We identify classes of food webs with regard to their stability and species diversity. Food webs are characterised by the topology of their inter-species relations, e.g. feeding on products of metabolism of another species or competition on nutrients or via a common predator. To gain insight into these structures we pursue a statistical approach: the starting point is the numerical implementation of food webs of with given inter-species network dependence. We consider different aquatic microbial communities. Each species is defined by parameters determining its attributes. A whole distribution of parameter combinations is then randomly generated and tested according to its temporal evolution. Individual systems evolve for some time in simulations and the outcome is monitored. Specifically, we deduce probabilities for the survival of a given number of species over distributions of network parameters at fixed network topology.

How molecular knots can pass through each other — Jonathan Trefz1,2,1, Benjamin Trefz2,1, and Peter Virnau3 — 1Department of Physics, Johannes Gutenberg University of Mainz, D-55128 Mainz, Germany — 2Graduate School Materials Science in Mainz, D-55128 Mainz, Germany

In our work a method is proposed that allows two molecular knots on a DNA strand to pass through each other. This results in interchanging their positions along the strand. By expanding its size, one of the knots allows the other to diffuse along its contour. As explained in PNAS, 111(22), 7948-7951 the free energy barrier for this particular mechanism only amounts to a few k_B T. Therefore, it is not only of aesthetic interest, but may also play a role in technological applications, e.g. nanopore sequencing.

Rigorous combination of molecular dynamics and biased or multi-temperature simulations with pytram — Christoph Wehmeier, Antonia Mey, Fabian Paul, Hao Wu, and Frank

The TRAM method is implemented in the pytram package, available at https://github.com/markovmodel/pytram.

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Rigorous combination of molecular dynamics and biased or multi-temperature simulations with pytram — Christoph Wehmeier, Antonia Mey, Fabian Paul, Hao Wu, and Frank

Not — Institut für Mathematik, Freie Universität Berlin

The reliable estimation of equilibrium and kinetic properties of complex dynamical systems is of general interest in the physical and life sciences. Despite well established theoretical frameworks, the underlying complexity in general renders analytical predictions impossible and requires a numerical treatment instead; which can still be costly due to rare events dynamics.

Enhanced sampling and multi-ensemble methods (e.g. parallel tempering, Hamiltonian replica exchange, or umbrella sampling) allow to sample such rare events feasibly in many cases and, in this way, to calculate equilibrium properties. In general, however, the simultaneous analysis of molecular dynamics and biased simulations lacks a rigorous and broadly applicable protocol.

To this aim, we present TRAM, a fully rigorous approach to combine molecular dynamics and multi-ensemble simulations to estimate equilibrium and kinetic properties of systems with rare event dynamics using the Markov state model framework.

The TRAM method is implemented in the pytram package, available at https://github.com/markovmodel/pytram.

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are strongly correlated to the so-called rank of the interaction scheme.

Modeling chromosomes during meiosis in fission yeast —
**Wenwen Huang***1, **Yen Ting Lin***1, **Daniela Frömberger***1, **Petrina Delivanis***2, **Mariana Chacón***1, **Iva Tolec***1, **Frank Jelicher***1, and **Vasily Zaburdaev***1 — 1Max Planck Institute for the Physics of Complex Systems, 01187, Dresden, Germany; 2Max Planck Institute of Molecular Cell Biology and Genetics, 01307, Dresden, Germany

During the prophase of meiosis in fission yeast, both ends of chromosomes are bound to the spindle pole body (SPB) and form a ring-like structure. Furthermore, the whole nucleus oscillates, moving from one pole of the zygote to the other. The dramatic movements of the nucleus are believed to promote the chromatin alignment and are required for proper recombination. Our goal is to understand the physical picture of chromosome alignment during nuclear oscillations. We perform extensive Brownian dynamics simulations of three pairs of homologous chromosomes during the oscillations. An individual chromosome is represented by a bead-rod ring, where the SPB is a special common bead shared by all the rings. A periodic force is applied to the SPB, which pulls the chromosomes through the viscous nucleoplasm and under the confinement of the cell walls. By setting parameters based on estimation of the available experimental data, we analyze the distance between the homologous loci as a function of time and amplitude of oscillations and compare it to the experimental data. Our results provide a quantitative characterization of both chromosome movements and help to understand the role of nuclear oscillations on the alignment of chromosomes during meiosis.

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Flux simulations of anisotropic particles in different geometries using lattice Boltzmann method — Lukas Schröder and Stephan Gehke — Biofluid Simulation and Modeling, Universität Bayreuth

Experiments by Trebbin et al. [1] have shown that anisotropic particles align perpendicular to the flow direction after passing through constricted parts of narrow microchannels. In order to gain additional insight into the microscopic orientation distribution characteristics of these particles, we simulate the flow of rod-like colloids within a restrictive geometry which contains a narrowing section. We use the lattice Boltzmann method as implemented in the software package ESPResSo [2]. We have expanded this software package by integrating cylinders with variable diameter and bifurcations to the alternatives of possible geometries.

Our simulations are performed at low Reynolds numbers and since the alignment process is likely to be a collective phenomena, a large amount of rods is investigated. Each of them consists of single point particles, bonded to each other by a harmonic potential. Stability of the alignment process is of particular interest.


Micropipette force sensors for biomechanics and soft matter adhesion studies — Marcin M. Makowski and Oliver Barumen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany

The precise determination of acting forces is fundamentally important for the characterization of mechanical properties of soft matter and biological processes, e.g. cell-cell and cell-substrate interactions. Optical or magnetic tweezers as well as AFM force probes can provide quantitative information on the interactions of objects such as single molecules and bacteria. However, these techniques are very much limited to objects within a certain force and size range. Inspired by the work of Colbert et al. (FPF 90, 117, 2009), we developed a micropipette deflection technique which is capable of quantifying forces down to the pN level (and up to mN) of objects of the size of µm (and up to mm), that are attached via a small negative pressure within the micropipette. As it is purely based on optical high-resolution (and eventually high-speed) imaging involving image cross-correlation analysis, the technique additionally allows for quantitative force-shape correlations and, e.g. in adhesion and friction studies, a direct access to the area of contact. Here, we present force spectroscopy measurements of vesicle adhesion on hydrophilic and hydrophobic substrates, based on micropipette force sensors.

Probing the inhomogeneity of intracellular fluids with fluorescence lifetime imaging — Olivia Stiehl and Matthias Weiss — University of Bayreuth, Bayreuth, Deutschland

Cellular fluids are crowded with a plethora of macromolecules, supramolecular complexes, and organelles. These fluids can therefore be expected to display a spatial inhomogeneity on small length scales, i.e. a coexistence of spatially varying environments. So far, the local diffusional mobility of tracer particles has been exploited frequently as a measure for such inhomogeneities. Here, we report on a different approach that is based on local changes of the photophysics of a tracer dye. In particular, we have used fluorescence lifetime imaging microscopy (FLIM) to quantify local variations in the photophysics of DASPMI in the cytoplasm of living cells. Due to shortened lifetimes in regions of lower viscosity, this method allowed us to explore local properties of the cytoplasm without a need to interpret complex diffusion data. Our results suggest that the cytoplasm's properties are altered in response to changes in the cells' substrate and alterations in intracellular traffic.

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The role of detailed balance in chemically active droplets — R. H. Varma, M. D. Erlandsson, J. M. Hoare, and J. Michelson
1 Max-Planck Institut für Physik komplexer Systeme, Dresden — 2School of Engineering and Applied Science, Harvard University, Cambridge, MA

Liquid systems that undergo phase separation coarsen with time. One mechanism for coarsening is Ostwald ripening, where large droplets grow at the expense of smaller ones by diffusive fluxes. We are interested in situations in which Ostwald ripening is suppressed due to chemical reactions. We consider a system consisting of three chemical components in which reactions occur between the components. Reaction rates in general obey local detailed balance conditions. We focus on the case where two of the components phase-separate while the third component does not participate in phase separation but represents a reservoir that provides chemical free energy to the system. In this case, the system can be effectively described as a two component phase-separating system with broken detailed balance. In this case, many droplets can coexist with a stable stationary droplet size. Thus, chemical reactions can suppress Ostwald ripening and stabilize active suspensions. Our work could be relevant to phase separation in biological cells where liquid-like structures such as centrosomes and germ granules coexist in the cytoplasm in presence of chemical reactions.

The mechanical properties of early Drosophila embryos measured by high-speed video micro rheology — Alok Daniel Wessel and Christoph F. Schmidt — Drittes Physikalisches Institut, Georg-August-Universität Göttingen

In early development, Drosophila melanogaster embryos form a syncytium, i.e. multiplying nuclei are not yet separated by cell membranes, but are interconnected by cytoskeletal polymer networks consisting of actin and microtubules. Between division cycles 9 and 13, nuclei and cytoskeleton form a 2D cortical layer. To probe the mechanical properties and dynamics of this self-organizing "pre-tissue", we measured shear moduli in the embryo by high-speed video micro rheology. We recorded position fluctuations of injected micron-sized fluorescent beads with kHz sampling frequencies and characterized the viscoelasticity of the embryo in different locations. Between nuclear layer and yolk the cytoplasm was homogeneous and viscously-dominated, with a viscosity three orders of magnitude higher than that of water. Within the nuclear layer we found an increase of the elastic and viscous moduli consistent with an increased microtubule density. Drug-interference experiments showed that microtubules contribute to the measured viscoelasticity inside the embryo whereas actin only plays a minor role. Myosin inhibition had only minor effects on the probe particle’s fluctuation. Measurements at different stages of the nuclear division cycle showed little variation, besides at anaphase where we observe directed motion.

BP 28.4 The mechanical properties of early Drosophila embryos measured by high-speed video micro rheology — Alok Daniel Wessel and Christoph F. Schmidt — Drittes Physikalisches Institut, Georg-August-Universität Göttingen

In early development, Drosophila melanogaster embryos form a syncytium, i.e. multiplying nuclei are not yet separated by cell membranes, but are interconnected by cytoskeletal polymer networks consisting of actin and microtubules. Between division cycles 9 and 13, nuclei and cytoskeleton form a 2D cortical layer. To probe the mechanical properties and dynamics of this self-organizing "pre-tissue", we measured shear moduli in the embryo by high-speed video micro rheology. We recorded position fluctuations of injected micron-sized fluorescent beads with kHz sampling frequencies and characterized the viscoelasticity of the embryo in different locations. Between nuclear layer and yolk the cytoplasm was homogeneous and viscously-dominated, with a viscosity three orders of magnitude higher than that of water. Within the nuclear layer we found an increase of the elastic and viscous moduli consistent with an increased microtubule density. Drug-interference experiments showed that microtubules contribute to the measured viscoelasticity inside the embryo whereas actin only plays a minor role. Myosin inhibition had only minor effects on the probe particle’s fluctuation. Measurements at different stages of the nuclear division cycle showed little variation, besides at anaphase where we observe directed motion.

BP 28.3 The mechanical properties of early Drosophila embryos measured by high-speed video micro rheology — Alok Daniel Wessel and Christoph F. Schmidt — Drittes Physikalisches Institut, Georg-August-Universität Göttingen

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BP 28.1 Raman spectroscopic analysis of drug-target interactions in malaria disease — Torsten Frosch1,2 and Jürgen Popp1,2
1 Leibniz Institute of Photonic Technology — 2 Institute of Physical Chemistry, Friedrich Schiller University Jena

Raman spectroscopy provides extremely high chemical selectivity for the identification and quantification of antimalarial active agents [1,2]. A Raman spectroscopic elucidation of drug-target-interactions was performed in physiological environment [3], while water did not cause a strong Raman signal. Raman spectra were acquired within intact cells. Highly spectrally resolved Raman difference spectra were acquired in order to elucidate small shifts of the molecular vibrations caused by the weak interactions. Defined stoichiometric ratios of heme (targets) and antimalarial drugs characterize the molecular interaction. With help of a thorough interpretation of these binding processes this work contributes towards the tailored design of new effective active agents against Malaria.

Acknowledgment: We thank Katja Becker for help with cell preparation.

A unified theoretical approach to the inelastic mechanics of biopolymer gels, cells and cell aggregates — Andrea Kramer, Matti Giraldo and Klaus Kremer — Institute for Theoretical Physics, Universität Leipzig, Germany — Department of Physics, University of California, Berkeley, USA

Whereas classical viscoelastic models can often be applied to describe the mechanical response of biomaterials to small deformations, they cannot adequately be used to model the response to large deformations. Here, the transient breaking of bonds, e.g., crosslinks in biopolymer networks or cell-cell adhesions in cell aggregates, leads to a new class of response reminiscent of (pseudo-)plastic phenomenology. We present a schematic modeling framework for the construction of inelastic models for biological materials based on the inelastic Glassy Wormlike Chain (iGWLC) model [1]. Decomposing the total deformation into viscoelastic and inelastic components, we provide a unified description that is able to qualitatively explain recent experimental data for the nonlinear mechanics of fibrin and collagen gels, cells and cell aggregates [2,3].

2. S. Münster et al., PNAS 110, 12197 (2013)

Time: Tuesday 14:00–16:00

BP 29.1 Tue 14:00 Poster A Control of ventricular tachycardia under myocardial ischemic conditions and infarction — Edda Boccia and Stephan Luther — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, Göttingen, Germany

Myocardial ischemia arises when blood supply of substrates doesn’t meet tissue’s metabolic demands. It can degenerate to acute ischemia and infarction. Ischemia is followed by profound metabolic changes: hyperkalemia (increment of extracellular potassium), hypoxia (deprivation of oxygen supply) and acidosis (increment of acidity in the blood). We present a modified version of the Luo-Rudy I model, adopted to investigate action potential propagation under ischemia and infarction. The domain is represented by a 2D virtual sheet of myocardial tissue, where heterogeneity is introduced by subdividing it in three distinct zones: a central circular ischemic area (CZ), a ring-shaped border zone (BZ, linear transition between physiological and ischemic values) and normal tissue. As a first approximation, hyperkalemia and acidosis were simulated and parameters were changed and ischemic values) and normal tissue. As a first approximation, hyperkalemia and acidosis were simulated and parameters were changed in the CZ and in the BZ at each time after the onset of ischemia. We study the interaction of propagating waves with ischemic regions and the onset of cardiac arrhythmias, including ventricular tachycardia (VT) and fibrillation (VF). We investigate pinning and unpinning of propagating waves to and from infarction zones using pulsed electric fields. (VT) and fibrillation (VF). We investigate pinning and unpinning of propagating waves to and from infarction zones using pulsed electric fields. We study the interaction of propagating waves with ischemic regions and the onset of cardiac arrhythmias, including ventricular tachycardia (VT) and fibrillation (VF). We investigate pinning and unpinning of propagating waves to and from infarction zones using pulsed electric fields.

BP 29.2 Tue 14:00 Poster A Combined x-ray phase contrast tomography and scanning x-ray micro-diffraction for multi-scale investigation in regenerative medicine — Alessia Cedola, Gertang Campi, Anna Bureeka, Michela Fratini, Giuliana Tromba, Madalena Mastrogiovanni, Ranieri Cancadden, and Manfred Burghammer — 1ips-cnr/o Physics Department- Sapienza University- Rome-Italy. — 1Istituto di Cristallografia- CNR, Monterotondo Rome, Italy. — 2Sincrotrone Trieste ScPa, 34149 Basovizza (Trieste), Italy. — 3Dipartimento di Medicina Sperimentale-Università di Genova. — 4esrf-Grenoble-France

The importance of investigating the engineered bone, which is formed when porous ceramic constructs are loaded with bone marrow stromal cells and implanted in vivo, is a key point for Regenerative Medicine. Several aspects of the mechanisms leading to the generation of the new bone, in particular the dynamics of collagen packing during mineralization, requires a deeper understanding. The hierarchical structure of bone makes the combination of X-ray micro-diffraction scanning technique (XR*D) and the X-ray phase contrast tomography (XRPTC) the most effective tool to investigate the structural features of this tissue at different length scales. In particular we use XRPTC to provide the direct 3D image of the collagen network organization and XR*D to probe the structural fluctuations of the collagen lateral spacing and orientation during the growth of mineral particles at molecular and atomic scale. Moreover, we imagine by XRPTC the 3D microvascular networks in different bone-engineered constructs.
suggestion that the RNAi machinery adopts to large variations in target mRNA level, independent of siRNA or Ago2 concentrations. These experimental findings are not explained by the common literature view of RNAi, here termed dissociative mechanism, where the departing ligand (i.e., cleaved RNA fragments) leaves the complex in a slow step. Here, we investigate an alternative, associative mechanism of target strand recognition by Argonaute 2 (Ago2). The associative model is compatible with the high multiple turnover rates of RNAi-based gene silencing in living cells and accounts for target miRNA concentration-dependent acceleration of the RNAi machinery. The associative model proposed here suggests that the efficacy of an siRNA or miRNA depends on the expression level of its target RNA such that high target levels allow better regulation via RNAi.

**BP 30: Posters: Biotechnology and bioengineering**

**BP 30.1** Tue 14:00 Poster A

"Mesofluidik" für Zell- und Gewebekulturen — Claus Fütterer — Translational Centre of Regenerative Medicine, Leipzig & Biophysical Tools GmbH, Leipzig

The durchschlagende Erfolg der Mikrofluidik is unter anderem der Laminarität der Strömung (Reynoldszahl << 1) sowie dem preiswer- ten Einsatz von sehr effizienten Mikrofabrikationsmethoden zu verdan- ken. Leider sind Mikrokanäle nicht immer geeignet, insbesondere, wenn man größere Zellkulturen, Co-Kulturen oder sogar Organkulturen un- tersuchen möchte. Es stellt sich die Frage: Können die Vorteile der Mikrofluidik "hochskaliert" werden? Was sagen die hydrodynamischen Gleichungen dazu?

Diese Frage wird theoretisch diskutiert, und als experimentelle Ant- wort präsentieren wir ein Perfusionssystem, welches laufende Strö- mungen im Bereich mehrerer Milliliter/Sekunde präzise schalten und steuern kann. Bis zu 8 verschiedene Lösungen können völlig unterbre- chungsfrei geschaltet werden. Als Anwendung werden Messungen an Chlorid-Kanälen präsentiert - eine Verbindung also von Meso- und Na- nofluidik. Dieses System eignet sich hervorragend für die Messung von Kinetiken und Dynamiken von der molekularen bis zur multizellulären 

**BP 31: Posters: Modelling of non-linear dynamics in biological movement**

**BP 31.1** Tue 14:00 Poster A

Intrinsic muscle design: influence on human motor control — Alexandra Bayer1,2, Syn Schmitt1,2, Michael Guenther3, and Daniel Fabian Benjamin Harupl1 — 1Universität Stuttgart, Institut für Sport- und Bewegungswissenschaft, Allmandring 28, D-70569 Stuttgart, Germany — 2Universität Stuttgart, Stuttgart Research Center for Simulation Technology, Pfaffenwaldring 5a, D-70569 Stuttgart

A key aspect of understanding human movement is the interaction of the control strategy with the musculoskeletal system. Recent studies have shown that Hill-type musculoskeletal models can be used as well-established biomechanical actuators. As it has never been investigat- ed, we address the question which characteristics are relevant for actuators to perform fast goal-directed arm movements.

In our simulation study, the human arm is modeled by a non- linear musculoskeletal model and four lumped muscle-tendon com- plexes. Each muscle-tendon model consists of biochemical activation dynamics and four biomechanical elements (CE, PEE, SEE, SDE). The motor control system is represented by a combination of feedforward and feedback-controller. We compared the effect of different math- ematical representation of the biochemical and biomechanical model parts on movement speed in fast goal-directed arm movements. Al- ready exchanging the description of activation dynamics revealed sig- nificant differences in peak arm speed. Exchanging the models of the biomechanical structures also influences arm kinematics. We discuss the implications of these results for motor control simulation studies.
Frequency-Dependent Selection at Rough Expanding Fronts

Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin

Microbial colonies are a formidable model system to study long-standing questions of population dynamics, ecology, and evolutionary dynamics. Growth on surfaces naturally allows to observe range expansions, where microbes colonize new territory. The small number of reproducing individuals introduces strong demoscopic fluctuations, which interact with mutations at the front.

We use generalized Eden models to explore statistical properties of multi-species range expansions, where the front’s geometry and evolutionary dynamics couple to each other. In earlier work we found that irreversible mutations entail a new type of non-equilibrium phase transition accompanied by enhanced surface roughening [1].

If reproduction rates depend on local species composition, we distinguish a variety of patterns. Focusing on social dilemmas, we obtain new exponents for both kinetic roughening and the transition between global defection vs. global cooperation. This is also reflected in the dynamics of single species domains which at large times show enhanced fluctuation statistics.


Evolutionary Fitness in Variable Environments — ANNA MELLINGER AND MASSIMO VERGASSOLA — University of California San Diego

One essential ingredient of evolutionary theory is the concept of fitness as a measure for a species’ success in its living conditions. Here, we quantify the effect of environmental fluctuations onto fitness by analytical calculations on a general evolutionary model and by studying corresponding individual-based microscopic models. We demonstrate that not only larger growth rates and viabilities, but also reduced sensitivity to environmental variability substantially increases the fitness. Even for neutral evolution, variability in the growth rates plays the crucial role of strongly reducing the expected fixation times. Thereby, environmental fluctuations constitute a mechanism to account for the effective population sizes inferred from genetic data that are often much smaller than expected.

Evolutionary Coalitional Games — KARL WIENAND1, MATTHIAS LECHNER1, FELIX BECKER2, HEINRICH JUNG2, and ERWIN FREY3 — 1Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians Universität, Munich, Germany — 2Biocentrum, Ludwig-Maximilian University, Munich, Germany

Selection results from the interplay between directed selection and fluctuation statistics. We found excellent agreement between experiments and theory. We also able to elucidate the importance of initial conditions on the steady state distribution on population compositions. In particular, the initial size of the populations can tune the relative importance of initial assortment and growth as noise sources for the final distribution.

Counterintuitive findings for evolution on networks — LAURA HINDERSIN and ARNE TRAULSEN — Max Planck Institute for Evolutionary Biology, Plió, Germany

How does spatial population structure affect the fixation time of a novel mutation? In the framework of evolutionary graph theory, individuals inhabit the nodes of a network. We study the Moran birth-death process, where reproduction happens with probability proportional to fitness. The links of a node determine which other individuals can be replaced by the offspring of that individual.

Intuitively, one might assume that adding a link to a given network would always decrease the fixation time. However, a simple counterexample disproves this intuition. We show analytically for small networks, that adding a link can increase the fixation time. Simulating the stochastic process on larger lattices, we find a similar result. By adding links to a 2D-lattice without boundary conditions, the fixation time can increase as well. This shows the validity of our counterintuitive result even for larger population sizes.


BP 32.5 Tue 15:00 MA 001

The Cost and Dynamics of Competence in Bacillus subtilis — JEFFREY POWER, MELNIK YUKSEL, and BERENIKE MAURER — Universität zu Köln, Cologne, Germany

When bacterial cells deplete all of the nutrients in their environment, they can enter a stationary growth phase. In Bacillus subtilis, the stationary phase is of particular interest as a fraction of a culture in the stationary phase will stochastically switch into a competent state, where cells can take up extracellular DNA and use it as a measure for a species’ success in its living conditions. Here, we demonstrate analytical calculations on a general evolutionary model and by studying the effect of environmental fluctuations onto fitness by analytical calculations on a general evolutionary model and by studying the effect of environmental fluctuations onto fitness.

This work is a fundamental start to better understanding the dynamics of the stationary phase and the evolutionary advantage of stochastically switching a population subset into a competent state.

A Two-Player Game with Linear State-Dependent Payoff Function — TIM HERRMANN1, MARK KIRENIN2, and KATHARINA FISCHER3 — 1TU Dresden — 2TU Dresden, Chair of Managerial Economics — 3TU Dresden, Institut für mathematische Stochastik

In classic game theory all elements of a game (set of players, set of strategies, payoff function) are static. In contrary, real-world strategic interactions are often characterized by changes of at least one of the three elements of a game over time. In our model a game with state-dependent payoff functions is analysed. The payoff function of the (n + 1)-st round depends linearly on the payoff of the n-th round. Thereby the structure of the game can change, e.g. from prisoner’s dilemma structure to a structure, where individual rationality coincides with collective rationality. Therefore, the concepts of short-term and long-term rationality are defined. It is shown for our game with a state-dependent payoff function, that the following criteria of long-term rationality are equivalent (besides a few special cases): Pareto optimality, collective rationality and the Nash equilibrium in recursive dominant strategies. For symmetric payoff functions these three criteria of (individual and collective) long-term rationality are additionally equivalent to the collective short-term rationality. The concept of ESS is refined to absolute ESS (ESSA) and relative ESS (ESSR). It is shown that ESSA-tuples are equivalent to the above mentioned criteria for symmetric payoff functions and long-term rationality.

Evolutionary Coalition Games — TADEUSZ PLATROWSKI — Faculty of Mathematics, Informatics, and Mechanics \ University of Warsaw, Warsaw, Poland

We introduce the concept of evolutionary coalition games played in a large population. The members of the population play a strategy chosen from a finite set, and interact in randomly formed coalitions. The interactions are described by a multiplayer strategic game. Each coalition generates a total utility, identified with the value of the coalition, and equal to the sum of the payoffs of its all members from the multiplayer game. The total utility is distributed among the coalition
members, proportionally to their Shapley values. Evolution of the whole population is governed by the replicator equations. Polymorphic stationary states of the population are studied for various types of the multiplayer social dilemma games. It is argued that application of coalitional game theory solution concepts to social dilemma models of evolutionary game theory can foster cooperation in the long run.

BP 32.8 Tue 15:45 MA 001


Condensation phenomena occur in many systems, both in classical and quantum mechanical contexts. Typically, the entities that constitute a system collectively concentrate in one or multiple states during condensation. For example, particular strategies are selected in zero-sum games, which are generalizations of the children’s game Rock-Paper-Scissors. These winning strategies can be identified with condensates.

In our work, we apply the theory of evolutionary zero-sum games to explain condensation in bosonic systems when quantum coherence is negligible. Only recently has it been shown that a gradient-dissipative gas of bosons may condense not only into a single, but also into multiple non-degenerate states. This phenomenon may occur when a system of non-interacting bosons is weakly coupled to a reservoir and is driven by an external time-periodic force (Floquet system). On a mathematical level, this condensation is described by the same coupled birth-death processes that govern the dynamics of evolutionary zero-sum games. We illuminate the physical principles underlying the condensation and find that the vanishing of relative entropy production determines the condensates. Condensation proceeds exponentially fast, but the system of condensates never comes to rest: The occupation numbers of condensates oscillate, which we demonstrate for a Rock-Paper-Scissors game of condensates.

BP 33: Cell adhesion, mechanics and migration I (joint BP/CPP)

Time: Wednesday 9:30–13:15

Invited Talk BP 33.1 Wed 9:30 H 1058

Feeling for cell function: Mechanical phenotyping at 100 cells/sec — J ochen Guck — Technische Universität Dresden, Germany

The mechanical properties of cells have long been heralded as a label-free, inherent marker of biological function in health and disease. Wide-spread utilization has so far been impeded by the lack of a convenient measurement technique with sufficient throughput. To address this need, we introduce real-time deformability cytometry (RT-DC) for the continuous mechanical single-cell characterization of large populations (> 100,000 cells) with analysis rates greater than 100 cells/s, approaching that of conventional fluorescence-based flow cytometers. Using RT-DC we can sensitively detect cytoskeletal alterations, distinguish cell cycle phases, track hematopoietic stem cell differentiation into distinct lineages and characterize cell populations in whole blood by their mechanical fingerprint. Our results indicate that cell mechanics can define cell function, can be used as an inherent cell marker and could serve as target for novel therapies. Mechanical phenotyping adds a new functional, marker-free dimension to flow cytometry with many applications in biology, biotechnology and medicine.

BP 33.2 Wed 10:00 H 1058

Characterizing viscoelastic properties of the cortex in mitotic cells — Elizabeth Fischer-Friedrich1, Jonne Helenius2, Anthony Hymann2, Daniel Müller3, and Frank Jülicher — 1(MPI PKS, Nöthnitzerstr. 38, 01187 Dresden, Germany — 2(MPI CBG, Pfotenhauerstr. 108, 01307 Dresden, Germany — 3D-BSES, ETHZ, Mattenstr. 26, 4058 Basel, Switzerland

Cell stiffness is a key parameter for our understanding of cell shape, cell migration and tissue organization. However, as the cell consists of several components, it is challenging to extract the force contribution and the elastic modulus of a specific component upon cell deformation. Here, we probe the stiffness of round, mitotic HeLa cells in a parallel plate compression setup, where we measure the force necessary to compress cells in between plates. An earlier study showed that in steady state, this force is due to cell surface tension. Here, we apply step strains and sinusoidal modulation of the plate distance at various frequencies allowing us to probe differential cell stiffness. We find strong indications that cell stiffness in mitosis is dominated by actomyosin and therefore by the mitotic cortex. This interpretation allows to extract an associated frequency-dependent area extension modulus. We show that myosin activity at the same time fluidizes and stiffens cells, where differential cell stiffness increases linearly in dependence of active prestress. On the other hand, the passive cross-linker α-actinin solidifies and stiffens mitotic cells. Our study shows how active and passive cross-linkers influence rheological properties of the cortical actin-network in vivo.

BP 33.3 Wed 10:15 H 1058

Biogenic cracks in porous medium — Arnaud Hemmerle1, Jörn Hartung1, Oskar Hallatschek1,2, Lucas Goehring1, and Stephan Herminghaus3 — 1Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — 2Department of Physics, University of California, Berkeley, CA, USA

Microorganisms growing on and inside porous rock may fracture it by various processes. Most of the studies have been on the chemical aspects of biofouling and bioweathering, while mechanical contributions have been neglected. However, as witnessed by the perseverance of a seed germinating and cracking up a concrete block, the turgor pressure of living organisms can be very significant. It is the effects of such mechanical forces on the weathering of porous media that will concern us here. We designed a model porous medium made of glass beads held together by polydimethylsiloxane (PDMS) capillary bridges. The rheological properties of this material can be controlled by the curing conditions and the crosslinking of the PDMS. Glass and PDMS being inert to most chemicals, we are able to focus on the mechanical processes of biodeterioration, excluding any chemical weathering. Inspired by recent measurements of the high pressure (>0.5 Mpa) exerted by a growing population of yeast trapped in a microfluidic device, we show that yeast cells can be cultured homogeneously within porous medium and investigate then the effects of such an inner pressure on the mechanical properties of the sample. We observe crack propagation for a certain range of bead sizes and cohesive ness, showing a clear interaction between biotic and abiotic processes.

BP 33.4 Wed 10:30 H 1058

Artificial tissue, Ultra-soft elastomers for cell mechanical in-
Molecular stress sensors constructed from DNA — Neenakshi Prabhune, Jonathan Bath, Andrew Turberfield, Florian Rehfeldt, and Christoph F Schmidt — Third Institute of Physics-Biophysics, Georg-August-Universität Göttingen

We present electrical impedance measurements of single amoeboid cells — Helmar Leonhardt — Universität Potsdam, 14476 Potsdam OT Golm

Molecular stress sensors constructed from DNA — Neenakshi Prabhune, Jonathan Bath, Andrew Turberfield, Florian Rehfeldt, and Christoph F Schmidt — Third Institute of Physics-Biophysics, Georg-August-Universität Göttingen

We present electrical impedance measurements of single amoeboid cells — Helmar Leonhardt — Universität Potsdam, 14476 Potsdam OT Golm

Shake and adhesion dynamics of amoeboid cells studied by cell-substrate impedance fluctuations — Helmar Leonhardt — Universität Potsdam, 14476 Potsdam OT Golm

We present electrical impedance measurements of single amoeboid cells on microelectrodes. Wild type cells and mutant strains are studied that differ in their cell-substrate adhesion strength. We recorded the projected cell area by time lapse microscopy and found a correlation between kinetics of the projected area (cell shape oscillation) and the internal cell’s morphology. We developed a data processing routine to extract such trends. We furthermore observed that cell-substrate attachment strength strongly affects the impedance in that the magnitude of fluctuations are enhanced in cells that effectively transmit forces to the substrate. For example, in talA- cells, which lack the actin anchoring protein talin, the fluctuations are strongly reduced. Such short-term fluctuations are extracted by high-pass filtering the original data. Typically, amoeboid motility advances via a cycle of membrane protrusion, substrate adhesion, traction of the cell body and tail retraction. This motility cycle results in the quasi-periodic oscillations of the projected cell area and the impedance. In all cell lines measured, similar periods were observed for this cycle, despite the differences in attachment strength. Based on the approach presented here, we can separate the changes in the impedance signal that are caused by the projected cell area from the fluctuations induced by the cell-substrate adhesion.

30 min break

Probing the role of cytoplasmic flows in embryogenesis — Matthias Mittasch, Peter Gross, Stephan Grill, and Moritz Kreyssig — Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany — Biotechnology Center, Technische Universität Dresden, 01307 Dresden, Germany

While the genetic basis of embryogenesis is increasingly well understood, it is also clear that gene expression needs to be coupled to physical transport phenomena to account for the genesis of spatial structure. A striking example of morphogenesis is the polarization of the egg cell of the nematode worm C. elegans prior to asymmetric cell division. This process relies on the active cortical transport of morphogens (PAR proteins), and is impaired upon myosin-2 motor down-regulation. However, little is known about the mechanistic role of the cytoplasmic flows that seem to stabilize cell polarization. Here, we adapt the previously described technique of light driven micro-fluidics (Weinert & Braun, J. appl. Phys. 2008), in order to now generate flows inside early stage embryos. Specifically, we report on the generation of micro-scale flow patterns confined in three dimensions, with velocities exceeding the wild type flows. By this, we aim to (i) rescue impaired embryos, (ii) manipulate wild-type cytoplasmic flow velocities, and (iii) introduce polarity multiples through the induction of well-controlled artificial cytoplasmic flows inside C. elegans eggs. We anticipate that our findings will add to the general understanding of how biological systems utilize active transport phenomena to establish spatial structure.

Force fluctuations in three-dimensional suspended fibroblasts — Florian Schur, Christian Schröder, and Florian Rehfeldt — Drittes Physikalisches Institut - Biophysik, Georg-August-Universität Göttingen

Cells are sensitive to mechanical cues from their environment and at the same time generate and transmit forces to probe and to adapt to their surroundings. Key players in the generation of contractile forces are acto-myosin structures. To test forces and elasticity of cells not adhered to a substrate, we used a dual optical trap to suspend 3T3 fibroblasts between two fibronectin-coated beads. We analyzed the correlated motions of the beads with high bandwidth. A combination of active and passive microrheology allowed us to measure the non-equilibrium force fluctuations as well as the elastic properties of the cell. We found that cortical forces deform the cell from its round shape in the frequency regime from 0.1 to 10 Hz. Biochemical perturbation experiments using blebbistatin for myosin inhibition and nocodazole for microtubule depolymerization show that cell stiffness and cortical force fluctuations highly depend on acto-myosin activity but not on microtubules. Serum-starvation also largely reduced the fluctuation amplitude. A force-clamp allowed us to observe cells under defined constant forces. Combining our optical trap with a confocal microscope allowed us to image the three-dimensional actin distribution of Life-Act transfected cells during the force measurements.

Buckling dynamics of freely diffusing single erythrocytes — Michael Gollner, Adriana C. Toma, and Thomas Pfohl — Department of Chemistry, University of Basel, Switzerland

Containing a wealth of information, human blood is the most used sample for diagnostic purposes. Microfluidics, with its unique advantages in performing analytical functions, has been increasingly used for whole blood and cell-based analysis. However, studies on the single-cell level using microfluidic techniques often require active immobilization in order to be investigated by optical methods. We developed a microfluidic setup for single red blood cell (RBC) assays starting with whole blood samples which permits diffusion-controlled variation of the external environment. Individual RBCs are freely held at a substrate, we used a dual optical trap to suspend ST3 fibroblasts between two fibronectin-coated beads. We analyzed the correlated motions of the beads with high bandwidth. A combination of active and passive microrheology allowed us to measure the non-equilibrium force fluctuations as well as the elastic properties of the cell. We found that cortical forces deform the cell from its round shape in the frequency regime from 0.1 to 10 Hz. Biochemical perturbation experiments using blebbistatin for myosin inhibition and nocodazole for microtubule depolymerization show that cell stiffness and cortical force fluctuations highly depend on acto-myosin activity but not on microtubules. Serum-starvation also largely reduced the fluctuation amplitude. A force-clamp allowed us to observe cells under defined constant forces. Combining our optical trap with a confocal microscope allowed us to image the three-dimensional actin distribution of Life-Act transfected cells during the force measurements.

Biomechanics of the Spinal Cord — David E. Kosher and Christian Franze — Department of Physiology, Development and Neuroscience, University of Cambridge, United Kingdom

In cell physiology and pathology mechanical signaling plays an important role. Many types of mechanical forces correspond to the mechanical cues in their environment. Yet, in spinal cord, data on tissue stiffness are sparse and therefore the mechanical environment is unknown. To fill this gap, we conducted atomic force...
microscopy indentation and tensile measurements on acutely isolated mouse spinal cord tissue sectioned along the three major anatomical planes (transverse, coronal and sagittal planes), and correlated local mechanical properties with the underlying cellular structures. Our measurements revealed that gray matter is significantly stiffer than white matter irrespective of directionality and force direction. While white matter behaved like a transverse isotropic material on all length scales, gray matter was isotropic at the tissue and anisotropic at the cellular scale. Most importantly, tissue stiffness correlated with axon orientation, cell body size, and cellular in plane proximity, which we combined into a linear model to estimate local central nervous system tissue stiffness. Our study may thus lay the foundation to predicting local tissue stiffness based on histological data, and hence contribute to the understanding of cell behavior in response to mechanical signaling under physiological and pathological conditions.

Properties of Single Squamous Cell Carcinoma Cells — ●Susanne Steeger1, Tanja Schreyer1, Stefan Hänse2, Jörg Schipper2, and Mathias Getzlaff1

In this contribution we report on measurements of the mechanoelastic properties of ENT squamous cell carcinoma cells. The study of these single cancer cells in culture medium is carried out by Atomic Force Microscopy. Our main interest is the determination of the Youngs Modulus calculated by the Hertzian Model. We identify the elasticity of cancer cells in order to compare it with that of similar benign cells. Because Live Cell Imaging is a challenging task we first focus on testing different cantilevers and various strategies to treat the cells carefully.

In order to determine the individual properties of the cancer cells we additionally analyse their cytoskeleton (actin and tubulin) by using a confocal fluorescence microscope. Cancer cells are known for their modified cytoskeleton which is reflected in the different elasticities of both cancer and comparable benign cells.

PAR polarity pattern in C. elegans zygotes establishes via a mechanochemical feedback module — ●Peter Gross1,2, K.Vilay Kumar1,2,3, Nathan W. Goehring4, Justin S. Bois5,2, and Thomas Höfer1,2,3, and Stephan W. Grill1,2,3,5

The interplay between biochemistry and cell mechanics is critical for a broad range of morphogenetic changes. A prominent example hereof is the emergence of cell polarity during the embryogenesis of C. elegans, resulting in a patterned state of the membrane-associated PAR polarity proteins. Crucial for the emergence of the patterned state are large-scale flows in the membrane-associated actomyosin cortex, which are observed concomitantly with the emergence of PAR polarization. The coupling of biochemistry and cortical flows, driving this mechanochemical patterning processes, remain poorly understood.

Here we establish that PAR polarization of C. elegans zygotes represents a coupled mechanochemical feedback system. We demonstrate that the biochemistry in form of the PAR domains controls mechanics by establishing a myosin gradient. We measure the spatio-temporal profile of the anterior and posterior PAR concentration, the myosin concentration and the induced flow-field. Furthermore we present a theoretical description of this process in the framework of active fluids combined with PAR biochemistry in a coupled reaction-diffusion active-fluids approach. We show that this mechanochemical feedback description quantitatively recapitulates the spatiotemporal profile of PAR polarity emergence.

Pinned polymer loops in external field: how to align chromosomes for recombination? — Yrin Ting Lin1, Daniela Prömmers1, Wenwen Huang1, Petrina Delvain12, Mariola Chacón12, Iva Tolić12, Frank Jülicher1, and Vasily Zaburdaev1

Chromatin movement and structure are central to many processes in cells such as mitosis, replication, and transcription, where physical properties of the chromatin fiber play an essential role. Motivated by the problem of chromosome alignment and recombination during meiosis we solve for the statistics of a pinned polymer ring in an external force field. We predict how the contact probability between two rings depends on the ratio of the force to the intrinsic noise level and how it changes upon addition of new recombination spots. Due to the underlying loop topology, our theoretical results are readily applicable to the description of bacterial DNA and polymer brushes.

Statistical Inference of E.Coli’s tumbling behavior and chemotaxis strategy using Kramers-Moyal coefficients — ●Oliver Pohl1, Marius Hintschke2, Carlos Betz1, and Holger Stark2

The bacterium Escherichia coli moves with alternating runs and tumbles that occur with a mean tumble rate. In the presence of gradients corresponding to the description of bacterial DNA and polymer brushes.

Statistical Inference of E.Coli’s tumbling behavior and chemotaxis strategy using Kramers-Moyal coefficients — ●Oliver Pohl1, Marius Hintschke2, Carlos Betz1, and Holger Stark2

In vitro Min protein patterns arise from self-controlled chaos — ●Jacob Halatek and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität, München, Germany

The mass-conserving reaction-diffusion dynamics of Min proteins act as spatial regulator for the assembly of the cell division machinery. A plethora of experiments has demonstrated a remarkable adaptability of oscillatory Min protein patterns to variations of system geometry. As such, the Min system serves as ideal basis to study the theoretical concepts underlying a real pattern-forming system that can be found in nature. The classical picture for pattern-forming reaction-diffusion systems is rooted in two distinct concepts: The diffusion driven instability proposed by Turing, and the concept of diffusively coupled, self-sustained oscillators proposed by Kuramoto. Here, we investigate the spatio-temporal instabilities of Min protein dynamics that lead to characteristic patterns observed in vivo and in vitro. We find that the in vitro instability cannot be ascribed to any of the two classical concepts but gives rise to a new one. We find transient Turing patterns at onset that loose stability to a chaotic attractor. Further from onset this chaotic attractor condenses into a global limit cycle, passing a regime with transient chimera states. As such, Min protein patterns arise in vitro from a state of self-controlled chaos, rather than from destabilization of uniform states. We find that such dynamics stem from generic properties of mass-conserved reaction-diffusion dynamics and are not specific to the Min system.

Stochastic Dynamics of IFN Type I Signaling — ●Nikolaus Schnellbächer1,2, Nils Becker3, Thomas Höfer1, and Ulrich Schwarz1,2

By analyzing experimental data on swimming trajectories, we infer the parameters of our model. To this purpose generalized Kramers-Moyal coefficients are calculated for our shot-noise model and matched to the ones obtained from the trajectories. In contrast to common tumbling recognition algorithms no free parameters need to be pre-determined. Furthermore, we can identify the bacteria’s chemotaxis strategy by exploiting the Kramers-Moyal coefficients.
The signaling molecules interferon (IFN) of type I are secreted by many nucleated cells to signal the presence of an intracellular viral infection to their environment and to inhibit viral replication. Once in the extracellular environment, they bind to a heterodimeric cell surface receptor (IFNAR – Interferon Alpha Receptor) to form an association with the receptor and release the binding complex, which then triggers an intracellular response. The most prominent pathway activated by interferons is the canonical JAK/STAT signaling pathway, where STAT molecules dock at the receptor associated Janus kinases (JAKs) at their cytoplasmic domains.

A central question of this system is to explain the differential information processing of different interferons through the same transmembrane receptor system. Moreover noteworthy low copy numbers of the receptors on the cell surface are a typical cause for a high degree of intrinsic stochasticity. We use stochastic computer simulations to analyze the activation dynamics in space and time. In particular we investigate spatial effects on the dose response behavior of the IFN type I signaling system.

**BP 34.5** Wed 10:30 H 1028

**Scaling Regimes for Confined Wormlike Chains under Tension**

Greg Morrison
dave thirumalai

1IMT Lucca Institute for Advanced Studies, Lucca Italy 55100
2University of Maryland at College Park, College Park MD 20742

In this talk, we study the scaling behavior of a wormlike chain (WLC) with persistence length $l_p$ confined to the surface of a cylinder of radius $R$ under the application of an external tension. Inextensibility and confinement effects are treated on a mean field level, and we show that the stationary solution for the mean field parameters can be related to simple equations that can be solved asymptotically. We are able to accurately recover the well known Odijk scaling of $F \sim l_p^2/R^3$, with the deflection length $l_d = (l_p R^2)^{1/3}$, for strongly confined chains and show that this scaling is robust to weak external forces. We show that the scaling regimes for both weakly and strongly confined polymers change drastically under application of large external tension, with $F \sim l_p^2/R$ for a tensile length scale $l_t \sim (l_p/\beta f)^{1/2}$. Our results may be relevant in the mechanical unbinding of hormone-bound DNA as well as a variety of experimental situations involving DNA confined to nanochannels.

**BP 34.6** Wed 10:45 H 1028

**Single molecule measurement of the effective temperature in nonequilibrium steady states**

Eckhard Dietrich
Joan Camunas-Soler
Marco Ribezi-Crivellari
Udo Seifert
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Temperature is a crucial concept for equilibrium systems. For glassy systems, it has been extended to the nonequilibrium regime as an effective quantity showing up in the fluctuation-dissipation theorem. However, direct supporting experimental evidence remains scarce. Here, we present the first direct experimental demonstration of the effective temperature by measuring correlations and responses in single molecules in nonequilibrium steady states generated under external random forces. We combine experiment, analytical theory and simulations for systems with different levels of complexity ranging from a single bead in an optical trap to two-state and multiple-state DNA hairpins. From these data, we can extract a unifying picture for the existence of an effective temperature based on the relative order of various time-scales characterizing intrinsic relaxation and external driving. Our study thus introduces driven small systems as a fertile ground to address fundamental concepts in statistical physics, condensed matter physics and biophysics.

**30 min break**

Invited Talk

**BP 34.7** Wed 11:30 H 1028

**Efficiently extracting thermodynamics and kinetics from molecular simulation data at multiple thermodynamic states**

Frank Nae
FU Berlin, Arminmalee 6, 14195 Berlin

I will present novel methods based on Markov modeling for extracting statistical information (thermodynamics and kinetics) from molecular simulation data that has been generated at multiple thermodynamic states. Such data may be obtained from enhanced sampling protocols, such as umbrella sampling or replica-exchange dynamics, and by mixing one of these protocols with direct molecular dynamics data. Here I will propose ways to optimally extract information from such data, including the reconstruction of the kinetics of rare events that are not directly sampled in the data. An application of our approach is the estimation of rare unbinding kinetics of protein-ligand complexes when only the more frequent binding process can be sampled in direct MD simulations.

**BP 34.8** Wed 12:00 H 1028

**Stochastic dynamics of adhesion bonds for a rod propelled by both force and torque**

Anna Battista and Ulrich Schwarz
Heidelberg University, Heidelberg, Germany

The stochastic dynamics of adhesion bonds has emerged as a powerful theoretical framework to explain many prominent features of sliding friction, including the stick-slip regimes often observed at intermediate driving velocity. Sliding friction occurs in a variety of physical contexts, ranging from tribology to cell motility. In particular, stochastic bonds have been employed to model the dynamics of adhesion between a cell and its substrate. Although much progress has been achieved with the help of stochastic bond models, up to now they have been restricted to sliding friction in one dimension. However, there are situations in which translation is coupled with rotation, as is the case of gliding cells with a shape asymmetry. Motivated by this observation, we develop a sliding friction model for a slider that is both translated and rotated, while being connected to the substrate by stochastic bonds. We find that torque enhances the tendency for stick-slip behaviour and that adhesive patches spontaneously form at the moving interface when the on-rate of the bonds has a velocity dependence. Interestingly, our results show an adhesion dynamics reminiscent of that observed during the migration of curved malaria parasites.

**BP 34.9** Wed 12:15 H 1028

**High stress levels lead to transition from heterogeneous timing to synchronized cellular response of the E.coli Colicin E2 operon**

Anna Battista
Benedikt von Bronk
Benedikt Ewald
Sara Kessel
Karín Schmiedt
Erwin Frey
Madeleine Opitz

1Faculty of Physics, LMU München, Germany
2Institute for Genetics, Universität zu Köln, Germany

The production of bacteriocins, such as colicins, is one means of bacteria to outcompete other microorganisms. In a single cell study, we analyze the heterogeneous gene expression of Colicin E2, expressed from the SOS inducible E.coli Colicin E2 operon. We quantitatively study the expression dynamics of the Colicin E2 operon in E.coli using fluorescence time-lapse microscopy. Different fluorescence reporter proteins allow us to observe heterogeneity in Colicin production and Colicin release separately. At low exogenous stress levels all cells eventually respond after a given time (heterogeneous timing), high stress levels lead to a synchronized stress response of all cells about 75 min after stimulation via stress-induced heterogeneous response in combination with heterogeneous timing can be biologically significant. It might enable a bacterial population to endure low stress levels, while at high stress levels an immediate and synchronized response may allow elimination of closely related bacteria competing for resources. Furthermore we could demonstrate that the amount of Colicin released is dependent on cell (lysis) gene expression. Future investigations will focus on transcriptional as well as post-transcriptional regulation affecting the dynamics of Colicin expression and release.

**BP 34.10** Wed 12:30 H 1028

**The fluidity of the cytoplasm is regulated by cytosolic pH**

Matthias Munder
Daniel Midtvedt
Elisabeth Nüske
Shovanayer Maharana
Sonja Kroischwald
Doris Richter
Vasily Zaburdaev
Simon Alberti

1Max Planck Institut für Physik komplexer Systeme – 2Max Planck Institut für molekulare Zellbiologie und Genetik

Upon sub-optimal growth conditions, many cells enter a quiescent state characterized by lack of cell division, low metabolic activity and decreased intracellular pH. The mechanisms by which cells enter and leave quiescence are as of yet largely unknown.

Using single-particle tracking, we investigate the mobility of foreign tracer particles under different cytosolic pH conditions. We find a significant decrease in the mobility of the particles under acidic conditions.

Indicative of obstructed motion in a crowded solution, at short times the velocity autocorrelation function (VACF) of the tracer particles is negative. We relate these findings to a structural phase transition in
the cytoplasm. Our findings indicate that cells may use cytosolic pH to change the material properties of the cytoplasm. We are currently investigating possible consequences of these changes. Our findings could have broad implications for the understanding of alternative physiological states in cells, and promotes a view on the eukaryotic cytoplasm as a viscoelastic material with widely tunable properties.

Detailed balance violations in mesoscopic biological systems

— Christopher Battle1, Chase P. Bhoderz2, Nitha Fakhri1, Fred C. MacKintosh3, and Christoph F. Schmidt4 — 1Drittes Physikalisches Institut, Georg-August-Universitaet, Goettingen, Germany — 2Lewis-Sigler Institute for Integrative Genomics and Department of Physics, Princeton University, Princeton, NJ, USA — 3Dept. of Physics & Astronomy, Vrije Universiteit, Amsterdam, Netherlands

LIVING SYSTEMS EXIST FAR FROM THERMAL EQUILIBRIUM, WITH ACTIVE PROCESSES POWERING MANY OF THEIR FUNCTIONS. AS SUCH, THEY ARE EXPECTED TO VIOilate FUNDAMENTAL TENETS OF EQUILIBRIUM, SUCH AS THE PRINCIPLE OF DETAILED BALANCE. WHILE SOME CELLULAR PROCESSES SHOW UNMISTAKABLE NON-EQUILIBRIUM CHARACTERISTICS, E.G. DIRECTED MOTION, OTHERS ARE MORE SUBTLE, EXHIBITING NON-THERMAL, RANDOM MOTION WHICH IS SIMILAR IN APPEARANCE TO BROWNIAN MOTION, E.G. CORTICAL STRESS FLUCTUATIONS OR ACTIVE CELLULAR STIRRING. IT IS NOT A PRIORI CLEAR WHETHER THE ACTIVE, RANDOM NATURE OF THE SECOND CLASS OF MOTIONS WILL TRANSLATE INTO OBSERVABLE VIOLATIONS OF DETAILED BALANCE ON THE MESOSCOPIC, I.E. CELLULAR, SCALE. HERE WE REPORT EXPERIMENTAL EVIDENCE OF DETAILED BALANCE VIOLATIONS FOR SUCH A CASE. SUCH VIOLATIONS CAN BE USED TO "FINGERPRINT" NON-EQUILIBRIUM SYSTEMS, AND DIFFERENTIATE ACTIVE PROCESSES FROM THERMAL ONES WITHOUT PERTURBING THE SYSTEM.

BP 35.2 Wed 15:30 H 1028

Lipid composition in fusion of model membrane systems studied by x-ray diffraction — Sebastian Köhler1, Yihui Xu2, Ziad Khattari3, and Tim Salzetti4 — 1Institut für Röntgenphysik, Georg-August-Universität Göttingen — 2Department of Physics, Hashemite University, Zarqa, Jordan

We have investigated the structure and interaction of solid-supported multilamellar phospholipid bilayers as model systems for membrane fusion in view of the formation of stalks (putative intermediate structures occurring during the fusion process). X-ray reflectivity and grazing incidence small angle x-ray scattering measurements have been performed on bilayer stacks of different ternary and quaternary lipid mixtures at varying osmotic pressure. Analysis of the obtained electron density profiles and pressure-distance curves reveals systematic changes in structure and hydration repulsion. The osmotic pressure needed to induce stalk formation at the transition from the fluid lamellar to the rhombohedral phase indicates how membrane fusion properties are modified by bilayer composition. We present phase diagrams for all studied lipid mixtures.
from structural changes induced in membranes upon binding; it increases membrane rigidity, facilitates vesicle fusion and rupture. However, the mechanisms for these processes are still not fully understood. Here, we elucidate the effect of Al3+ ions on neutral and charged mixed supported lipid membranes (SLMs) using a variety of surface sensitive experimental techniques in combination with molecular dynamic (MD) simulations.

Our results show that Al3+ affects lipid packing, bilayer thickness, diffusivity as well as it does induce irreversible domain formation in a mixed bilayer. The observed effects for neutral SLMs are mostly reversible whilst the effects observed for mixed SLMs are mostly irreversible. Notably does MD simulations reveal that Al3+ changes the order parameter of the fatty acid chains.

BP 35.5 Wed 16:15 H 1028
Ultra-thin self-hydrated artificial membrane composed of DPPC and chitosan deposited without solvents — 
MARE J RETAMAL,1,2, MARCELO A. CISTERNAS1,2, SEBASTIAN E. GUTIERREZ-MALDONADO1, TOMAS PEREZ-ACLE1,3, BIRGER SEIFERT2,1,2, MARK BUSCH4, PATRICK HUBER5, and ULRICH G. VOLKMANN1,2 — 
1SurfLab UC, Instituto de Fisica, Pontificia Universidad Catolica de Chile (UC), Santiago, Chile — 2CIEN-UC, Santiago, Chile — 3DLab, Fundación Ciencia y Vida, Santiago, Chile — 4Institute of Materials, Physics and Technology, Hamburg University of Technology (TUHH), Hamburg-Harburg, Germany

We present the formation and characterization of a phospholipid bilayer (dipalmitoylphosphatidylcholine, DPPC) on a mattress of a polysaccharide (Chitosan) that keeps the membrane hydrated. The deposition of Chitosan (~25 Å) and DPPC (~60 Å) was performed from the gas phase in high vacuum onto a substrate of Si(100). The layer thickness was controlled in situ using Very High Resolution Ellipsometry (VHRE). Raman spectroscopy studies show that neither Chitosan nor DPPC molecules decompose during evaporation. With VHRE and AFM we have been able to detect phase transitions in the membrane. The presence of the Chitosan interlayer as a water reservoir is essential for both DPPC bilayer formation and stability. Our experiments at SurfLab UC show that the proposed sample preparation from the gas phase is reproducible and provides a natural environment for the DPPC bilayer. Reference: www.aip.org/publicating/journal-highlights/artificial-membranes-silicon

BP 35.6 Wed 16:30 H 1028
Attraction between hydrated hydrophilic surfaces — 
MATJ KANDUC,1 EMMANUEL SCHNECK2, and ROLAND NETZ3,4 — 
1Department of Physics, Free University Berlin — 2Max Planck Institute of Colloids and Interfaces, Research Campus Golm

According to common knowledge, hydrophilic surfaces repel via hydration forces while hydrophobic surfaces attract, but mounting experimental evidence suggests that also hydrophilic surfaces can attract. Using a custom molecular dynamics simulations at prescribed water chemical potential [1] we study the crossover from hydration repulsion to hydrophobic attraction between planar surfaces. We cover the complete spectrum from very hydrophobic surfaces (characterized by high repulsion) to hydrophilic surfaces exhibiting complete hydration repulsion at the molecular level and probe peptide folding because of its inherent surface specificity. In this study, two different peptides are shown to interact with membranes in very different ways. The cell membrane is the most important biological surface as its interaction with peptides is an integral part of transport, communication, energy transduction and survivability. However, an intrinsic difficulty in monitoring peptide interaction with membranes is the required surface sensitivity. Sum frequency generation (SFG) vibrational spectroscopy is well suited to study protein monolayers at lipid surfaces because of its inherent surface specificity. In this study, two different peptides are shown to interact with model membranes in very different ways.

GALA, a peptide mimicking viral fusion proteins, can disrupt membranes and escape from endosomes when triggered at low pH. We follow GALA activity at the molecular level and probe peptide folding as well as the disturbance and hydration of individual leaflets within model bilayers. We show that the cell-penetrating peptide SAP(E) solely interacts with the lipid headgroup region proving the first step of its proposed uptake mechanism. Peptides can also help stabilize lipid membranes. We discuss preliminary results about the effects of specific antifreeze proteins on the temperature stability of lipid monomeric bilayers.

BP 35.9 Wed 17:30 H 1028
From destruction to protection - following peptide interactions with membrane interfaces — 
JOHANNES FRANZ1, DENISE SCHACH1, JOE E. BAIQ2, DAN GRAHAM3, DAVID G. CASTNER2, MISCHA BONN4, and TOBIAS WEIDNER5 — 
1Max Planck Institute for Polymer Research, Mainz, Germany — 2Oregon State University, Corvallis, OR, USA — 3University of Washington, Seattle, WA, USA

The cell membrane is the most important biological surface as its interaction with peptides is an integral part of transport, communication, energy transduction and survivability. However, an intrinsic difficulty in monitoring peptide interaction with membranes is the required surface sensitivity. Sum frequency generation (SFG) vibrational spectroscopy is well suited to study protein monolayers at lipid surfaces because of its inherent surface specificity. In this study, two different peptides are shown to interact with model membranes in very different ways.
Multivalent interactions are observed in a multitude of biological processes (e.g., association of viruses or bacteria to their host cells). The involved receptors are nano-sized objects, making it challenging to assess the exact number of attachment points under physiological conditions. Using TIRF microscopy of fluorescently labelled, small unilamellar vesicles, which serve as a model system for the interaction of viruses with cell membranes, we show that multivalent interactions can be assessed by single particle tracking (SPT). The vesicles are linked to a supported lipid bilayer (SLB) using DNA-tethers carrying cholesterol groups at their ends, which automatically insert into the membranes and which allow a 2D diffusion of the vesicle above the SLB. The number of attachment points can be manipulated by the concentration ratio of vesicles to DNA-tethers. SPT allows to extract the diffusion coefficients on the level of single vesicles and histograms of the observed diffusion coefficients exhibit a spectrum of distinct peaks, which are related to subpopulations of vesicles differing by their number of DNA-tethers. This enables to recalculate fluctuations of the diffusion constant of a certain vesicle into fluctuations of the number of attachment points linking the vesicle to the SLB. The extension of this analysis to virus particle tracking including a comparison between SPT with fluorescence correlation spectroscopy will be discussed.

**BP 35.11** Wed 18:00 H 1028

**Fast tracking with nanometer precision of individual proteins on the cell membrane** — **Richard Taylor and Vahid Sandoogh Dar** — Max Planck Institute for the Science of Light, Erlangen, Germany

The diffusion dynamics of membrane-incorporated proteins in the live cell is of great biological significance, but its studies are complicated and nuanced due to the diversity and heterogeneity of the membrane landscape. While fluorescence microscopy is routinely employed to investigate membrane phenomena, a low fluorescence rate and photobleaching limit this technique both on the short and long time scales.

Furthermore, fluorescence microscopy suffers from a poor axial resolution.

Here, we report on the use of interferometric scattering (iSCAT) imaging with high three-dimensional spatio-temporal resolution. By labelling the proteins with a small gold nanoparticle, we are able to track indefinitely the protein diffusion in and out of plane, to an unparalleled nm-level accuracy at many thousands of frames per second. We present recent work on tracking of EGFR proteins in the model HeLa cell. Furthermore, we discuss the use of iSCAT imaging for studying out-of-membrane movement, thus allowing investigation into endocytic reactions.

**BP 35.12** Wed 18:15 H 1028

**The interaction of patterned amphiphilic dendritic nanomaterial with a lipid-monolayer** — **M. Alejandra Sanchez, Katharina Bücher, Klaus Müllen, Mischa Bonn,** and **Ellen H. G. Bachus** — Max Planck Institute for Polymer Research, Mainz, Germany

Well-defined amphiphilic dendrimeric macromolecules are biomimetic nanomaterials that can be used for drug delivery into cells. By organic synthesis, functional groups can be positioned in an atomically defined way, resulting in alternating patches of polar and apolar nature. Here we study systematically the interaction of various dendrimers with a model membrane consisting of a self-assembled monolayer of the lipid DPPC (1,2-dipalmitoyl-sn-glycero-3-phosphocholine) on water. By using sum frequency generation spectroscopy we obtain molecular specific information about the membrane molecules and the water molecules in the vicinity of the lipid. Although the dendrimers do not surface-active at the bare water-air interface, they do interact strongly with the aqueous monolayer. The extension of the interaction below the monolayer causes changes in the water orientation as well as the alignment of the lipid molecules. Remarkably, details of the interaction depend on the surface groups present on the dendrimer. Very small changes (e.g. n-propyl vs iso-propyl) result in a different behavior. We link the molecular level picture with the efficiency of penetrating into the cells.

**BP 36.1** Wed 15:00 H 1058

**The mechanics of invasion: How contraction sets the stage for invasive migration.** — **Katarzyna Kopanska** and **Timo Betz** — Physical-Chemistry Curie, UMR168, Institut Curie, Paris, France

To move out of the primary tumor, cancer cells start a complex process of migration in the surrounding tissue called invasion. Understanding the mechanisms responsible for the onset of cancer cell invasion remains an urgent research subject on the path to new strategies to prevent malignant invasion, and thus improve the prognosis of many cancer types.

We focus on the mechanical events that can be observed before and during invasion of the colon cancer cell line CTC26. The experimental system consists of a spheroid of about 2000 cells that is embedded in a collagen I matrix. Before the onset of invasion, a contraction of the collagen gel is observed that shows 3 different phases. Our results suggest that an increase in mechanical tension within the collagen matrix facilitated the outgrowth of cells and hence triggers invasion. In this sense, the cells in the spheroid may optimize the mechanical properties of their environment via force application to facilitate invasion.

**BP 36.2** Wed 15:15 H 1058

**Forces and flows in adhesion-independent cell migration** — **Anna Ernberger1, Martin Bergeier2,3, Ewa Paluch3,** and **Guillaume Salbreux1** — 1Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — 2currently at: Laboratory of Thermodynamics in Emerging Technologies, ETH Zuerich, Switzerland — 3MRC Laboratory for Molecular Cell Biology, UCL, London, UK

When cells move using specific substrate adhesions, they pull in the direction of motion with large stresses that contract the substrate. In confined environments however, cells exhibit directed migration modes which are independent of specific adhesions. Here, we combine hydrodynamic theory and experiments on motile cancer cells to investigate the forces involved in adhesion-free migration. We show that actin cortex flows and deformations move the cells via non-specific substrate friction. Strikingly, the forces propelling the cell forward are several orders of magnitude lower than during adhesion-based motility, while achieving similar cell velocities. Moreover, the force distribution in adhesion-free migration is inverted: it acts to expand, rather than contract, the cell substrate in the direction of motion. We discuss the implications of this fundamentally different mode of force transduction for cell-cell and cell-substrate interactions during migration.

**BP 36.3** Wed 15:30 H 1058

**Experimental Exploration of the Phase Space of Actin Waves** — **Eric Bernitt, Maite Ohmstedt,** and **Hans-Gönter Dörrbecker** — Institut für Biophysik, Universität Bremen, Bremen, Germany

We study actin waves in fibroblast cells that noticeably undulate the cell surface forming Circular Dorsal Ruffles (CDRs). We are interested in the currently unknown mechanism underlying these waves. Previous research in our lab revealed that the cell shape strongly influences the wave dynamics of CDRs, which complicated an analysis of the wave mechanism due to the irregular morphology of fibroblasts. When forced into a well-defined, disk-like morphology, however, cells form waves in a highly regular manner allowing detailed studies of the wave mechanism. We place these cells in flow channels allowing for rapid switching of the cellular biochemical state.

We ask which active role actin plays in the propagation mechanism of CDRs. From the behavior in the phase space of theoretical models we expect that the amount of free g-actin plays a pivotal role. Our setup gives us access to this phase space experimentally. With our approach, experimental and theoretical data can easily be matched, because CDRs on disc-shaped cells propagate laterally between cell edge and nucleus, forming an effectively one-dimensional system with periodic boundary conditions. Here we report our latest experiment in which we shift the cell’s position of the chemical equilibrium between f- and g-actin using latrunculin A.
Catching a target with directed run and tumble motion — Paweł Romanczuk and Guillaume Salbreux

The movement of single cells or entire cell populations is a fundamental mechanism for various biological processes. The ability of cells to change their direction of motion, a phenomenon known as run-and-tumble motion, is crucial for processes such as colony formation, migration, and chemotaxis. In this talk, we present a phenomenological model for crawling cells on patterned substrates. Here we present a phenomenological model for crawling cells on patterned substrates. The model reproduces experimental observations, like the response of a cell on a gradient in substrate elasticity (durotaxis). Collective states of motion such as concerted rotation arise for multiple interacting cells on patterned substrates.}

30 min break

Spontaneous actin dynamics in contractile rings — Victoria Wollrath, Raghavan Thijagarajan, Daniel Rivelin, and Karsten Kruse

Cell migration is a complex process that involves the dynamic rearrangement of the cell cytoskeleton. In this talk, we will focus on the spontaneous actin dynamics in contractile rings, which are key structures involved in cell migration. Contractile rings form during cell division and are also involved in other biological processes such as cytokinesis and morphogenesis. We will discuss recent experimental findings and theoretical models that aim to understand the mechanisms underlying the spontaneous actin dynamics in these rings. The talk will cover the latest advances in this field, including insights into the role of cell polarity, the influence of cytoskeletal dynamics, and the potential implications for cell behavior in various biological contexts.

Characterizing Cell Motility and Transmigration on Ring Shaped Micro Patterns — Christoph Schaffer, Felix Jakob, Jörg Segher, and Joachim Oskar Rädler

Cell migration is a fundamental biological process that is crucial for various physiological and pathological scenarios. In this talk, we will discuss recent advances in characterizing cell migration on ring-shaped micro patterns. These patterns are designed to mimic the natural microarchitecture of biological tissues and provide a controlled environment for studying cell behavior. We will present methods and tools for characterizing cell migration, including quantitative assessments of cell velocity and directionality. The talk will also cover the potential implications of these findings for understanding cell behavior in vivo and for developing new therapeutic strategies.

Is the wound healing mechanism an accelerating one? — Damir Vurnek, Sara Kalmar, and Ana-Suncićana Smith

Wound healing is a complex biological process that involves the repair of damaged or lost tissue. In this talk, we will discuss recent findings on the mechanism of wound healing, with a particular focus on the role of cell migration. We will present evidence suggesting that the wound healing mechanism is an accelerating one, which is consistent with the observed rapid tissue regeneration in some cases. The talk will cover the latest advances in this field, including insights into the mechanisms underlying the acceleration of wound healing and the implications of these findings for understanding tissue repair.

Migration patterns of dendritic cells in response to chemokines — Veronica Bierbaum, Jan Schwarz, Eva Kiermaier, Michael Sixt, and Tobias Bollembach

Dendritic cells (DCs) play a crucial role in the immune system by capturing and processing antigens, presenting them to T cells, and activating adaptive immune responses. In this talk, we will discuss how DCs migrate in response to chemokines, which are small leukocyte chemoattrac-
Stuttgart — Syn Schmitt

• new method applied to complex biological movement

Quantifying control error in complex biological movement: a new method applied to complex biological movement

Am Campus 1, 3400 Kloten-neuburg

Dendritic cells are key components of the adaptive immune system. They navigate through tissues by sensing two different chemokines, CCL19 and CCL21. We develop a physical description of dendritic cell migration as a function of the surrounding chemokine field formed by both immobilized and soluble chemokines. We perform in vitro assays to characterize key properties of migration. In this focus session, dendritic cell models are exposed to well-controlled concentration profiles of the two chemokines. We monitor the gradients and the cellular motion using time-lapse microscopy and obtain a large number of cell trajectories. These trajectories are well captured by Langevin equations, enabling us to separate the stochastic and deterministic contributions to cell migration. Direct Collocation was used to translate the ODE’s were specially designed to be able to independently change the costs at the three levels. Direct Collocation was used to translate the ODE’s into transistor level equations. Additionally, four types of spreading and motility can be identified, depending on the on normal stress at the boundaries: Uniform deformation, non-uniform deformation, uniform gliding and peristaltic ("worm-like") progression. Analytical and numerical solutions are presented along with bifurcation diagrams using normal stress and active force as control parameters.


BP 36.12 Wed 18:15 H 1058

Polarization of motile amoeboid cells under confinement — • Oliver Naegel1, Can Guven2, Matthias Thiebes3, Megan Dreiscol4, Wolfgang Losert2, and Carsten Bets1 — 1Institute of Physics and Astronomy, University of Potsdam, Germany
2Department of Physics, University of Maryland, College Park, Maryland, USA

The typical environment of motile eukaryotic cells, like leukocytes, cancer cells, and amoeba, is dominated by the narrow interstitial spacings of tissue or soil. While most of our knowledge of actin-driven eukaryotic motility is based on cells that move on planar open surfaces, recent work has demonstrated that confinement can lead to strongly altered motile behavior. Our experiments show that motile amoeboid cells undergo a spontaneous symmetry breaking under confinement. Cells inside narrow channels switch to a highly persistent, unidirectional mode of motion, moving at a constant speed along the channel. They remain in contact with the two opposing channel side walls and alternate protrusions of their leading edge near each wall. The actin cytoskeleton of the cells exhibits a characteristic arrangement that is dominated by dense, stationary actin foci at the side walls, together with less dense dynamic regions at the leading edge. Our experimental findings can be explained based on an excitable network model that accounts for the confinement-induced symmetry breaking and correctly recovers the spatio-temporal pattern of protrusions at the leading edge.

BP 37: Modelling of non-linear dynamics in biological movement (focus session)

Time: Wednesday 15:00–16:30

Invited Talk

BP 37.1 Wed 15:00 EW 202

The cost of moving optimally — • Di Jannet Krist emaker — VU, Amsterdam, The Netherlands — UWO, London, Canada

The field of Human Motor Control is concerned with how the brain deals with the very many kinematic and mechanical degrees of freedom (DoF) to control posture and movement. In this field, mathematical models of the musculoskeletal system are indispensable as they provide answers to questions that are inaccessible by experimental studies alone. In a recent set of studies, predictions using a detailed model of the arm together with behavioural data were used to investigate if the DoF are exploited by the brain to minimize costs at three distinct levels: the motor system’s input (e.g. control effort), the motor system’s mechanical output (e.g. energy) and kinematics (e.g. jerk). Subjects performed goal-directed arm movements while holding on to a robotic manipulandum in combination with visual perturbations of seen hand position. The force fields created by the robot and visual perturbations were specially designed to be able to independently change the costs at the three levels. Direct Collocation was used to translate the ODE’s of the model into nonlinear constraints and were solved together with task and boundary constraints using SNOPT, while minimizing several costs at the three levels. It was found that the behavioural data was consistent with the notion that the brain minimizes energy expenditure. Furthermore, it was found that in selecting a kinematic path, the brain does not take into account costs that relate to the output level or the dynamic level. Movement patterns observed experimentally were only consistent with a cost function based solely on kinematic costs.

BP 37.2 Wed 15:30 EW 202

 quantifying control error with information entropy: a new method applied to complex biological movement — • Daniel Haufe1, 2 Michael Günther1, Günter Wunser2, and Syn Schmeits1, 3 — 1Human Movement Simulation Lab, Universität Stuttgart — 2Institut für Theoretische Physik 1, Universität Stuttgart

The model further exhibits a stress accumulation within the tissue that proceeds in form of a mechanical wave, starting at the wound edge. Additionally, four types of spreading and motility can be identified, depending on the normal stress at the boundaries: Uniform deformation, non-uniform deformation, uniform gliding and peristaltic ("worm-like") progression. Analytical and numerical solutions are presented along with bifurcation diagrams using normal stress and active force as control parameters.
The paper outlines an alternative and highly non-linear mechanism capable of physically pushing the pointer's location reliably into the goal position using also the pointer's velocity, which has, too, been available in continuous visual feedback. It is the phase relationship between velocity and position, both emitted by a pattern generator, which jointly enables predicting the stop position from any intermediate state of the movement. This provides a prediction of the error, based on which one or several scaled force impulses can be released annihilating the error at movement end.

BP 37.4 Wed 16:00 EW 202
Reafferee Principle 2.0 — Kim Jong Bostrom and Heiko Wagner — Motion Science, University of Münster, Germany

The reafferee principle was introduced 1950 by Holst and Mittelstaedt, and its basic features have been confirmed by many experiments. It holds that the neural systems makes an efference copy that is compared with the reafference, i.e. the afferent signal resulting from movement caused by the efference, and the difference is passed to higher centers. However, efferent and afferent signals encode very different kinds of information, between which there need not exist a linear relationship. To address this problem it has been suggested that the brain involves a forward simulator to calculate the expected reafference from the efferent signal. Such mechanism, however, would require a considerable amount of neural resources and would introduce unavoidable latencies. We propose a more efficient and latency-free mechanism that does not require an efference copy but generates the movement directly together with the corresponding expected reafference. The mechanism involves a recurrent neural network that learns to generate movements from abstract movement commands, and at the same time leverages the resulting reafference from the sensory system. Afterwards, the network is able to generate both the movements together with the corresponding reafferences, and due to its intrinsic morphing capability, the network is able to flexibly interpolate and extrapolate the learned movements in synchrony with the expected reafferences. We demonstrate the modified reafferee principle by computer simulations.

BP 37.5 Wed 16:15 EW 202
Wobbling masses: definite costs and potential benefits — Michael Günther,¹ and Syn Schmitt¹,² — Universität Stuttgart, Human Movement Simulation Lab — ²Stuttgart Research Centre for Simulation Technology — Friedrich-Schiller-Universität Jena, Lehrstuhl für Bewegungswissenschaft

Humans seem biomechanically unique in the animal kingdom. It is, though, certainly neither bipedalism nor the strung-out leg that constitutes human’s uniqueness. Some birds can even sleep on just one extended leg. Rather, it is the amount of muscle mass in the legs that makes humans unique animals. Muscle masses are soft tissue attached to the skeleton. They “wobble” when the bones are mechanically excited by impacts. Macroscopic units of soft tissue can be modelled as rigid bodies (“wobbling masses”) interacting visco-elastically with the skeleton. As the corresponding energy dissipation is expected to roughly scale with wobbling mass volume, we examined how much energy is actually dissipated by human wobbling masses after a leg impact. We calculated numbers from wobbling mass kinematics of the stance leg, estimated on the basis of high-speed camera sequences of human running. Comparing dissipated energy to axial leg work and joint energy balances during ground contact provides a measure of relevance for the irreversible energy loss by leg wobbling masses. We discuss functional explanations for such a unique amount of wobbling masses in human legs. We also try and explain how they yet pay off although any significant amount of irreversible energy loss would seem inefficient and thus expectably avoided by nature as good as possible.

BP 38: Electrolytes at Interfaces - Stern Layer (focus session, joint CPP/BP/O)

Time: Wednesday 15:00–18:00

Invited Talk
BP 38.1 Wed 15:00 C 130
Ultrasound dynamics of hydrated metal ions at the water-solid interface observed by atomic force microscopy — Kislon Voitkovsky — Durham University, Durham, UK

The lateral organisation and dynamics of ions in the Stern layer of immersed solids is central to many electrochemical and biological processes. However, measuring the lateral organisation and dynamics of single adsorbed ions remains challenging experimentally. Recently we showed that atomic force microscopy could be used to image single metal ions at the surface of various solids in water [1, 2]. Our results indicate that, depending on the hydration landscape of the solid, adsorbed ions can form ordered structures within the Stern layer, through correlation effects that are driven purely by the interfacial water [2]. The dynamics of the adsorbed ions appears surprisingly slow, typically exhibiting residence times above the millisecond. This suggests that water can also dramatically alter the ions dynamics and play a key role in stabilizing adsorbed ions at a given location of the interface. The existence of long-lived ionic structures at interfaces could have important implications for charge transfer and at biointerfaces.


BP 38.2 Wed 15:30 C 130
Direct observation of ionic structure at solid-liquid interfaces: A deep look into the Stern Layer — Igor Siretanu, Daniel Ebeling, Martin P. Andersson, Cunlu Zhao, Dirk van den Ende, and Frieder Mugele — Physics of Complex Fluids and MESA+ Institute for Nanotechnology, Department of Science and Technology, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands

The distribution of ions and charge at solid-water interfaces plays an essential role in a wide range of processes in biology, geology and technology. While study of the solid-electrolyte interface date back to the early 20th century, a detailed picture of the structure of the electric double layer has remained elusive, largely because of experimental techniques that have not allowed direct observation of the behaviour of ions, i.e. with subnanometer resolution. Making use of recent advances in Atomic Force Microscopy with atomic level precision, herein, we reveal the local surface charge and the ordered adsorption of the divalent ions, unlike monovalent ions, to heterogeneous clay surfaces in contact with aqueous electrolytes. Complemented by density functional theory, the experiments produce a detailed picture of the formation of surface phases by templated adsorption of cations, anions and water, stabilized by hydrogen bonding.

BP 38.3 Wed 15:45 C 130
Probing surface chemistries at mineral surfaces in nanometer-confined electrolytes with atomic force microscopy — Cunlu Zhao, Daniel Ebeling, Igor Siretanu, Dirk van den Ende, and Frieder Mugele — Physics of Complex Fluids and MESA+ Institute for Nanotechnology, Department of Science and Technology, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands

We adopt atomic force microscopy (AFM) to investigate the chemistries of mineral surfaces in nanometer-confined electrolyte solutions. Firstly, AFM was used to measure interaction forces between tip and solid surfaces with nanometer separation in ambient electrolytes. Then a charge regulation (CR) boundary was formulated for the Poisson-Boltzmann equation to establish a linkage between AFM measurements and the surface chemistries (e.g., pK values of surface (de)protonation and ion adsorption). Finally, we analyzed force vs. distance curves recorded between a silica tip and a heterogenous silica-gibbsite substrates in aqueous solutions of NaCl and KCl within the framework of CR boundary-complemented Derjaguin-Landau-Verwey-Overbeek (DLVO) theory. By fitting experimental force vs. distance curves down to tip-sample separation of 2nm, we determined for both silica and gibbsite surfaces pK values of surface (de)protonation and ion adsorption. The various pK values determined from our AFM experiments are quite consistent with the macroscopic titration measurements tabulated in the literature. This indicates that AFM could be potentially used as a titration tool, but with an unprecendentedly high resolution.

BP 38.4 Wed 16:00 C 130
Ion adsorption-induced wetting transition in oil-water-
mineral systems — •FRIEDER MUGGLE, BIJOY BERA, ANDREA CAVALLI, IGOR SIRENTANU, ARMANDO MAESTRO, DIRK VAN DEN ENDE, MICHEL DUTS, AND MARTIN COHEN-STUART — University of Twente, MESAs+ Institute for Nanotechnology, Physics of Complex Fluids, Enschede, The Netherlands

The relative wettability of oil and water on solid surfaces is crucial to many environmental and technological processes including soil contamination/remediation, oil-water separation, and oil recovery. Good wettability of one fluid generally implies strong retention of that fluid in a porous solid matrix and simultaneously easy displacement of the other one. Here, we demonstrate that the contact angle of aqueous solutions of common chloride salts on mica in ambient oil displays a transition from near zero to finite contact angles up to 70° upon replacing monovalent Na+ and K+ cations in the aqueous phase by divalent Ca2+ and Mg2+ at neutral to elevated pH. This wetting transition is driven by electrostatic forces and originates from charge reversal of the mica-water interface upon adsorption of divalent cations. The ion-induced wettability alteration is synergistically enhanced by small amounts of polar molecules, stearic acid, added to the ambient oil, leading to water contact angles up to 70°.

BP 38.5 Wed 16:15 C 130 Cardiolipin Monolayers — •RENKO KESSBÖCK, HEIKO AHRENS, ANDREAS GRÖNING, THOMAS ORTMANN, AND CHRISTIANE A. HELM — Physik, Uni Greifswald, 17487 Greifswald, Germany

Cardiolipin-cytochrome c binding in the inner mitochondrial membrane is pertinent to apoptotic processes involving positively charged cytochrome c, motivating a characterization of cardiolipin membranes. Cardiolipins are negatively charged lipids with four alkyl chains. Our approach is to analyse cardiolipin monolayers at the water-air interface, using isotherms and Brewster angle microscopy. The calculation of the in-plane electrostatic pressure consists of an electrostatic contribution using Grahame’s equation and a chemical part reflected by the law of mass action. A nonmonotonic ionic strength dependence with a maximum at 0.1 M (NaCl, KCl) is observed for the phase transition surface pressure. This finding is in accordance with the calculations predicting the dominance of charge screening by monovalent counterions only for concentrations above 0.1 M. For lower salt content, its increase causes an elevation of the degree of dissociation and thus electrostatic repulsion within the cardiolipin membrane. The results will be reported, showing pH, concentration, temperature influences on the surface potential, and thus the ability to bind cytochrome c.

15 min. break

Invited Talk

BP 38.6 Wed 16:45 C 130 Water flow along a solid interface affects the Stern layer — •MIASCHA BONN — Max Planck Institute for polymer research, Mainz, Germany

At the surface or interface of water, the water hydrogen-bonded network is abruptly interrupted, conferring properties on interfacial water different from bulk water. Owing to its importance for disciplines such as electrochemistry, atmospheric chemistry and membrane biophysics, the structure of interfacial water has received much attention.

We elucidate the structure and structural dynamics of interfacial water using ultrafast surface-specific sum-frequency generation (SFG) vibrational spectroscopy. We make use of the fact that the SFG signal depends critically on the interfacial organization of water molecules.

We attempt to bridge continuum models of laminar flow along interfaces, with molecular-level descriptions of the Stern and diffuse layer, which describe the near-surface distribution of ions. For water at two different mineral interfaces, we report a dramatic effect of water flow water along the mineral surface on the organization of water at the interface. Our observations can be explained by considering the coupling between the flow and the dissolution chemistry at the interface. Even for low-soluble quartz at neutral pH, dissolution plays a key role in determining the interfacial water organization through the charge on the surface.

BP 38.7 Wed 17:15 C 130 Breaking the Symmetry of Ions at the Air-Water Interface — •ENSA BRANDERS, PETER KARACHOGEV, PADMAPARISH, VISWANATHI, AND HUBERT MOTSCHMANN — 1Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany — 2Centre for Nano and Soft Matter Sciences, Jalahalli, Bangalore 560013, India

The air-water interface is a widely discussed system. Controversial opinions exist especially for the arrangement of dissolved ions close to the interface; while the classical picture predicts depletion, more recent investigations suggest a nonmonotonous concentration profile with an enrichment layer followed by a depletion layer. A sophisticated method to investigate the air-water interface is the IR-vis sum frequency generation (SFG) spectroscopy, because this method is intrinsically surface specific for soft media.

In this contribution we investigate the behavior of octahedral metal complex ions close to the air-water interface. No SFG signal is expected for octahedrons unless there is a reduction in symmetry. This distortion can only take place close to the interface because only there is a non-isotropic environment. We got SFG responses from the octahedrons, revealing that they are close to the interface. Furthermore we measured the surface excess via a surface tension isotherm, which turns out to be negative. The combined measurements suggest a non-monotonous concentration profile.

BP 38.8 Wed 17:30 C 130 Macro- and Microeology of Heterogeneous Microgel Packings — •FANY DI LORENZO, 1,2 STEPHAN SCHAAF, CHRISTIANE A. HELM — Freie Universität Berlin, Germany

Cardiolipins are negatively charged lipids with four alkyl chains. Our approach is to analyse cardiolipin monolayers at the water-air interface, using isotherms and Brewster angle microscopy. The calculation of the in-plane electrostatic pressure consists of an electrostatic contribution using Grahame’s equation and a chemical part reflected by the law of mass action. A nonmonotonic ionic strength dependence with a maximum at 0.1 M (NaCl, KCl) is observed for the phase transition surface pressure. This finding is in accordance with the calculations predicting the dominance of charge screening by monovalent counterions only for concentrations above 0.1 M. For lower salt content, its increase causes an elevation of the degree of dissociation and thus electrostatic repulsion within the cardiolipin membrane. The results will be reported, showing pH, concentration, temperature influences on the surface potential, and thus the ability to bind cytochrome c.

BP 38.9 Wed 17:45 C 130 Dielectric Response of the Water Hydration Layer and its Application on the Solvation Energy — •CHRISTIAN SCHAAF and STEPHAN GEKLE — University Bayreuth, Bayreuth, Germany

The electric field caused by a charged solute molecule introduced into a dipolar liquid solvent leads to a reorientation of the solvent molecules which is quantified by the solvent’s local dielectric constant.

We calculate this dielectric response function using two different methods: linear response for a system with the explicit solute and theoretical calculations using the wave-vector dependent, non-local bulk permittivity. The good agreement leads to our central result: while the water dielectric constant for a radial field in the hydration layer of spherical solutes is strongly different from bulk water, this difference is not due to significant restructuring of the hydrogen bond network, but can be traced back almost entirely to bulk properties of pure water.

Finally, integrating our dielectric profiles, we calculate the solvation energies for Na+, Cl−, I−, and Cs+ and find quantitative agreement with experimental data.


Topical Talk

BP 39.1 Wed 16:45 MA 001
The Industrial Society’s natural Sustainability — HANS G. DIELMEYER and THOMAS MARTINETZ — Institut für Neuro- und Bioinformatik, Uni Lübeck

Human nature and industrial engineering form a predictable macro-system with six S-functional variables and biologically stabilized parameters [1]. S-functions display storing lifetimes with time shifts like sinus functions with phase shifts. Since 18th century UK the real GDP per capita increased 100-fold; only a factor of 2.7 yields for the G7 the biologic limit of 118 years for the life expectancy.

This is orders of magnitude below all earlier predictions. The industrial society will be materially sustainable. But the present financial system is unsustainable because saturating growth and interest rates dry out saving, life insurances, and pension funds. This caused the Great Depression and the crash of 2008, not neoclassical excuses [2]. The only cure is bringing finance in line with human biology: return to the sustainable income distribution between World War II and 1980; increase retirement age; continue innovation; and decrease the G7 population globally. Believing in the Neoclassical Paradigm of exponential growth is already Chinas problem because it wastes resources with unsustainable investments.


BP 39.2 Wed 17:15 MA 001
The decoupling of CO2 emissions and human development — KAI KORNHUBER1, DOMINIK REUSKER1, LUISA COSTA1, JÜRGEN KROPP1–3, RVBSKI DIEGO1, and SCHELLHUBNER JOACHIM1–3
1Potsdam Institute for Climate Impact Research, Potsdam, Germany — 2University of Potsdam, Potsdam, Germany — 3Saná Fe Institute

Evidence of a decoupling between greenhouse gas emission and socioeconomic development would benefit international climate negotations in two ways. First, it would communicate to emerging countries that socioeconomic progress is not strictly connected with ever-growing emissions. Secondly, it informs developed economies on reduction targets that do not jeopardize progress. Using the Environmental Kuznets Curve as background and country-panel data between 1990 and 2013, a model was established to test postulated relationships between socioeconomic progress (measured using the Human Development Index (HDI)) and CO2 emissions from fossil fuels. An inverted U-curve with a time-dependent maximum moving towards higher HDI and lower per capita CO2 mission was established as the relationship delivering the lower fitting error. Extrapolating the global decoupling trend until 2050 returns global cumulative emissions of CO2 that are incompatible with meaningful with long-term climate protection targets. Individual countries presented remarkable differences in their decoupling dynamics. Further insights and implications of the analysis will be discussed, as well as future research needs.

BP 39.3 Wed 17:30 MA 001
The size distribution, scaling properties and spatial organization of urban clusters: a global and regional perspective — TILL FLUSCHNICK, STEFFEN KRIEWALD, ANSELMO GARCÍA CANTÚ ROS, BIN ZHOU, DOMINIK REUSKER, JÜRGEN PETER KROPP, and DIEGO RVBSKI — Potsdam Institute for Climate Impact Research (PIK)

Human development has far-reaching impacts on the surface of the globe. The transformation of natural land cover occurs in different forms and urban growth is one of the most eminent transformative processes. We analyze global land cover data and extract cities as defined by maximally connected urban clusters. The analysis of the city size distribution for all cities on the globe confirms Zipf’s law. Moreover, by investigating the percolation properties of the clustering of urban areas we assess the closeness to criticality. We study the Zipf-exponent and find a function of the closeness to percolation and find a systematic decrease with increasing scale, which could be the reason for deviating exponents reported in literature.

BP 39.4 Wed 17:45 MA 001
Limits and opportunities of a regionalized food production for cities: A global analysis — STEFFEN KRIEWALD, ANSELMO GARCÍA CANTÚ ROS, TILL STEEREL, PRALAD PRADHAN, and JÜRGEN P. KROPP — Potsdam Institute for Climate Impact Research, Potsdam, Germany

The massive ongoing urbanisation in the 21st century is a major challenge for societies and therefore crucial developments towards a sustainable future will take place in cities. Together with many other issues a proper food supply is essential. Today, the necessary transport of food, especially the increasing transport by plane due to the global food supply chain, leads to a significant amount of greenhouse gas emissions. A reorganisation of cities in terms of their food allocation could save a considerable amount of emissions. We provide a global overview of the potential of peri-urban agriculture based on land-use, population, yield and dietary datasets. Our analysis indicates that up to 2 billion city dwellers can be fed by local grown products. However, Climate Change will drastically decrease the possibility of a local food supply for many regions.

BP 39.5 Wed 18:00 MA 001
Food demand and supply under global change: need for sustainable agricultural intensification — PRALAD PRADHAN1, DOMINIK REUSKER1, MATTHIAS LÜDEKE1, and JÜRGEN KROPP1,2
1Potsdam Institute for Climate Impact Research, Potsdam, Germany — 2University of Potsdam, Dept. of Geo- and Environmental Sciences, Potsdam

Global food demand is expected to increase by 60–110% between 2005 and 2050. Meeting growing food demand along with reducing agricultural impacts is a global sustainability challenge. We investigated diet shifts, emissions, livestock feed, local food, and yield gaps to address this challenge. Globally, we identified sixteen dietary patterns. Diets common in developed world, exhibit higher emissions. Currently, 40% of global crops is fed to livestock. Two billions people are self-sufficient within 5’ grid, while 1 billion Asians and Africans require inter-continental trade. However, they can become self-sufficient by closing yield gaps. By 2050, the global agricultural emissions will approach 7–20 Gt CO2eq./yr and feed demand may increase up to 1.3 times. The number of trade dependent people will range 1.5–6 billion which may be further increased by 4–16% due to climate change. In future, diet shifts will significantly increase crop demand, emissions, and trade. These can be reduced by technological change, consuming local food, and closing yield gaps. Sustainability of inputs and management required to close yield gaps depends on how options are chosen and implemented. Hence, a combination of sustainable intensification, expansion, trade and diet shifts is required to feed growing population.

BP 39.6 Wed 18:15 MA 001
Sustainability for a Warming Planet — HUMBERTO LLAVADOR1, JOHN ROEMER1, and JOAQUIM SILVESTRE2
1Universitat Pompeu Fabra (Barcelona) — 2Barcelona GSE — 3Yale University — 4University of California, Davis

A clean biosphere is a resource in jeopardy due to man-made GHG emissions. What is the fair way to share this scarce global resource across present and future generations, and across regions of the world? This study proposes that the guiding ethics should be sustainability and egalitarianism. Sustainability is interpreted as a pattern of economic activity over time that sustains a given rate of growth of human welfare indefinitely; in doing so, the atmospheric concentration of carbon must be capped at some level not much higher than exists today. Human welfare depends not only upon consumption, but also upon education, knowledge, and a clean biosphere. The analysis shows that we should be investing more in education and substantially more in knowledge creation than is currently the case.

International cooperation is vital in capping global greenhouse gas emissions at a sufficiently low level. We propose that solving the barrier problem emerging from the decoupling of income and welfare, termed ‘sustainable development’, will be an essential ingredient for bridging the gap between the current human welfare and the biologic biologic limit of 118 years for the life expectancy.
not be altered by the agreement. This principle, along with sustain-
ability, suffices to determine how emissions should be allocated across
regions and time.

BP 40: BP Mitgliederversammlung (Annual General Meeting of the Biological Physics
Division)

Time: Wednesday 19:00–20:00

Discussion

Invited Talk

BP 41.1 Thu 9:30 H 1058
Probing the downhill folding kinetics of Lambda repressor
variants with optical tweezers — ANN MUKHORTOVA, ANDREAS
HARTMANN, and •MICHAEL SCHLIERF — B CUBE - Center for Molecu-
lar Bioengineering, TU Dresden, Dresden, Germany

Protein folding is a process of molecular self-assembly during which a
disordered polypeptide chain collapses to form a compact and well-
defined three-dimensional structure. The process of folding is described
as a path on a multi-dimensional energy landscape.

Here, we present a comparative study of single-molecule protein fold-
ing using optical tweezers that provide the possibility to measure struc-
tural dynamics with sub-millisecond and nanometer resolution. We
characterize the folding dynamics of three different lambda repressor
variants: a two-state folder LambdaWT (Y22W) and two downhill
folding variants, LambdaYA (Y22W/Q35Y/G46,48A) and LambdaHA
(Y22W/Q33H/G46,48A). We show that force perturbation of the en-
ergy landscape slowed down the ultrafast kinetics of downhill folders,
making them accessible to single-molecule studies. Interestingly, the
downhill variants of lambda repressor appeared as two-state folders
under load with significantly different folding kinetics and force de-
pendence. A comparison between these variants allowed us to extract
fine details of their underlying energy landscape.

BP 41.2 Thu 10:00 H 1058
Insulin at the air-water interface: Monomers or dimers? —
•SERGIO MAURIL,1,2, TOBIAS WEIDNER,2, and HEIKE ARNOLD3 —
1Surface Science Research Centre, University of Liverpool, UK —
2Max Planck institute for polymer research, Mainz, Germany

The adsorption of insulin at surfaces is a ubiquitous problem of inter-
est in various fields of biotechnology and pharmaceutical applications.

Studying protein structure at surfaces is generally though a challeng-
ing task: Conventional techniques like IR and Raman spectroscopy,
can achieve surface sensitivity, but different states (aggregates) of the
same protein have often similar spectral signatures. Here we combine
sum frequency spectroscopy (SFG) spectroscopy with spectra calcu-
lations to identify specific oligomeric species of insulin at interfaces.

In particular we study the air/water interface due to its relevance in
the production, storage and delivery of insulin-based medications.
In-
sulin is present in Nature mainly as hexamers, dimers and monomers.

While the first two are stable, monomers do denature and aggregate
under certain conditions. Eventually, monomers further aggregate in
amyloid-like structures, which are undesired. We find that only insulin
monomers segregate at the air/water interface. This advance helps to
solve the long standing puzzle of insulin fibril formation. The versat-
ility of the proposed experimental approach could be used to investigate
a large variety of proteins and surfaces.

- Mauri et al., PCCP, 2014, 16, 26722-26724

BP 41.3 Thu 10:15 H 1058
Structural changes of proteins at interfaces — •LARS SCHÜSSEL,1, NADJA HELLMANN,2, MISCHA BONN,2, and TOBIAS
WEIDNER1 — Max Planck Institute for Polymer Research, Ackern-
mannweg 10, 55128 Mainz, Germany — 1Institute for Molecular Bio-
physics, Jakob Wedler Weg 26, 55128 Mainz, Germany

Information about the 3D structure of proteins at interfaces is essen-
tial for understanding of interfacial biological mechanisms. Structural
insight can aid the design of tailored proteins with specific functions,
structures or binding sites. However, static snapshots of protein struc-
ture are insufficient to understand many protein functions, which arise
from protein dynamics: Protein folding, refolding and motion. A
well-established tool to study static protein structures is X-ray crystal-
lography. But with this method it is still challenging to follow protein
conformational change, folding or refolding in real time. We use vibra-
tional sum frequency generation spectroscopy (SFG) to follow confor-
national changes of proteins at interfaces. The aim is to combine time
resolved SFG with molecular dynamics simulations to glean informa-
tion about protein dynamics and intermediate structures at interfaces
during folding. For a pump-SFG probe detection scheme, an optical
trigger for conformational change is a core requirement. We will
discuss the design, preparation and characterization of model protein
films with optical triggers.

BP 41.4 Thu 10:30 H 1058
The initial adsorption stages of fibrinogen at mica and
graphite — •STEPHAN KÖHLER1,2 and GIOVANNI SETTANN1,3
1Johannes Gutenberg-Universität Mainz, Institut für Physik,
Staudinger Weg 7, D-55128 Mainz — 2Graduate School Materials
Science in Mainz, Staudinger Weg 9, D-55128 Mainz — 3Max Planck
Graduate Center mit der Johannes Gutenberg-Universität Mainz,
Staudinger Weg 9, D-55128 Mainz

Fibrinogen is a large glycoprotein in the blood of vertebrates. It is
an essential factor in blood clotting where it forms fibrin after being
activated by thrombin. Furthermore, adsorbed fibrinogen is known to
be an important factor for the biocompatibility of materials. The pro-
tein contains binding sites for leukocytes and platelets. Consequently,
adsorbed fibrinogen has been implicated as a cause for thrombosis and
inflammation at implants. The molecular underpinnings of this have
been investigated in many experimental studies. These studies often
use model surfaces like mica and graphite to investigate the structure
of adsorbed fibrinogen.

Here we present the first fully atomistic simulations of the initial
adsorption stages of a fibrinogen protomer at such model surfaces.

The simulations reveal a weak adsorption at mica that allows frequent
desorption and reorientation events. This adsorption is driven by elec-
trostatic interactions between the protein and the silicate surface as
well as the counter ion layer. Preferred adsorption orientations for the
globalar regions are identified. As a contrast to mica, adsorption at
graphite is more permanent and the onset of denaturation is observed.

BP 41.5 Thu 10:45 H 1058
Biomolecules at gold-water interfaces: the role of the metal
polarization — •ISIDRO LORENZO1,2, HADI RAMEZANI-DAKHEL1,2,
HENDRIK HEINZ2, and MARIALOPE SULFIJIK2,3 — 1Johannes Gutenberg
University Mainz, Staudinger Weg 7 55099 Mainz — 2Department of
Polymer Engineering, University of Akron, Ohio 44325

Microscopic understanding and control of protein-surface interactions
is gaining an increasing interest due to the new development of bio-
interfaces for medical and bio-technological applications. In this con-
tribution we aim to provide a characterization of different peptides /
gold interactions at a molecular level in order to explain and inter-
pret recent surface experimental results [1]. We have devised a novel
scheme to include the metal polarization (image charge effect) induced
by the adsorbed molecules into atomistic simulations. Our scheme
can easily complement currently used 12-6 Lennard-Jones potentials
[2], as included in simulation packages as GROMACS and LAMMPS.
Extensive tests have been performed for the force field validation and
comparisons with quantum mechanics (QM) density functional the-
ory (DFT) calculations are also discussed. Results for aminoacids and


30 min break

BP 41.6 Thu 11:30 H 1058
Self-assembled protein nanofibres as novel biomaterials — Christian Helbing1, Gang Wei2, Tanja Deckert-Gaudig1, and Klaus D. Jandt1 — Chair of Materials Science (CMS), Otto-Schott-Institute of Materials Research (OSIM), Friedrich Schiller University Jena, Jena, Germany — 1Hybrid Materials Interfaces Group, University of Bremen, Bremen, Germany — 2Institute for Photonic Technology, Jena, Germany

Protein nanofibers (PNF) are promising materials for numerous applications in the field of biotechnological engineering. Especially, self-assembled PNFs based on plasma proteins have a high importance due their easy fabrication and high biocompatibility. However, knowledge about the self-assembly mechanism and the properties of such PNFs is limited. The aim of the current study is to deepen the understanding of the formation mechanism. We tested the hypotheses that properties, morphology, and inner structure of PNF depends on environmental conditions. In this work, we present first results of self-assembled PNF structures formed in solution from different plasma proteins and plasma protein combinations. The observed morphology and mechanical properties of the formed PNFs depended strongly on the formation conditions. The structural analysis suggest that a partial denaturation, i.e., a change in the secondary structure, of the plasma proteins is a necessary requirement for the formation of PNFs. The comparison of the secondary structure of the PNFs and the native proteins helps to improve the understanding of the self-assembly mechanism. The current results leads to a better control during the PNF formation.

BP 41.7 Thu 11:45 H 1058
Ultrafast Infrared Spectroscopy Reveals Water-mediated Coherent Dynamics in an Enzyme Active Site — Katrin Adamczyk1, Niall Simpson2, Gregory M. GheeTham2, Andrea Guimond2, Martin A. Walsh2, Michael Towner2, Anthony W. Parker2, and Neil T. Hunt3 — 1University of Strathclyde, Glasgow, UK — 2Central Laser Facility, Rutherford Appleton Laboratory, Didcot, UK — 3Diamond Light Source, Didcot, UK

Understanding the impact of fast dynamics upon chemical processes occurring within the active sites of proteins and enzymes is a key challenge that continues to attract interest. Similar gaps in our knowledge exist in understanding the role played by water, either as a solvent or as a structural/dynamic component of the active site. In order to investigate further the potential biological roles of water, ultrafast infrared spectroscopy is employed that directly probe the vibrational dynamics of NO bound to the ferric haem of the catalase enzyme from Corynebacterium glutamicum in both H2O and D2O. An isotope decomposition with the protein number. This feature could be beneficial to organelle maintenance in ageing bacteria.

BP 41.10 Thu 12:30 H 1058
Refractive index regulation of the vertebrate retina — Alfonso Garcia-Ulloa, Heike Petzold, Alexandr Dibrov, Kaushikaram Subramanian, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Due to its similarity, the vertebrate retina serves as a model system for the brain, and it yet is different. Whereas brain tissue is opaque on sub-millimeter scale, the retina is of high optical quality and manages to suppress the backscattering of photons on their way to the sensitive photoreceptors.

Although the molecular basis of the retina’s optical quality is largely unknown so far, physical optics clearly states that the magnitude of scattering at given particle sizes mostly depends on the refractive index contrast. Also, based microscopy technique yields small signals when applied to retinal tissues. These observations raise the question of what regulates the retinal refractive index distribution.

We hypothesize that proteins with housekeeping functions, highly soluble and with high weight-specific refractive indices fulfill the role of refractive index regulators in the retina. In mouse models, the expression of crystallins has been localized in regions of high refractive index contrast like the nuclei, in the inner nuclear layer and in between nuclei, in the outer nuclear layer.

Our study establishes the role of refractive index regulators in specific retinal layers by combining fluorescent localization, quantitative phase-contrast microscopy and quantitative mass spectrometry.

BP 41.11 Thu 12:45 H 1058
Hierarchical nanoscale dynamics of proteins in solution — Marco Grimaldo1, Felix Roosen-Runge1, Fajun Zhang2, Frank Schreiber3, and Tilo Seydel1 — 1Institut Laue-Langevin, Grenoble, France — 2Institut für Angewandte Physik - Universität Tübingen, Tübingen, Deutschland

The dynamics of proteins in solution is essential for both protein function and cellular processes. The hierarchical protein dynamics, from the global center-of-mass diffusion to the motions of side-chains and chemical groups renders a complete understanding challenging. Profiting from the very high flux of the new backscattering spectrometer IN16, the translational and rotational diffusion of the proteins can be self-consistently separated from the internal molecular motions. The global protein diffusion on the nanosecond time scale is consistent with predictions for colloidal suspensions of effective hard spheres even when the molecular structure differs considerably from a sphere [1]. The internal motions on nanometer length scales are characterized both geometrically and dynamically, suggesting a picture of methyl rotations and restricted diffusion of side chains. We also systematically explore the temperature-dependence of both the global and internal diffusive motions in protein solutions, including unfolding and aggregation at temperatures beyond the thermal denaturation [2].

Invited Talk

**BP 42.1 Thu 9:30 H 1028**

**Microtubules adapt to mechanical stress through spontaneous intra-lattice repair** — *Laure Schneider*, *John John*, *Jeremie Gaillard*, *Maxence Nachury*, *Laur- rent Blanchoin*, and *Manuel Thery*

Microtubules within the microtubule overlaps. Microtubule arrays define the shape of axons, flagella, and provide tracks for intracellular transport. Although microtubules assembled in vitro are stiffer than other cytoskeletal polymers by several orders of magnitude, intracellular forces lead to the formation of highly bent microtubules. It is currently not known how microtubules tolerate the vast forces exerted on them. It is likely that physical constraints affect microtubule structure and stiffness. Using a newly developed microfluidic device, we find that microtubule stiffness decreases incrementally with each cycle of bending and release. Similar to other cases of material fatigue, rather than a homogenous distribution of stress, the concentration of mechanical stresses turns pre-existing defects in the microtubule lattice into larger damages. Strikingly, damaged microtubules are able to recover their initial stiffness by spontaneously incorporating tubulin into their lattice. These findings demonstrate that microtubules are ductile materials with self-healing properties. Microtubule dynamics is thus not exclusive to the ends and intra-lattice incorporation of tubulin enables spontaneous adaptation to mechanical stresses.

**BP 42.2 Thu 10:00 H 1028**

**Molecular wear of microtubules propelled by surface-adhered kinesins** — *Emmanuel Lp Dumont*, *Catherine Do*, and *Henry Hess*

Wear, the progressive loss of material from a body caused by contact and relative movement, is a major concern not only in engineering but also in biology. Advances in nanotechnology both enable the study of the origins of wear processes at the atomic and molecular scale and demand the prediction and control of wear in nanoscale systems. Here we discuss wear that occurs in an in vitro system consisting of microtubules gliding across a surface coated with kinesin-1 motor proteins, and that energetic considerations suggest a molecule-by-molecule removal of tubulin proteins. The rates of removal show a complex dependence on sliding velocity and kinesin density, which - in contrast to the friction behavior between microtubules and kinesin - cannot be explained by simple chemical reaction kinetics.

**BP 42.3 Thu 10:15 H 1028**

**Diffusible crosslinkers generate directed forces in microtubule networks** — *Zdenek Lanský*, *Marcus Braun*, *AnneMarie Lédecker*, *Michael Schlierf*, *Pieter ten Wode*, *Marcel Janets*, and *Stefan Diez*

Remodeling of cytoskeletal filament networks is essential to cell division and morphogenesis. The mechanical forces driving the restructuring are attributed to the action of molecular motors and filament dynamics, which both consume chemical energy. By contrast, non-enzymatic filament antagonists are regarded as mere friction-generating entities. Here, we experimentally demonstrate that non-enzymatic, diffusible microtubule crosslinkers of the Ase1/PRC1/Map65 family generate directed microtubule sliding when confined between partially-overlapping microtubules. The Ase1-generated forces, directly measured by optical tweezers to be in the piconewton-range, were sufficient to antagonize motor-protein driven microtubule sliding. Force generation can be quantitatively explained by the entropic expansion of confined Ase1 molecules diffusing within the microtubule overlaps. The thermal motion of confined crosslinkers is thus harnessed to generate mechanical work analogous to compressed gas propelling a piston in a cylinder. As confinement of diffusible crosslinkers is ubiquitous in cells, the associated entropic forces are likely to be of importance for cellular mechanics beyond cytoskeletal networks.

**BP 42.4 Thu 10:30 H 1028**

**The Dynamics of cross-linked Microtubules in Neurons** — *Maximilian Jäger*, *University of Cambridge — Universität zu Köln*

Microtubule bundles play a central role in the initiation and growth of cellular processes such as neuronal axons and dendrites. However, a quantitative understanding of the involved mechanisms is still lacking. Here, we developed computer simulations that mimic the 1D dynamics of microtubule bundles, cross-linked by ensembles of molecular motors, to investigate the mechanics of growth. We demonstrated that unipolar motors (such as cytoplasmic dynein and most kinesins) are much more effective in initiating axon growth than bipolar motors (such as kinesin 5). The latter, however, are in turn more efficient in filament sorting. We furthermore investigated axon growth dynamics as a function of the restoring forces acting on MT bundles. Our calculations demonstrated that the maximum force such bundles may exert increases monotonically with the elastic rigidity of the opposing membrane, and that it is insensitive to the polarity of filaments in the bundle. Finally, we found that the motor density must exceed a percolation threshold, which depends on the number of filaments in the bundle, before any force can be exerted. Future experiments and considerations might reveal an important contribution of microtubule-generated forces to neuronal symmetry breaking.

**BP 42.5 Thu 10:45 H 1028**

**Cross-linking proteins facilitate formation of microtubule bundles** — *Marcel Prelogovic*, *Lora Winters*, *Iva Tolj*, and *Nesrin Pavin*

During mitosis, microtubules (MTs) form a spindle which is responsible for proper segregation of chromosomes. In the fission yeast Schizosaccharomyces Pombe, the spindle is a bundle of MTs emanating from two spindle pole bodies and held together by cross-linking proteins. Our goal is to understand the dynamic properties of MTs interacting with cross-linking proteins and the role of cross-linking proteins in the formation of MT bundles. We introduce a theoretical model of MT bundling which describes angular movement of MTs around the spindle pole body driven by thermal forces and forces exerted by cross-linking proteins, described as elastic springs. If the number of cross-linking proteins connecting the MTs is above a critical number, attractive forces exerted by cross-linking proteins dominate over thermal forces at very small angles between MTs, causing MT-s to bundle. We identify stable bundles formed in the cases where MTs are more likely to be bundled than not. Theory yields bundling probability as a function of length and cross-linking protein concentration and predicts parameters for which stable bundles form. In conclusion, these results provide an explanation for how the angular brownian motion and cross-linking proteins affect the formation of stable MT bundles.

**BP 42.6 Thu 11:00 H 1028**

**Quantifying protein diffusion and capture on filaments** — *Emmanuel Reichmann*, *Louis Reese*, and *Erwin Frey*

The functional relevance of regulating proteins is often restricted to specific binding sites such as the ends of microtubules or actin filaments. A localization of proteins on these functional sites is of great importance. In this respect, recent experimental studies suggested that several key players involved in regulation of microtubules and actin filaments utilize a one-dimensional diffusive motion on the respective filament to target the functional end. We present a quantitative theory for a diffusion and capture process, where proteins diffuse on a filament and stop diffusion when reaching the filament’s end. It is found that end-association after one-dimensional diffusion is highly efficient as compared to direct binding from solution/cytosplasm. As a consequence, diffusion and capture substantially enhances the reaction velocity of enzymatic reactions, where proteins and filament ends are to each other as enzyme and substrate. We show that the reaction ve
Cellular chirality arising from the self-organization of the actin cytoskeleton – ALEXANDER BERSHADSKY – Department of Molecular Cell Biology, Weizmann Institute of Science, Rehovot 76100, Israel — Mechanobiology Institute, National University of Singapore, Singapore 117411, Singapore

Cellular mechanisms underlying the development of left-right asymmetry in tissues and embryos remain obscure. Here, the development of a chiral pattern of actomyosin was revealed by studying actin cytoskeleton self-organization in cells with isotropic circular shape. A radially symmetrical system of actin bundles consisting of α-actinin-enriched radial fibers (RFs) and myosin-IIA-enriched transverse fibers (TFs) evolved spontaneously into the chiral system as a result of the unidirectional tilting of all RFs, which was accompanied by a tangential shift in the retrograde movement of TFs. We showed that myosin IIA-dependent contractile stresses within TFs drive their movement along RFs, which grow centripetally in a formin-dependent fashion. The handedness of the chiral pattern was shown to be regulated by α-actinin-1. Computational modeling demonstrated that the dynamics of radial-transverse fiber system can explain the pattern transition from radial to chiral. Thus, actin cytoskeleton self-organization provides built-in machinery that potentially allows cells to develop left-right asymmetry.

Invited Talk

BP 42.7 Thu 11:30 H 1028

Organisation dynamics of stress fibers in adult stem cells –

CARINA WOLLNIK1, BENJAMIN ELZTNER2, STEPHAN HUCKEMANN3, and FLORIAN REHFELDT1 – 1Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — 2Institute for Mathematical Stochastics, Georg-August-University, Göttingen, Germany — 3Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

Adult human mesenchymal stem cells (hMSCs) differentiate into various cell types. Here substrate stiffness is sufficient to guide hMSCs towards different lineages without additional biochemical stimuli [1]. Stress fibres (SFs) composed of actin filaments, cross-linkers and myosin motor-proteins generate and transmit tension throughout the cell. Myosin inhibition stops the differentiation [1], implying importance of SF tension for this process. Characteristic SF patterns can be detected within 24 hours and used as an early morphological marker [2]. We use 24h long-term live-cell imaging of RFP-Lifeact transfected hMSCs on substrates of different stiffness, recording many cells in parallel for better statistics in comparable conditions. SFs are traced with a sophisticated filament tracking program [3] and a tool to extract filament modes [4], to gain a deeper understanding of SF formation dynamics in early stem cell differentiation. This leads to a non-monotonic dependence of SF polarization on the Young’s modulus of the underlying substrate [2].


BP 42.8 Thu 12:00 H 1028

Spontaneous polarization in an interfacial growth model for actin filament networks with a rigorous mechanochemical coupling – KARIN JOHN1, DENIS CAILLERIE2, THOMAS STÖPPELER3, and CHAOUGI MISBAH1 – 1Université Grenoble Alpes/ CNRS, LIPHY, F-38000 Grenoble, France — 2Université Grenoble Alpes/CNRS, 3SR, F-38000 Grenoble, France — 3Otto-von-Guericke Universität Magdeburg

Many processes in eukaryotic cells, including cell motility, rely on the growth of branched actin networks from surfaces. Despite its central role the mechanochemical coupling mechanisms that guide the growth process are poorly understood, and a general continuum description combining growth and mechanics is lacking. We develop a theory that bridges the gap between mesoscale and continuum limit and propose a general framework providing the evolution law of actin networks growing under stress. This formulation opens an area for the systematic study of actin dynamics in arbitrary geometries. Our framework predicts morphological instability of actin growth on a rigid sphere, leading to a spontaneous polarization of the network with a mode selection corresponding to a comet, as reported experimentally. We show that the mechanics of the contact between the network and the surface plays a crucial role, in that it determines directly the existence of the instability. We extract scaling laws relating growth dynamics and network properties offering basic perspectives for new experiments on growing actin networks.

BP 42.9 Thu 12:15 H 1028

Contractile actin bundles without molecular motors – JÖRG SCHNAUS1, TOM GOLDES2, CARSTEN SCHULZE2, SEBASTIAN SCHMIDT2, MARTIN GLASER1, DAN STREHLE1, JOSÉF KAS1, and CLAUS HÜBINGER2 – 1Institute for Experimental Physics I, University of Leipzig , Linnéstraße 5, 04103 Leipzig , Germany — 2Institute for Theoretical Physics, Georg-August-University of Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen, Germany

Since the 1940, interactions of actin and its molecular motor myosin are known as the fundamental process for biological force generation. These interactions convert chemical energy into mechanical work by ATP hydrolysis. The dogma of molecular motors being the basis of all contractile forces has never been disproven. In this study we show an alternative force generation mechanism in the absence of molecular motors. The system is not driven by ATP hydrolysis and solely relies on minimization of free energy based on filament-filament interactions induced by a crowded environment. Dynamics of these contractions behave differently to a single filament pair shown in theoretical and experimental studies. We are able to show that the behavior of contractile actin bundles can be well described as an emergent phenomenon of multiple filament pairs. This finding demonstrates that the mechanics of the contact between the network and the surrounding matter play a crucial role, in that it determines directly the existence of macro-molecular content of cells and crowding effects have to be considered in cellular systems. We measured contraction velocities ranging from 0.10 to 0.65 µm/s and evaluated a force regime of 0.5 to 3.0 pN. Dynamics and forces of this non-dissipative process correspond to an active behavior of single myosin motors.

BP 42.10 Thu 12:30 H 1028

Elasticity of 3D networks with rigid filaments and compliant crosslinks – KURT M. HEIDEMANN1, ABHINAV SHARMA2, FLORIAN REHFELDT3, CHRISTOPH P. SCHMIDT2, and MAX WARDETZKY1 – 1Institut für Numerische und Angewandte Mathematik, Georg-August-Universität, Göttingen – 2Drittes Physikalisches Institut – Biophysik, Georg-August-Universität, Göttingen

Disordered filamentous networks with compliant crosslinks exhibit a low linear elastic shear modulus at small strains, but stiffen dramatically at high strains. Experiments have shown that the elastic modulus can increase by up to three orders of magnitude while the networks withstand relatively large stresses without rupturing. Here, we perform an analytical and numerical study on model networks in three dimensions. Our model consists of a collection of randomly oriented rigid filaments connected by flexible crosslinks that are modeled as wormlike chains. Under the assumption of affine deformations in the limit of infinite crosslink density, we show analytically that the nonlinear elastic regime in 1- and 2-dimensional networks is characterized by power-law scaling of the elastic modulus with the stress. In contrast, 3-dimensional networks show an exponential dependence of the modulus on stress. Independent of dimensionality, if the crosslink density is finite, we show that the only persistent scaling exponent is that of the single wormlike chain. Consequently, unlike non-entangled networks, the model system studied here cannot provide an explanation for the experimentally observed linear scaling of the modulus with the stress in filamentous networks.
Sensitivity against author name disambiguation of a motif-based success score in coauthorship networks — David F. Klosik, Stefan Bornholdt, and Marc-Thorsten Hütt — Institut für Theoretische Physik, Universität Bremen — School of Engineering and Science, Jacobs University Bremen

Motivated by the question whether large-scale citation datasets allow for a quantitative assessment of social influences in form of coauthorship of publications we investigate a success score [L. Krumov, C. Fretter, M. Müller-Hannemann, K. Weiße, and M.-T. Hütt, EPJ B (84), 535 (2011)] for small collaboration patterns in coauthorship networks. We find that when applied to a network compiled from aggregated citation data provided by the American Physical Society this score which is based on the scale of small induced subgraphs (as known from motif-analysis) is highly sensitive to details of the network construction from the data; especially to the inevitable disambiguation of author names (i.e., the scheme applied to group instances of author names into a vertex). We argue that these findings might not be exclusive to coauthorship networks since similar ambiguities are present in the network representations of other data [D.F. Klosik, S. Bornholdt, M.-T. Hütt, Phys. Rev. E 90, 032811 (2014)].

Restricting the h-index to a citation time window: A case study of a timed Hirsch index — Michael Schreiber — Institute für Physik, TU Chemnitz

The h-index has been shown to increase in many cases mostly because of citations to rather old publications. This inertia can be circumvented by restricting the evaluation to a citation time window. Here I report results of an empirical study analyzing the evolution of the thus defined timed h-index in dependence on the length of the citation time window.

An Interacting Network Perspective on Global Trade — Julian Mal lucr and Reik V. Donner — Potsdam Institute for Climate Impact Research, Germany

In the last years the International Trade Network (ITN) has caught rising attention among the scientific community. By decomposing countries into national industry sectors, data provided by multi-regional input-output tables allow for a more detailed investigation into the substructure of the ITN. We introduce an interacting network approach to quantify trends and extreme events in global trade patterns between 1990 and 2011. Different definitions of subgraphs exhibit different characteristic topological features of the ITN. This study compares and evaluates partitions that are defined by industry sector and by country, respectively. We assess how meaningful the notion of national economies in present-day globalized economy still is and show that the approach of interacting networks provides suitable methods to perceive important patterns in global trade.

Invited Talk

Molecular Systems Engineering with DNA: Four pieces, one rule, and many possibilities. — Hendrik Dietz — Technische Universität München, Munich, Germany

It is notoriously difficult to observe, let alone control, the position and orientation of molecules because of their small size and the constant thermal fluctuations that they experience in solution. Molecular self-assembly with DNA provides a route for placing molecules and constraining their fluctuations in user-defined ways, thereby opening attractive and unprecedented avenues for scientific and technological exploration. In my talk I will introduce some of the key concepts and methods, and highlight a number of recent applications.

Mechanisms of backtrack recovery by RNA polymerases I and II — Ana Lisica, Marcus Jaini, Christoph Engler, Edgar Rodlan, Patrick Cramer, and Stephan Gulli — Biotec, Dresden, Germany — MPI CBG, Dresden, Germany — MPI PBC, Göttingen, Germany — MPI PKS, Dresden, Germany — GSB, Madrid, Spain

RNA polymerases (Pol) backtrack frequently during transcription elongation. To recover from the backtrack state, Pol I uses a strong transcription cleavage activity, while that of Pol II is weak but can be enhanced by transcription factor TFIIS. However, backtrack recovery can also proceed by 1D diffusion, and the mechanisms that underlie the choice of backtrack recovery pathway have not been investigated. Here, we use dual-trap optical tweezers to compare Pol I and Pol II transcription and backtrack dynamics. We find that Pol I is faster than Pol II, pauses less often, and can transcribe against higher opposing forces. Neither enzyme can recover alone from backtracks beyond a threshold depth, and only Pol II with TFIIS can rapidly recover from deep backtracks. Comparing recovery times from varying backtrack depths with expectations from the theory shows that the choice of backtrack recovery pathway is determined by a kinetic competition between 1D diffusion and transcript cleavage. In Pol I, this balance is influenced by the TFIIS-homologous subunit A12.2, which both decreases the rate of 1D diffusion and increases the rate of cleavage. Our data identifies the distinct backtrack recovery behaviours of Pol I and Pol II that evolved to serve specific cellular roles of these enzymes.

BP 44: DNA/RNA and related enzymes

Location: H 1058

DNA/RNA and related enzymes

Past Chromatin Assembly facilitated by Nucleosome Breathing and Replication-Guided Packing — Johannes Nuebler, Brendan O’Regan, Philippe Korchin, and Ulrich Gerland — Theory of Complex Biosystems, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — Adolf-Butenandt-Institut, University of Munich, Schillerstrasse 44, 80336 Munich, Germany

The condensation of eukaryotic DNA into chromatin entails the formation of dense nucleosome arrays. These arrays are frequently destroyed...
by transcription and replication, such that reassembly is required. Due to a jamming effect in the random adsorption of mutually exclusive objects (the ‘car parking problem’), the question was raised how in vivo nucleosome densities, and patterns, can be reached in the biological relevant timescale of minutes [1]. We show that the ‘softness’ of nucleosomes alleviates this kinetic challenge [2]. Nucleosome softness arises due to transient DNA unwrapping (breathing) and stepwise nucleosome assembly. From a physics perspective, the ‘soft car parking problem’ differs fundamentally from its hard counterpart by exhibiting non-monotonic density and rapid equilibration. We also discuss scenarios how the progression of the replication fork can promote rapid reassembly in its wake. For example, tight packing arises naturally if the fork progresses slowly compared to the reassembly rate.


Gene regulation on the RNA level. The B12 dependent btuB riboswitch studied with single molecule FRET. — RICHARD BÖHNER, MICHELLE SCHAEFFER, SOPHIA GALLO, AND ROLAND K.O. SIGEL — Department of Chemistry, University Zurich, Switzerland

The btuB riboswitch is one of the promising candidates for understanding the gene regulation at the RNA level (1). This B12 specific RNA is encoded in the 5’-untranslated region (UTR) of the btuB gene encoding a coenzyme B12 (AdoCbl) transporter found among other bacteria, especially in E. coli. Upon binding of B12, a conformational switch of the btuB aptamer occurs, thus inhibiting the expression of the cellular B12 transporter. Although studied intensively on a bulk level (2), the kinetics and in particular the exact structural information of this riboswitch is still missing, as neither a crystal nor a NMR structure exists.

Herein, we use Förster resonance energy transfer on a single molecule level (smFRET) as a versatile tool to characterize the conformational states and the folding kinetics of the aptamer region of the btuB riboswitch. Thereby, we will especially focus on the influence of AdoCbl and the function of Mg²⁺ for folding and switching. As FRET is known to be used as molecular ruler, we are aiming at absolute rather than apparent distance measurements (3). Thus, a study of the global structure of the btuB riboswitch will complement our experiments.


For simplicity, cartoons often depict DNA replication on a straight 1D line. In fact, we deal with a polymer that is packed and modified on different levels yielding higher order structures of organisation. Processing a DNA piece (as for example during DNA synthesis in clusters of replication factories) requires proper coordination amongst all individual machines (replicons) on it. However, it remains unknown how such replicons are organised at each replication factory.

We apply a 2 bead on a string model for two neighbouring replicons. We calculate analytically the probability for replicons to meet using Boltzmann statistics and then fit this with experimental data of replicon association in yeast to determine binding energies. This suffices to link our model to the dynamics of replicon activation and movement along DNA during the synthesis phase, to extrapolate from 2 neighbour interactions to the whole yeast-genome, and to describe properties of measured experimental distributions of fork numbers per cluster. Our model yields a near perfect match with the data suggesting that actively replicating units of DNA randomly associate with each other to form replication factories rather than being controlled by the cell.

Vibrational dynamics and hydration of the DNA backbone — BISWAJIT GUCHARIT, YINGLIANG LIU, RENE COSTARD, TORSTEN SIEBERT, AND THOMAS ELSAESSER — Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born-Str. 2a, 12489 Berlin, Germany

The DNA double helix and its aqueous environment display structural dynamics on the ultrafast time-scale of molecular motions. Two-dimensional (2D) infrared spectroscopy is employed in a frequency range from 950 to 1300 cm⁻¹ to map and discern the vibrational excitations of the fully hydrated DNA backbone, their couplings and the interactions with the surrounding water shell. The mutual couplings and corresponding delocalized nature of vibrational modes of the phosphate group, phosphodiester linkage and furanose ring structure within the backbone are evident from the rich cross peak pattern observed in the 2D spectra. The couplings further facilitate a picosecond transfer of vibrational energy from the phosphate to the sugar linkage and ring modes. The phosphate modes further play a key role for the interaction with the surrounding water shell, where structural fluctuations of interfacial water are limited and slowed down compared to bulk H₂O. This behavior is attributed to steric hindrance and the action of strong electric fields at the interface.

Continuous, sequence dependent gelation of nucleic acids driven by a thermal gradient. — CHRISTOP MAST, MATTHIAS MORASCH, AND DIETER BRAUN — Systems Biophysics, Faculty of Physics, LMU Munich, Amalienstrasse 54, 80799 Munich

Under equilibrium conditions, the phase transition of bio-polymers like DNA toward a compacted state requires mutual binding forces from high polymer concentrations or multivalent ions. We demonstrate that the physical non-equilibrium of a thermal gradient across an elongated chamber accomplishes this task from dilute DNA solutions without the help of multivalent ions, proteins, evaporation or encapsulation. The gelation process is governed by the base pair interactions between respective DNA strands, leading to a highly nonlinear sequence dependency of the gelation process. DNA of different sequences are compacted at distinct sites, yielding a sequence-based physical sorting mechanism. DNA strands with low hybridization energies do not form a gel within the measurement time. The DNA gel is continuously rebuilt inside the thermal gradient in a dynamic turn-over fashion and remains stable for days under dilute equilibrium conditions. The process implements a basic prebiotic machine that selects and stores sticky sequence motifs out of a random sequence pool.
We are able to directly visualise mutants via fluorescent proteins. Mutants gaining the ability to modify their pili by glycosylation and mutants no longer producing pili, were seen to spread more easily within the population. We attribute this effect to decreased cell-to-cell interaction by either changing the pilus or lacking it.

We conclude that fine-tuning of physical interactions can lead to segregation into sub-populations, thus maintaining the heterogeneity and co-existence of multiple phenotypes.

Centrosomes are membrane-less organelles, which are important for cell division. A centrosome consist of liquid-like pericentriolar material that accumulates around a centriole pair. We describe the centrosome as an active droplet, where the pericentriolar material is created from soluble building blocks by chemical reactions that are catalyzed both inside the droplet and at the centrioles [D. Zwicker, M. Decker, S. Jaensch, A. A. Hyman, F. Jülicher, PNAS 111 E2636-45 (2014)]. This model accounts for the observed nucleation and growth behavior as well as the suppression of Ostwald ripening.

Here, we analyze this model further and focus on the effects of the material fluxes that are created by the interplay of chemical reactions and diffusion. In particular, we show that centrosomes exhibit an effective centering force if their catalytic activity is large enough. Furthermore, fluctuations of the spherical droplet shape are suppressed, even for an arbitrarily small surface tension. The non-equilibrium conditions created by the chemical reactions thus allow to control important properties of active droplets.

Centrosomes are membrane-less organelles, which are important for cell division. A centrosome consist of liquid-like pericentriolar material that accumulates around a centriole pair. We describe the centrosome as an active droplet, where the pericentriolar material is created from soluble building blocks by chemical reactions that are catalyzed both inside the droplet and at the centrioles [D. Zwicker, M. Decker, S. Jaensch, A. A. Hyman, F. Jülicher, PNAS 111 E2636-45 (2014)]. This model accounts for the observed nucleation and growth behavior as well as the suppression of Ostwald ripening.

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BP 45.4 Thu 15:45 H 1028

Scaling and regeneration of self-organized patterns — Steffen Werner1, Tom Stückemann2, Manuel Behän Amigo1,3, Jochen C. Rink2, Frank Jülicher1, and Benjamin M. Friedrich1 — 1Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — 3Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — 3Universidad Autónoma de Madrid, Madrid, Spain

Biological patterns and morphologies, generated during development and regeneration, often scale with organism size. Some organisms such as flatworms can even regenerate an appropriately scaled body plan from tissue fragments of varying sizes. Turing proposed a general principle for self-organized chiral pattern formation, yet our understanding of the Turing patterns usually do not scale with system size, but are governed by characteristic length scales. Here, we introduce a generalization of the Turing patterns that is both self-organized and self-scaling. We analytically characterize this novel class of pattern forming systems, for which a Turing instability is coupled to the reaction kinetics of diffusing expander molecules. This expander regulates reaction rates of the Turing system, thereby adjusting its intrinsic length scale proportional to system size. Using dynamical systems theory, we identify minimal requirements for self-scaling. We address robustness of emerging patterns with respect to parameter variations as well as structural robustness of the feedback logic itself. Our model captures essential features of body plan regeneration in flatworm fragments as observed in amputation experiments. For more information: arXiv:1411.2359
Dynamic and static force measurements on (PLL/HA)n multilayer films by atomic force microscopy — Brigitte Neugirg, Rudo Heimann, Benedikt Neugirg and Regine von Klitzing — Strankski-Laboratorium, TU Berlin, Berlin

In recent years smart biomaterials have become a highly developing field of interest for biomedical applications, e.g. drug delivery(1). The layer-by-layer (LbL) technique (2) gives the opportunity to build up self assembled polyelectrolyte multilayer films (PEM) with defined architecture, physical and chemical properties. PEM made of poly(L-lysine) (PLL) and hyaluronic acid (HA) were produced by using the LbL technique. Potential applications of these PEMs require controlling of the adhesion behaviour by tuning their elastic-viscoelastic properties.

In this study elastic(3) and viscoelastic properties of LbL coated poly(L-lysine)/hyaluronic acid PLL/HA films were studied by colloidal probe atomic force microscopy. It was shown that the indentation modulus of PLL/HA films measured in different pH, ionic strength and temperature of the surrounding medium changes. Furthermore the viscoelastic film behaviour was measured and calculated by dynamic force measurements.


Mechanical characterization of recombinant spider silk: yarn tensile testing and single fiber deformation via AFM —

Benedikt Neugirg1, Gregor Lang2, Thomas Scheibel2, and Andreas Ferry3 — 1Physical Chemistry II, University of Bayreuth — 2Biomaterials, University of Bayreuth

Outstanding mechanical properties combined with biocompatibility render spider silks one of the most promising materials with respect to biomedical applications. Recombinant routes to e.g. dragline silk core proteins of Araneus diadematus provide access to material fabrication at industrially relevant scales. Together with the electrospinning technique, morphologies based on fibrillar structures, from single fiber to nonwovens are readily producible.

In our work, we mechanically characterize recombinant silk yarns and the individual sub-um diameter fibers which the yarns consist of. For this purpose we use macroscopic tensile testing and nanoscopic AFM lateral bending experiments. Furthermore, we investigate the influence of the relative humidity (RH) which is known to have a huge impact on silk mechanics.

In the recombinant silk to resemble rubber-like properties at higher levels of RH. Enhancing structure crystallinity by post-treatment of the fibers dramatically increases the energy uptake at high RH prior to rupture. In this (physiologically relevant) humidity range, recombinant spider silk can keep up with its natural analog in terms of toughness, the most prominent mechanical characteristic.

Wang-Landau simulation of protein-like G5 model molecules — Arne Böker and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg

The Wang-Landau method is a recent contribution to the Monte Carlo family, able to provide complete thermodynamic information about a system. Contrary to Markovian Monte Carlo, it is a general statistical ensemble, giving the opportunity to access quantities of microcanonical and canonical ensembles in one simulation.

G5-like protein models have been successful for several decades owing to their simplicity, allowing fast simulation to achieve mostly reasonable results. Thus, they provide a suitable model system for the relatively complicated Wang-Landau algorithm.

We applied this method to a basic G5 model consisting of hard tangent spheres with a square-well attraction to investigate the phase behaviour and especially the influence of the length scale used to define neighbours within the G5 model on these properties.
Investigation of the lateral arrangement of phospholipid monolayers with respect to the adsorption of hyaluronan* — •Florian Wieland1, Thomas Zander1, Sören Geyer1, Andrea Dedinaite2, Per Claesson2, Vasyl Haramus3, and Regine Willumset-Römer3 — Helmholtz Zentrum Geesthacht, Max Planck Str. 1, 21502 Geesthacht — 2KTH Royal Institute of Technology, School of Chemical Sciences and Engineering, Department of Chemistry, Surface and Corrosion Science, Drottning Kristinas väg 51, SE-10044 Stockholm, Sweden

The unmatched tribological performance of articulated joints is due to both the properties of the cartilage itself and the assumed self-organization of the molecules in the synovial fluid and at the surface of cartilage. Phospholipids form lamellar structures on cartilage surfaces and are able to reduce friction and wear. We performed x-ray reflectivity and grazing incidence diffraction measurements on Langmuir layers of Dipalmitoylphosphatidylcholine and investigated how the adsorption of hyaluronan (HA) changes the arrangement of the lipids. In the course of the experiment we changed parameters like the molecular weight (MW) and the salt concentration in the subphase, in order to determine the key parameters.

Our data indicate that the adsorption strongly depends on the MW of HA and further on the presence of divalent ions in the subphase.

Interaction of Hyaluron and Phospholipids at high hydrostatic pressure — •Thomas Zander1, Florian Wieland1, Min Wang2, Akanksha Raj3, Per Claesson2,3, Andrea Dedinaite2,3, Vasyl Haramus3, Regine Willumset-Römer3, and Andreas Schreyer1 — Helmholtz Zentrum Geesthacht, Institute for Materials Research, DE-21502 Geesthacht — 2KTH Royal Institute of Technology, School of Chemical Sciences and Engineering, SE-10044 Stockholm — 3SP Technical Research Institute of Sweden, SP Chemistry, SE-11486 Stockholm

Articular joints are bio-lubrication systems with the lowest friction coefficients found in nature. The friction coefficient is provided by the synovial fluid, which is an intricate composition of different macromolecules (e.g. phospholipids and hyaluronan) and which keep the exceptional good lubrication properties even under high loads and shear rates. It is thought that the different constituents form complex structures in order to enable this low friction coefficients.

X-ray reflectivity measurements at different hydrostatic pressures (60bar - 2kbar) on silicon supported phospholipid- and phospholipid hyaluronen composite layers have been performed in order to gain information about their structural arrangement. Parameters like, temperature, molecular weight of the hyaluronan and ions in the solvent solution have been varied, to identify possible key parameters for good lubrication. Our results clearly reveal differences in the behaviour of the phospholipid hyaluronen composites due to different solvent conditions.

Establishing Short-Range Gradients of Cytokines to Mimic Paracrine Cell Interactions in vitro — •Michael Ansorge and Tilo Pompe — Universität Leipzig, Institute of Biochemistry

Cells in various tissues receive myriads of exogenous signals, which in sum determine their fate. Many signaling molecules act in a gradient fashion to guide cell migration, differentiation and proliferation. We set up a microparticle-based system for generating biomimetic short-ranged gradients to analyze dynamic cell behavior with high resolution in vitro. The modification of agarose microbeads with glycosaminoglycans (GAG) with different degree of sulfation provides a toolbox to tune the binding and release of various cytokines.

Using chemically sulfated hyaluronic acid (HA) as GAG we were able to load the microbeads with different cytokines (SDF-1, TGF-beta, IL10) in dependence on their affinity to sulfated and non-sulfated HA. By following the local concentration decrease of fluorescently labeled cytokine inside the microbeads over days with confocal microscopy we could determine released amounts and diffusion-based transport properties. We were able to calculate local cytokine gradients surrounding the microbeads, which are estimated to be in the range of some tens of micrometers at physiological concentrations of pg/ml. We currently verify these local gradients using fluorescence correlation spectroscopy.

Studies on the dynamic cell behavior within the cytokines gradients address biomedical questions on cell fate of hematopoietic stem cells and fibroblasts in 3D collagen-based matrices.

Kinetics of mutarotation in fucose-saccharides as monitored by dielectric and infrared spectroscopy — •Wilhelm Kossack1, Wycliffe Kiprop Kipsusu1, Mateusz Dulski2, Karolina Adriansoniczi2, Olga Madejczyk2, Emanuel Urandu Mapessa1, Martin Tröss1, Kamil Kasinski2, and Friedrich Kremer3 — 1University of Leipzig, Linnestr. 5, Leipzig, Germany — 2University of Silesia, Katowice, Poland

Fourier Transform Infrared Spectroscopy and Broadband Dielectric Spectroscopy are combined to trace kinetics of mutarotation in L-fucose. After quenching molten samples to temperatures between T = 313 K and 328 K, the concentrations of two anumeric species change according to a simple exponential time dependence, as seen by the increasing absorbance of specific IR-vibrations. In contrast, the dielectric spectra reveal a slowing down of the structural (a-) relaxation according to a stretched exponential time dependence (stretching exponent of 1.5 ± 0.2). The rates of change in the IR absorption for α- and β-fucopyranose are (at T = 313 K) nearly one decade faster than that of the intermolecular interactions as measured by the shift of the a-relaxation. This reflects the fact that the α-relaxation monitors the equilibration at a mesoscopic length scale, resulting from fluctuations in the anomeric composition.
Invited Talk

BP 47.1 Thu 15:45 PC 203
Flagellar synchronisation through direct hydrodynamic interactions — •MARCO POLIN1, DOUGLAS COSTA2, MIT, Boston, MA, US — 2University of Warwick, Coventry, UK — 3University of Cambridge, Cambridge, UK

Microscale fluid flows generated by ensembles of beating eukaryotic flagella are crucial to fundamental processes such as development, motility and sensing. Despite significant experimental and theoretical progress, the underlying physical mechanisms that drive this striking coordination remain unclear. We describe a novel series of experiments in which the flagellar dynamics of two micropipette-held somatic cells of Volvox carteri, with measurably different intrinsic beating frequencies, are studied by high-speed imaging as a function of their mutual separation and orientation. From analysis of beating time series, we find that the interflagellar coupling, which is constrained by the lack of chemical and mechanical connections between the cells to be purely hydrodynamical, exhibits a spatial dependence that is consistent with theoretical predictions. At close spacings it produces robust synchrony which can prevail for thousands of flagellar beats, while at increasing separations this synchrony is systematically degraded by stochastic processes. Through tracking we quantify the associated waveforms and show that they are significantly different in the synchronised state. This study unequivocally reveals that flagella coupled only through a fluid medium are capable of exhibiting robust synchrony despite significant differences in their intrinsic properties.

Invited Talk

BP 47.2 Thu 16:15 PC 203
Active motion: From single microswimmers to their emergent collective behavior — •HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Active motion of artificial and biological microswimmers is relevant in microfluidics and biological applications but also poses fundamental questions in nonequilibrium statistical physics. Mechanisms of single microswimmers need to be understood and a detailed modeling of microorganisms helps to explore their complex cell design and their behavior. The collective motion of microswimmers generates appealing dynamic patterns.

In this talk I review some of our work modeling biological microswimmers such as E. coli [1] and the African trypanosome [2], the causative agent of the sleeping sickness, in order to contribute to their better understanding. Using simpler model microswimmers such as active Brownian particles, I will demonstrate their emergent collective behavior. Hydrodynamic interactions lead to a clustering transition dependent on swimmer type [3] or to the formation of fluid pulses in 3D harmonic traps [4]. Self-phoretic active colloids show biomimetic auto-chemo-mechanical behavior, which can include dynamic clustering, oscillating clusters, or a chemotactic collapse [5].


BP 47.3 Thu 16:45 PC 203
Collective behavior and clustering of self-propelled rod shaped catalytic motors: A theoretical study — •DAVID POULADAS2 and ZAHA ESKANDARI1 — 1Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — 2Max Planck Institute for Intelligent Systems, Stuttgart, Germany

In the last few years, catalytic micro-motors have attracted considerable attention and different experiments have performed in order to investigate their applicability in biology, e.g. colloidal cargo transportation. The collective behaviour of these micro-engines and their dynamic self-organization have recently been studied in experiments. In our study, we did Brownian dynamics simulation of rigid rods as a model for the interaction of catalytic motors, in a framework of stochastic processes which explain the force generating chemical reactions, and theoretically investigated the effect of spatial geometry of these active rods in the pattern formation of their clusters.

BP 47.4 Thu 17:00 PC 203
Vortex pattern formation of curved active polymers — •LORENE HUBER, JONAS DENK, EMANUEL REITTMANN, and ERWIN FREY — Ludwig-Maximilians-Universität, München, Deutschland

During bacterial cytokinesis FtsZ filaments assemble into a ring-like structure. Recent experiments with reconstituted FtsZ-dependent recruitment of FtsZ filaments to supported membranes have observed self-organization into vortex patterns. Accounting for the treadmilling dynamics of curved FtsZ on the membrane, we propose a model for systems of polymers with equal length and curvature that undergo collective reorganization in the presence of a mechanical force. We numerically simulate the evolution of the system and study the effects of the magnitude of the mechanical force on the characteristic length scales of the resulting vortex patterns. These results provide a framework for interpreting experiments with multiple rings and for using vortex patterns to study the mechanical properties of FtsZ filaments.

BP 47.5 Thu 17:15 PC 203
The many faces of drag in micro-swimming — •JAYANT PANDE1, LAURA MERCHANT1,2, JENS HARTING2, and ANA S. SMITH3 — 1Inst. for Theor. Phys., Friedrich-Alexander Univ. Erlangen, Germany — 2School of Phys. and Astronomy, Univ. of St. Andrews, Scotland — 3Dept. of Appl. Phys., Eindhoven Univ. of Technology, Eindhoven, the Netherlands — 4Ruder Bošković Inst., Zagreb, Croatia

Although the theoretical study of micro-swimming is becoming increasingly important, the role of the drag force faced by swimmers—clearly one of the cornerstones of micro-locomotion—remains inadequately understood. We shed light in this talk on some of the fundamental ways in which this force affects micro-swimming, using a very simple yet versatile model of a bead-spring swimmer, based on the three-sphere design of Najafi and Golestanian. The drag force on these swimmers enters in various guises—through the influence of the mean bead shape, through any induced transitory shape changes during the swimming cycle if the beads are non-rigid, and through the fluid viscosity. We consider the effect of each contribution separately by letting the beads be of any shape as well as of rigid or flexible material, and by analyzing the various forces on them in fluid. We show that in general an increase in the drag force can have a net positive or a negative impact on the velocity, and it is the swimmer elasticity which decides this. Depending on the latter, we present precise expressions for the parameter ranges where the drag has opposing effects. We support the theory using lattice Boltzmann method-based simulations, and discuss the parts of the theoretical parameter space which are accessible to the simulations.

BP 47.6 Thu 17:30 PC 203
Formation, compression and surface melting of colloidal clusters by active particles — •FELIX KÖMMEL1, PARMIDA SHABESTARI1, and CLEMENS BECHINGER1,2 — 1Max-Planck-Institut für Intelligente Systeme, D-70569 Stuttgart, Germany — 2Max-Planck-Institut für Physikalisches Institut, Universität Stuttgart, D-70569 Stuttgart, Germany

Artificial active swimmers, i.e. Janus particles, suspended in a critical binary mixture, are capable of a self-driven, persistent macroscopic motion upon illumination [1][2]. In previous experiments, the dynamics of such swimmers close to walls and periodic arrays of rigid obstacles has been investigated [1]. Here, we experimentally examine the structural changes in a mixture of passive and a small number of active colloidal particles of equal diameters in a two-dimensional system. With increasing passive particle area fraction, we observe the formation of clusters with passive particles in the interior and active particles at their boundaries. Further increase of the passive particle area fraction leads to the merging and compression of such clusters and eventually to local melting of crystalline regions by enclosed microswimmers. Our results demonstrate that the addition of only a small amount of active particles largely changes the structure and the dynamics of colloidal suspensions.

BP 47.4 Thu 17:00 PC 203
Detention times of microswimmers close to surfaces —

Andreas Zöttl, Konstantin Schäffner, and Holger Stark

Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin — Robert Koch-Institut, D-13355 Berlin — Institut für Theoretische Biologie, Humboldt Universität Berlin, D-10115 Berlin

The locomotion of biological microswimmers such as bacteria in aqueous environments is determined by low-Reynolds-number hydrodynamics and influenced by thermal and intrinsic biological noise. In many relevant environments such as in the human body or in the ocean, microorganisms swim in the presence of soft or solid boundaries. When bacteria approach surfaces they accumulate there and form aggregates such as biofilms. A key ingredient for the observed near-wall accumulation are the relatively large times the microswimmers reside at a surface before leaving the surface. Recently, the role of noise compared to hydrodynamic interactions with the surface has become the subject of a debate.

We introduce a general framework to calculate their wall detention time distribution, i.e., the time they stay at the surface. We map the escape of the microswimmer from the surface to the surface to a mean-first passage problem and apply our theory to different swimmer models (pusher, puller, source-dipole swimmer). While source dipole swimmers have a reduced and pullers an increased detention time compared to a simple active Brownian particle, pushers can have both.

Evaluating a Socio-environmental Complex Adaptive System: The Case of Self-Organized Socio-environmental Development in State Chiapas. — Felipe Lara-Rosano and Adriana Quiroga-Carapia

Universidad Nacional Autónoma de Mexico (UNAM), Mexico City, Mexico — Colegio de la Frontera Sur (ECOSUR), San Cristobal las Casas, Mexico

The project "Social and Environmental Innovation for Development in Areas of High Poverty and Biodiversity in the Southern Border of Mexico" was proposed by a research institute: the Colegio de la Frontera Sur (ECOSUR), and financed by the Mexican Research Council.

Its central objective: to create opportunities for social and environmental innovation on the southern border of Mexico, seeking to strengthen the local capacity for sustainable management of natural resources and the welfare of its inhabitants. Because of the complex system and environment dynamics the solution of the problem is not a fixed one but it is a process that must be continuously evaluated and adapted based on the standpoint of the complex systems paradigm. The assessment of the socio-environmental development project is performed conceptualizing and organizing the community as a complex adaptive system in interaction with its environment. The system has properties expressed as state variables associated with a value that is changing through the development process. The analysis of the system dynamics is based on the behavior of its state variables. The Colegio de la Frontera Sur (ECOSUR) successfully applied this method in rural development projects in state Chiapas in 2013.

Macroscopic description of complex adaptive networks coevolving with dynamic node states —

Marc Wiedermann, Jonathan F. Donges, Joost Heitzig, Wolfgang Lüchtt, and Jürgen Kurths

Potsdam Institute for Climate Impact Research, Germany — Humboldt University, Berlin, Germany — Stockholm Resilience Centre, Stockholm University, Sweden

When investigating the causes and consequences of global change, the collective behavior of human beings is believed to have a considerable impact on natural systems. Here, we study opinion formation and imitation of nodes on a complex network depending on the state of individual resource stocks that are harvested by each node. Numerical simulations reveal that high interaction rates between nodes cause a likely depletion of the resource whereas low interaction rates ensure their sustainable existence. However, adaptively rewiring the nodes' neighborhood structure with an appropriate frequency guides the system into an equilibrium state where all nodes behave sustainably and a full depletion of the resource stocks is avoided. In order to explain these observations, we derive a consistent macroscopic description of the system, which provides a general framework to model and quantify the influence of single node dynamics on the macroscopic state of a network and is applicable to many fields of study, such as epidemic spreading or social modeling. Our results suggest that with the current trend to faster imitation and ever increasing global network connectivity, societies are becoming more vulnerable to environmental collapse if they remain myopic at the same time.

Exploring the safe and just operating space in an inhomogeneous world —

Wolfram Barford, Boyan Beronov, Marc Wiedermann, and Jonathan Donges

Stockholm Resilience Centre, Stockholm University, Sweden

The Anthropocene has become reality during the 20th century, meaning that our species is pressuring the Earth’s ecosystems on a global scale. In the meantime the challenge of eradicating poverty has not yet come to an end. Effectively dealing with these issues requires us to better understand the driving forces, feedback loops and tipping elements in the whole earth system, constituted from natural and social components. To take a step forward in this direction, we refine existing conceptual evolutionary model between social and ecological domains by adding inhomogeneities modelled after real-world data. We then propose an analysis framework, ‘the safe and just space’-plot, which aligns with the current debate of simultaneously staying within the Planetary Boundaries and ensuring the social foundations and transforms it into a practical tool for studying socio-ecological
models as well as real-world observations. First results from comparing the model outcome with real-world data indicate that the current state of the world is neither particularly safe nor particularly just.

BP 48.5 Thu 18:15 MA 001
Topology of Sustainable Management of Dynamical Systems with Desirable States — Jobst Heitzig1 and Tim KITTEL1,2 — 1Potsdam Institute for Climate Impact Research — 2Humboldt University Berlin
The sustainable management of systems mainly governed by an internal dynamics for which one desires to stay in a certain region of their state space requires an understanding of the topology of the system's state space in terms of what regions are "safe" to stay in, and to what qualitative degree, and which of these regions can be reached from which others by the internal dynamics or by management.

The paradigm of optimal control on the one hand does not provide sufficient concepts for such a qualitative analysis and on the other hand typically requires quite a lot of structural knowledge about the problem, in particular, some or other form of quantitative evaluation or states.

In this talk, we will derive in a purely topological way a thorough qualitative classification of the possible states and management options of a system with respect to the possibility of avoiding or leaving some given undesired region by means of some given management options. Our results indicate that the sustainable management of a system may require discrete decisions such as choosing between ultimate safety and permanent desirability, or between permanent safety and increasing future options, etc.

BP 49: Molecular motors

Invited Talk
BP 49.1 Thu 16:45 H 1028
Directional bias in the kinesin superfamily of molecular motors — Robert Cross — Warwick Medical School, Coventry CV4 7AL, UK
The molecular stepping mechanisms of various members of the kinesin family are being dissected by a number of labs using experimental protein engineering and single molecule mechanics. The mechanisms of directional bias are of major interest. Kinesin-1 walks towards microtubule plus ends, holding on with one motor head and biasing the attachment direction of the other. Some of this bias may originate in electrostatic steering. The stability of microtubule binding is strain-dependent, and this gives rise to biased detachment, in which the probability of detachment of each motor head depends on the magnitude and direction of the strain it experiences. Docking and undocking of the C-terminal neck linker domain will be strain dependent and can influence both microtubule binding and binding of the ATP fuel and the ADP product of ATP hydrolysis. Altering the tethering point of the motor domains can influence direction, but does not always do so. Other contributors to directional bias are also emerging. Recently, it has emerged that kinesin-5, the architect of bipolarity in the mitotic spindle, slows down and ultimately reverses direction as the number of motors engaged with the microtubule is progressively increased. Our own most recent work addresses the influence of the ATP:ADP ratio in the bathing solution on the directionality of kinesin-1.

BP 49.2 Thu 17:15 H 1028
Microfluidic setup for highly-parallel force-velocity measurements on single motor proteins — Marta Urbanska1, Karl Duderstadt2, Annemarie Liethack1, Wim Walter1, Anne van Ojen2, and Stefan Diez3 — 1B CUBE, TU Dresden, Germany — 2Zernike Institute for Advanced Materials, University of Groningen, Netherlands — 3Biozentrum Klein Flottbek, Uni Hamburg, Germany
Cytoskeletal motor proteins are essential for long-range, directed transport in cells. In vitro, it has been shown that external loads alter the velocity with which these ATP-driven molecules step along their filamentous tracks. So far, such force-velocity studies have been performed almost exclusively using optical traps. While optical trapping provides the highest force and spatio-temporal accuracy, it allows for one measurement at a time only. Here, we describe an alternative method to simultaneously measure multiple force-velocity relations based on the application of calibrated hydrodynamic forces to stepping motors via DNA-tethered beads. In particular, 1-μm beads were attached to the SNAP-tag-labelled tails of kinesin-1 motors via A-DNA linker. Such motor-DNA-bead complexes were applied to surface-attached to the SNAP-tag-labelled tails of kinesin-1 motors via a C-terminal domain and controlled flow was used to exert forces onto the motors. By observing the bead positions over time we were able to simultaneously track stepping of hundreds of individual motors with nanometer precision. The highly parallel nature of the measurements enables efficient collection of statistically significant quantities of data. Moreover, our approach is readily applicable to other motors and constitutes a new methodology for single-molecule force studies.

BP 49.3 Thu 17:30 H 1028
Control of cytoplasmic dynein force production and processes by its C-terminal domain — Matthew Nicholas4, Peter Höök2, Shylibre Brenner1, Caitlin Lazar3, Richard Vallée5, and Arne Gerschler1 — 1Albert Einstein College of Medicine, Bronx, NY 10128 — 2University of Notre Dame, Notre Dame, IN 46556 — 3Columbia University, New York, NY 10027
Cytoplasmic dynein is a microtubule motor involved in cargo transport, nuclear migration and cell division. Despite structural conservation of the dynein motor domain from yeast to higher eukaryotes, the extensively studied S. cerevisiae dynein behaves distinctly from mammalian dyneins, which produce far less force and travel over shorter distances. However, isolated reports of yeast-like force production by mammalian dynein have called interspecies differences into question.

We report that functional differences between yeast and mammalian dynein are real and attributable to a C-terminal motor element absent in yeast, which resembles a "cap" over the central pore of the mammalian dynein motor domain. Removal of this cap increases the force generation rate of dynein from 1 pN to a yeast-like 6 pN and greatly increases its travel distance. Our findings identify the CT-cap as a novel regulator of dynein function.
parameters influence the cooperativity.

Filamin Inhibition of Myosin Groups Potentiates with Group Size — Zsombor Balassay1, Leonard Hilbert2, Natasima B. Zitouni1, and Anne-Marie Lauzon3 — McGill University, Montréal, Canada — 2Center for Systems Biology, Dresden, Germany

Filamin is an actin-actin crosslinker found in smooth muscle and non-muscle cells and inhibits actin filament sliding in vitro motility assays. Here, we investigate how inhibition by filamin scales with myosin group size. In our in vitro motility assay (smooth muscle myosin), filamin did not disrupt the bistable stop-and-go motion of actin [1], did not affect the velocity of sliding actin, but decreased the fraction of actin in the sliding state (f_mot). Full arrest occurred for [Filamin] = 15 nM ([Actin] = 30 nM). For [Filamin] = 5 nM, f_mot had a maximum (f_mot = 0.6) at intermediate actin length (L = 1.0 μm). For shorter actin, f_mot displayed the typical reduction to lower f_mot. For longer actin, however, an atypical decrease of f_mot with L was observed (f_mot = 0.45 for L = 1.7 μm). We extended our mathematical model of actin propulsion by myosin groups [1] and reproduced these results. The model now explicitly treats the location of myosin and filamin binding sites on actin (spacing 35.5 nm), mechanical coupling strength decays exponentially along actin (characteristic length 175 nm). In the model, filamin binding is established and resolved in localized confined domains, each of which can lead to global arrest of actin sliding. On longer actin there are more localized domains, each of which can independently arrest the whole filament, leading to a greater likelihood of arrest. [1] Hilbert et al., Biophys J, 2013

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

Many single molecule experiments for molecular motors comprise not only the motor but also large probe particles coupled to it. The theoretical analysis of these assays, however, often takes into account only the degrees of freedom representing the motor. We present a coarse-graining method that maps a model comprising two coupled degrees of freedom which represent motor and probe particle to such an effective one-particle model by eliminating the dynamics of the probe particle in a thermodynamically and dynamically consistent way. The coarse-grained rates obey a local detailed balance condition and reproduce the net currents. Moreover, the average entropy production as well as the thermodynamic efficiency is invariant under this coarse-graining procedure. Our analysis reveals that only by assuming unrealistically fast probe particles, the coarse-grained transition rates coincide with the transition rates of the traditionally used one-particle motor models. Additionally, we find that for multicyclic motors the stall force can depend on the probe size. We apply this coarse-graining method to specific case studies of the F1-ATPase and the kinesin motor.

Real-time deformability cytometry: On-the-fly mechanical phenotyping for label-free cell functional assays — Oliver Otto1, Philipp Rosendahl1, Alexander Mietke1,2, Stefan Golff01, Angela Jacob1, Christoph Herold1, Daniel Klau1, Nicole Töppner1, Salvatore Girardo1, Elisabeth Fischer-Friedrich2, and Jochen Guck3,4,5 — 1Biotechnology Center, Technical University of Dresden, Dresden, Germany — 2Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany — 3Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

The mechanical properties of cells are considered as a label-free, inherent marker of biological function in health and disease. Wide-spread utilization has so far been impeded by the lack of a convenient measurement technique with sufficient throughput, sensitive to cytoskeletal changes. Here, we introduce real-time deformability cytometry (RT-DC) for continuous mechanical single-cell characterization with analyze rates in excess of 100 cells/s. Cells are driven through a microfluidic channel leading to deformations due to hydrodynamic stresses, which are described by an analytical hydrodynamic model. Experiments with RT-DC demonstrate sensitivity to cytoskeletal alterations and specificity for different cell cycle phases. RT-DC can also track the differentiation of hematopoietic stem cells into different lineages and identify cell types in whole blood by their mechanical properties. In summary, RT-DC enables continuous mechanical phenotyping of heterogeneous cell populations with a throughput comparable to standard flow cytometry.

Interaction between Polyelectrolytes and Proteins in aqueous solution — Shun Yu1, Xiao Xu1, Joachim Demuynck1, and Matthias Ballauff1 — Helmholtz-Zentrum Berlin, Institute of Soft Matter and Functional Materials

Complex self-assembling systems of interacting polyelectrolyte (PE) and proteins are a growing topic in recent research in pharmacy, biochemistry, and physics [1]. The adsorption of unwanted short polyelectrolytes upon proteins in blood plasma and thus hindering their function is a crucial medical problem. To improve the removal of low molecular weight toxins, a deeper understanding of the interaction between the toxin and the protein is crucial. We use Polyacrylic acid (PAA) as a model polymer and study its interaction with Human Serum Albumin (HSA) at a pH well above the isoelectric point of HSA. It has been recognised, that complex formation can occur at the "wrong side of pH", where both protein and polyelectrolyte are same charged [2]. Driving forces of the interaction can be very well studied using Isothermal Titration Calorimetry (ITC) to analyse binding strengths, entropy and enthalpy [3]. In the present work, we show a full thermodynamic analysis of the binding behavior and find a strong dependency of the interaction on ionic strenght and temperature. Moreover, theoretical modelling using MD simulations supports experimental results and quantifies the role of electrostatic field in the binding process. [1] Kayitmazer et al., Soft Matter 9, 2953 (2013) [2] Dubin et al., Separation & Purification Reviews 23, 1 (1994) [3] Welsch et al., Polymer 12, 2835 (2013)

Diamondoid-functionalized Au(111) nano-electrodes as probes for detecting DNA and mutations — Ganesh Sivaraman1, Rodrigo Garcia Asorim1, Ralph Scheuerm1, and Maria Fyta1 — 1Institute of Computational Physics, University of Stuttgart, Germany — 2Division of Material Theory, Department of Physics and Astronomy, Uppsala University, Sweden

Solid state nanoprobes embedded with gold electrodes have been proposed to be strong candidates for the electrical read out of DNA. However, reduction in the noise in the electrical measurement is critical for an error free read out of DNA. A possible solution would be to use functionalized nanoprobes by which the specific interaction of a “functionaizing molecule” with the DNA should increase the signal-to-noise ratio in the measurements. Recently, we have proposed that amine and thiol doped diamond-like cages, known as diamondoids, as a candidate for functionalizing molecule.

In the first part of this theoretical investigation, we characterize the structure, electronic, and transport properties of Au(111) electrodes and diamondoid-modification on the Au(111) electrode surface. In the second part, a small bias voltage is applied across the Au(111) electrodes. The aim is to use the tunneling current across the functionaized junction as a means for distinguishing between individual DNA nucleobases/mutations. We will evaluate the tunneling current across the electrodes by inserting separately the 4 nucleotides, one mutant, and one epigenetic marker between the electrodes.

Highly controllable synthetic neuronal circuits: Poly-L-lysine patterned semiconductor microtube substrates — Jann Harberts1, Aune Kottmä1, Gabriele Loer1, Cornelius Bausch1, Daniel Diedrich1, David Sonnensberg1, Christian Heys1, Wolfgang Hansen1, and Robert H. Bliss1 — 1CHYN & INF, University of Hamburg, Germany — 2ZMNH, University Medical Center Hamburg-Eppendorf, Germany
Detailed understanding of the human brain is a central field of research. Due to high complexity of neuron interaction, the experimental set-up has to be reduced to a manageable amount of neurons with predefined axon growth. It has been shown that microtubes can influence the direction of axon growth. The preparation is based on lattice mismatched layers. The arrangement of the tubes is defined by photolithography. Etching of the sacrificial material reduces the strain between the layers and creates tubes.

In order to produce controllable neuronal circuits we print poly-L-lysine (PLL), which supports cell adhesion, in front of the tube notches. The challenge is to find the right printer settings for PLL. We determined suitable parameters to print with PLL. The droplets we use reach a diameter of roughly 25 μm. The advantage of this method is the flexibility of patterning. It serves a fast way to adapt new patterns to different layouts, where the minimum definable drop spacing is 5 μm. Printing droplets of PLL enhances the yield of the axonguiding through the tubes and creates a highly controlled neural network.

Time: Thursday 18:00–18:30

**BP 50.5  Thu 18:30  H 1058**

**IR-Spectroscopy and Multivariate Data Analysis in Point of Care Testing** — Peter Hegemann, Tobias Unruh — Physik Department, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudstr. 3, 91058 Erlangen, Germany

Tetracosane (C24), TC5 w/o nanoemulsions stabilized by the lecinthin 1,2-dimyristoyl-sn-glycerol-3-phosphocholine (DMPC) were prepared by high-pressure melt homogenization. The droplets (diameters of about 65 nm as measured by photon correlation spectroscopy) exhibit a strong supercooling (ΔT about 20 K) and crystallize in a for TC5 unusual orthorhombic crystal structure (space group Pca21 as verified by wide-angle x-ray scattering).

Using small-angle x-ray and neutron scattering and nanodispersions with different neutron scattering contrast for the TC5 core and the DMPC stabilizer layer, the molecular arrangement of DMPC in the interfacial layer was studied. For the nanoemulsions a dense monolayer of DMPC with a thickness of about 16.2 Å was found with only a minor interpretation between TC5 and the acyl chains of DMPC. For the nanoemulsions a monolayer thickness of 10.5 Å is found, indicating a more flat arrangement of the DMPC molecules at the interface. This could be explained by the expanded surface of the nanocrystals with respect to the emulsion droplets.

The structure of the interfacial stabilizer layer of lipid emulsions and suspensions is highly relevant with regard to lipid oxidation of bioactive compounds in food and the crystallization of nanoemulsions.

**BP 51: Physics of Food (joint CPP/BP)**

**Time:** Thursday 18:00–18:30

Small-angle scattering study on the structure of the lecinthin stabilizer layer in tetracosane-water nanoemulsions and suspensions — Martin Schmiele and Tobias Unruh — Physik Department, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudstr. 3, 91058 Erlangen, Germany

Tetracosane (C24), TC5/w/o nanoemulsions stabilized by the lecinthin 1,2-dimyristoyl-sn-glycerol-3-phosphocholine (DMPC) were prepared by high-pressure melt homogenization. The droplets (diameters of about 65 nm as measured by photon correlation spectroscopy) exhibit a strong supercooling (ΔT about 20 K) and crystallize in a for TC5 unusual orthorhombic crystal structure (space group Pca21 as verified by wide-angle x-ray scattering).

Using small-angle x-ray and neutron scattering and nanodispersions with different neutron scattering contrast for the TC5 core and the DMPC stabilizer layer, the molecular arrangement of DMPC in the interfacial layer was studied. For the nanoemulsions a dense monolayer of DMPC with a thickness of about 16.2 Å was found with only a minor interpretation between TC5 and the acyl chains of DMPC. For the nanoemulsions a monolayer thickness of 10.5 Å is found, indicating a more flat arrangement of the DMPC molecules at the interface. This could be explained by the expanded surface of the nanocrystals with respect to the emulsion droplets.

The structure of the interfacial stabilizer layer of lipid emulsions and suspensions is highly relevant with regard to lipid oxidation of bioactive compounds in food and the crystallization of nanoemulsions.

Lipid migration in multicomponent food products such as chocolate — Svenja Reinke², Stephan V. Roth³, Gonzalo Santoro², Josélia Vieira², Stefan Palzer¹, and Stefan Heinrich¹ — ¹Hamburg University of Technology, Denickestr. 15, 21073 Hamburg, Germany — ²DESY, Notkehstr. 85, 22607 Hamburg, Germany — ³Nestlé Product Technology Centre York, P.O. Box 204, Haxby Road, York YO91 1XY, United Kingdom — Nestlé SA, Avenue Nestlé 55, 1800 Vevey, Switzerland

Our aim is to obtain a deeper understanding of the preferred pathways of lipid molecule migration in multicomponent food materials. A profound understanding of the mechanisms is the basis for controlling undesired fat migration leading to degradation of the material quality, e.g., fat blooming of chocolate, resulting in large sales losses for the food industry. Synchrotron X-ray tomography revealed voids in an industrial chocolate sample, which are considered as having a strong impact on the plausible migration pathways. In addition, oil migration into particles with cocoa butter, which resulted in structural changes, were tracked using spatially resolved small angle X-ray scattering (SAXS).

Oil migration has been observed in artificial pores produced in cocoa butter matrices with embedded particles and the DMPC properties of the material has provided further insights into the migration mechanism. Although we have not yet elucidated the exact migration mechanism, our results suggest that migration could occur through the pores of the material. Future research will further clarify the role of the porous structure in chocolate fat blooming.
sität Linz, Altenberger Strasse 69, 4040 Linz, Austria
Rhodopsins are biological pigment-proteins found in photoreceptor cells of the retina. Within the framework of a quantum chemical/electrostatic calculation scheme that has recently been successfully applied to reveal the functional states of BLUF photoreceptors [1], we estimated absorption shifts of the retinal cofactor for a series of site-directed mutants. Our calculations accurately reproduce a series of spectroscopic data and eventually the variations of the maximal absorption in the red- and green-sensitive visual pigments.


BP 52.3 Fri 10:15 H 1028
Photo-dynamics of photo-activated adenyl cyclase NgPAC3 from the amoeboidflagellate Nae
gleria gruberi NEG-M strain — Alfons Penzkofer1, Meenakshi Tanwar2, Sindu Kan
doth Veettil2, Suneel Katekiri2, Manuela Stierl3, and Peter Hегgemann3
1 Fakultät für Physik, Universität Regensburg, Uni
versitätstraße 31, D-93053 Regensburg, Germany — 2Department of Biochemistry, University of Delhi South Campus, Benito Juarez Road, New Delhi 110021, India — 3Institut für Biologie/Expermentele Bion
physik, Humboldt Universität zu Berlin, Invalidenstraße 42, D-10117 Berlin, Germany
The absorption and emission spectroscopic behavior of the photo-
activated adenyl cyclase NgPAC3 from the amoeboidflagellate Nae
gleria gruberi NEG-M strain was studied [1]. The flavin cofactor was found to be partly fully oxidized and partly fully reduced. The typ
ical BLUF domain (BLUF = Blue Light sensor Using Flavin) fully oxidized flavin absorption photo-cycle with an environmental
flavin absorption red-shift in the signaling state was observed. The quantum efficiency of signaling state formation was determined to be φs = 0.66 ± 0.03. A bi-exponential signaling state recovery to the dark-adapted receptor state was observed with the time constants τs,1 = 275± (fraction 0.29) and τs,2 = 45± (fraction 0.71). The thermal irreversible protein unfolding was studied and a protein melting temperature of θm ≈ 50°C was found. NgPAC3 showed light-gated adenylate cyclase activity upon illumination with blue light.


15 min break

BP 52.4 Fri 10:45 H 1028
Conformational Change of the Neuronal Calcium Sensor GCAP1 — Jörg Robin, Jens Brauer, Stephan Sulmann, Christoph Lienau, and Karl-Wilhelm Koch — Carl von Ossi
etzky Universität, 26129 Oldenburg
The ability of photoreceptor cells to adjust to changing light conditions on a millisecond timescale relies on a well balanced interplay of two
second messengers, cGMP and calcium [1]. Upon decrease of intracel
lular calcium due to closure of cGMP gated ion channels the guanylate cyclase is stimulated to replenish cGMP. Two sensor proteins, GCAP1 and GCAP2, regulate the activity of the guanylate cyclase in a sequen
tial step by step order mechanism [2] by conformational change due to binding of calcium. This conformational change has recently been in
vestigated by time-resolved fluorescence spectroscopy for GCAP2 [3].
In this study, we have site-specifically labelled each cysteine residue in GCAP1 mutants by the fluorescent dye Alexa647 and probed its lo
cal environment via time-resolved fluorescence spectroscopy. We have observed both an increase in fluorescence lifetime and in rotational correlation time for the apo compared to the calcium bound state. Our findings are supported by analysing the motional restriction of the dye in a wobbling-in-a-cone model and by molecular dynamics simula

BP 52.5 Fri 11:00 H 1028
Phase behavior of deacyclic lysozyme solutions — Julian Schule1, Johannes Möller2, Michael Paulus3, Julia Nare4, Metin Tolan4, and Roland Winters2 — 1Fakultät Physik/Delta, Technische Universität Dortmund, 44221 Dortmund, Germany — 2Fakultät für Chemie und Chemische Biologie, Technische Universität Dortmund, 44221 Dortmund, Germany
In previous studies, small angle X-ray scattering (SAXS) in combi
nation with liquid-state theoretical approaches and DLVO theory was used to study the intermolecular interaction potential, V(r), of lysozyme solutions under the influence of varying environmental con
ditions as protein concentration c, temperature T, pressure p or salt concentration I. While the repulsive Coulomb term of the DLVO po
tential remains almost constant as a function of p, the depth of the attractive part, J(p), exhibits a non-monotonic p-dependence with a minimum at 1.5 kbar at selected T. Adding 0.5 M NaCl leads to more prominent short range interactions, especially at high c and low T. Here, the homogeneous protein solution becomes turbid due to for
mation of a metastable liquid-liquid phase separation (LLPS) region, where lysozyme forms small droplets of high concentration within the more dilute liquid phase. At elevated pressures, this phase separa
tion is suppressed, but due to the non-monotonic behavior of J(p), a further pressure increase leads to a re-entrant LLPS. The analysis of the SAXS data allows the construction of the c-p-T phase diagram of lysozyme solutions. As crystallization occurs in this c-p-T region as well, the diagram will help optimize crystallization conditions.

BP 52.6 Fri 11:15 H 1028
Exploring the multiscale signaling behavior of phototropin1 from Chlamydomonas reinhardtii using a full-residue space kinetic Monte Carlo molecular dynamics technique — Emanuel Peter, Bernhard Dick, Ivan Stambolic, and Stephan Baerule — Institut für Physikalische und Theoretische Chemie, Uni
versität Regensburg, 93040 Regensburg
Devising analysis tools for elucidating the regulatory mechanism of complex enzymes has been a challenging task for many decades. It generally requires the determination of the structural-dynamical in
formation of protein solvent systems far from equilibrium over multi
ple length and time scales, which is still difficult both theoretically and experimentally. To cope with the problem, we introduce a full
residue space multiscale simulation method [1] based on a combina
tion of the kinetic Monte Carlo and molecular dynamics techniques, in which the rates of the rate-determining processes are evaluated from a biomolecular forcefield on the fly during the simulation run by taking into account the full space of residues. To demonstrate its reliability and efficiency, we explore the light-induced functional behavior of the full-length phototropin1 from Chlamydomonas reinhardtii (Cy-phot1).
Our results demonstrate that in the signaling state the kinase is activ
ated through the disruption of the Jα-helix from the light-oxygen

BP 52.7 Fri 11:30 H 1028
Dynamics of the Orange Carotenoid Protein (OCP) under Photoactivation — Evgeny Maskinov1, Franz-Josef Schmitt2, Thomas Friedrich2, and Vladimir Paschenko2
1 Institute of Chemistry, Bioenergetics, TU Berlin, Straße des 17. Juni 87, D-10623 Berlin, Germany — 2Department of Biophysics, Biology Faculty, Lomonosov Moscow State University, 119991 Moscow, Russia
The cyanobacterium Synechocystis sp. PCC6803 contains a photo-
switchable protein, the orange carotenoid protein (OCP) which under
goes conformational changes under illumination in the blue spectral regime. After activation by light the OCP binds to the membrane ex
trinsic phycobilisome (PBS) complexes and leads to non-photochemical quenching (NPQ) of the PBS fluorescence reducing the flow of energy into the photosystems under high light conditions as protection mech
anism. Time- and wavelength-resolved fluorescence spectroscopy was used to image the dynamics during the photoinduced conformation change and subsequent change in the NPQ efficiency. We suppose that there is a β-ring rotation of the echinenone during photoactiva
tion of OCP that leads to a significant red shift of the absorption spectrum. A distance change between Tyr-201, Trp-288 and the keto
ring rotation of the echinenone during photoactiva
tion of OCP that leads to a significant red shift of the absorption spectrum. A distance change between Tyr-201, Trp-288 and the keto
Biomolecule dynamics in microfluidic pH gradients and pre-biotic FeS membranes — FRIEDERIKE M. MÖLLER1, DOMINIC REINHOLD1, FRANZESKA KAPFER1, MICHAEL RUSSELL2, and DIETER BRAUN1 — 1Systems Biophysics, LMU München, Germany — 2Jet Propulsion Laboratory, Pasadena, USA

What are possible driving forces to reduce local entropy in early evolution? Early earth creates a marked redox potential of >600mV between the CO2-dominated atmosphere, creating an ocean around pH 6 and the alkaline outflow of geological serpentinization reactions at pH 10. How is these phenomena coupled to the FeS-rich, potential gradient? Its equilibrium version was studied by Huber and Wächtershäuser to form the first organic molecules starting from CO. The FeS clusters created in the membrane are central parts in ancient electron-transfer proteins.

What are the physical characteristics of this membrane? In a microfluidic replica, the pH gradient leaks through the membrane. However, we find yet unexplained attractive forces: hydrophobic and charged molecules are strongly attracted towards the membrane center. As reference system, we create pH gradients in water by uncaging of OH- or H+ ions. The phoretic motions and pH gradients are measured by fluorescence. The rich non-equilibrium dynamics are explained with finite element modeling. They offer a microscopic view back in time into the geological setting of early Earth.

A simple array of NIR laser beams is spatially varied with a periodic dynamics in order to optically 'shake' single cells. A detector bead, which is optically trapped with an independent laser beam, is used to simultaneously map the resulting microfluidic flow. We demonstrate a first application of this novel technique by resolving mechanobiological differences in the hypotonic state of individual human erythrocytes. By analyzing the Fourier spectra of cell and detector bead movements, we show that tracking a single detector particle is sufficient to distinguish between soft and hard cells.

We present a technique to measure the mechanics of cellular microenvironment within living tissues and organs. We use ferrofluid oil droplets as mechanical actuators. Once injected in developing zebrafish embryos, we obtain the mechanical properties by tracking the dynamical response of the droplet when actuated by an external magnetic field. In particular, this technique allows us to measure the changes in mechanical properties underlying zebrafish gastrulation.

This technique opens the door to experiments which uniquely relate biological signals to the underlying mechanical properties.

Time: Friday 9:30–12:15

Location: H 1058

BP 53.1 Fri 9:30 H 1058

Anisotropic Diffusion of Macromolecules in the Contiguous Nucleo-cytoplasmic Fluid during Embryonic Cell Division — NISHA PAWAR, CLAUDIA DONTTH, and MATTHIAS WEISS — Experimental Physics I, University of Bayreuth, Bayreuth, Germany

Protein diffusion in intracellular fluids is a crucial determinant of many vital biochemical pathways. Frequently an anomalous diffusion of macromolecules in the cytoplasm and nucleoplasm of eukaryotic cells has been reported, and associated changes in biochemical reactions have been discussed in some detail. Here we show that the contiguous nucleo-cytoplasmic fluid in dividing cells features an anisotropically varying diffusion of macromolecules [1]. In metaphase, diffusion in the contiguous nucleo-cytoplasmic fluid appears less anomalous along the spindle axis as compared to perpendicular directions. As a consequence, the long-time diffusion of macromolecules preferentially points along the spindle axis, leading to a prolonged residence of macromolecules in the spindle region. An anisotropic diffusion may support the dynamic formation of a spindle matrix which guides later steps in mitosis.


BP 53.2 Fri 9:45 H 1058

Optical Shaking of Single Cells — CARLA ZERENZ1,2, ISIS E. FERNANDEZ3, OLIVER ECKELBERG2,3, THIBOALD LOHMÜLLER1,3, and JOCHEN FELDMANN1,3 — 1Chair for Photonics and Optoelectronics, Physics Department and CeNS, Ludwig-Maximilians-Universität, Munich, Germany — 2Comprehensive Pneumology Center, Institute of Lung Biology and Disease, Ludwig-Maximilians-Universität and Helmholtz Zentrum, Munich, Germany — 3Nanosystems Initiative Munich (NIM), Schellingstr. 4, Munich, Germany

We report on a new strategy to dynamically manipulate single cells by exposing them to an applied optical force field which varies periodically in time and space. The mechanical transient response of the cell is monitored both by optical imaging and by a microfluidic detector bead [1] positioned in the cell vicinity. These optical 'shaking' experiments give insight into the mechanobiological properties of single cells.

A predefined array of NIR laser beams is spatially varied with a periodic dynamics in order to optically 'shake' single cells. A detector bead, which is optically trapped with an independent laser beam, is used to simultaneously map the resulting microfluidic flow. We demonstrate a first application of this novel technique by resolving mechanobiological differences in the hypotonic state of individual human erythrocytes. By analyzing the Fourier spectra of cell and detector bead movements, we show that tracking a single detector particle is sufficient to distinguish between soft and hard cells.


BP 53.3 Fri 10:00 H 1058

In vivo mechanics measurements using ferrofluid droplets — FRIEDREICH SERWANE, ALESSANDRO MONGERA, PAVON ROWHAMAN, DAVID KEALHOFER, and OTGER CAMPS — Department of Mechanical Engineering, University of California, Santa Barbara, USA

The development of living tissues and organs depends on cell behaviors. First results of such experiments will be presented as well.

The results of both the QENS experiments and the MD simulations coincide nicely and confirm the benefit of the combination of these complementary methods. These results provide a basis for extended studies on more complex systems e. g. lipid mixtures and lipid-protein interactions. First results of such experiments will be presented as well.

BP 53.4 Fri 10:15 H 1058

Bridging the scales: How is the large-scale deformation of a cellular network related to cell-scale processes? — MATTHIAS MEREKEL1, RAPHAEL ETOUNRAY2, SUZANNE EATON2, and FRANK JULICHER1 — 1MPI for the Physics of Complex Systems, Dresden — 2MPI of Molecular Cell Biology and Genetics, Dresden

We propose a method to study the deformation of two-dimensional cellular networks. We use ferrofluid oil droplets as mechanical actuators. Once injected in developing zebrafish embryos, we obtain the mechanical properties by tracking the dynamical response of the droplet when actuated by an external magnetic field. In particular, this technique allows us to measure the changes in mechanical properties underlying zebrafish gastrulation.

This technique opens the door to experiments which uniquely relate biological signals to the underlying mechanical properties.

BP 53.5 Fri 10:30 H 1058

Dynamics of biological membrane mimics - A combined QENS and MD simulation study — LEA LAUTNER1, MARTIN SCHMIEDEL1, SEBASTIAN BUSCH2, MICHAELA ZAMPONI3, and TOBIAS URNBR1 — 1Chair for Crystallography and Structural Physics, FAU Erlangen-Nuremberg, Germany — 2University of Oxford, United Kingdom — 3Heinz Maier-Leibnitz Zentrum, Garching

Phospholipids are of high interest in the fields of biology and biophysics. As a main component of biological cell membranes the lipids are involved in lipid-lipid and lipid-protein interactions and therefore essential in a variety of cell functions. Many of these processes, e.g. binding to or transport through the membrane, are coupled to their structure and dynamics. Quasileonelshlight Scattering (QENS) experiments and state-of-the-art Molecular Dynamics (MD) simulations yield a complementary view on these processes, with high spatial as well as temporal resolution. A combination of QENS experiments and MD simulations was used to obtain a detailed understanding of the dynamics of biomimetic POPC (1-palmitoyl-2-oleoyl-sn-glycerol-3-phosphocholine) bilayers in the liquid crystalline (L*O) phase. Special emphasis was thereby the study of the temperature dependent behaviour of the phospholipid dynamics. The results of both the QENS experiments and the MD simulations coincide nicely and confirm the benefit of the combination of these complementary methods. These results provide a basis for extended studies on more complex systems e. g. lipid mixtures and lipid-protein interactions. First results of such experiments will be presented as well.

15 min break

BP 53.6 Fri 11:00 H 1058

Nanosystems Initiative Munich — BP 53.1 Fri 9:30 H 1058

Optical Shaking of Single Cells — CARLA ZERENZ1,2, ISIS E. FERNANDEZ3, OLIVER ECKELBERG2,3, THIBOALD LOHMÜLLER1,3, and JOCHEN FELDMANN1,3 — 1Chair for Photonics and Optoelectronics, Physics Department and CeNS, Ludwig-Maximilians-Universität, Munich, Germany — 2Comprehensive Pneumology Center, Institute of Lung Biology and Disease, Ludwig-Maximilians-Universität and Helmholtz Zentrum, Munich, Germany — 3Nanosystems Initiative Munich (NIM), Schellingstr. 4, Munich, Germany

We report on a new strategy to dynamically manipulate single cells by exposing them to an applied optical force field which varies periodically in time and space. The mechanical transient response of the cell is monitored both by optical imaging and by a microfluidic detector bead [1] positioned in the cell vicinity. These optical 'shaking' experiments give insight into the mechanobiological properties of single cells.

A predefined array of NIR laser beams is spatially varied with a periodic dynamics in order to optically 'shake' single cells. A detector bead, which is optically trapped with an independent laser beam, is used to simultaneously map the resulting microfluidic flow. We demonstrate a first application of this novel technique by resolving mechanobiological differences in the hypotonic state of individual human erythrocytes. By analyzing the Fourier spectra of cell and detector bead movements, we show that tracking a single detector particle is sufficient to distinguish between soft and hard cells.

the key idea, we introduce a tiling of the cellular network into triangles. This allows us to define the precise contribution of each of kind of cellular process to large-scale deformation. Additionally, our rigorous approach reveals subtle effects of correlated cellular motion, which constitute a novel source of large-scale tissue deformation. Finally, we introduce our new method on the wing of the fruit fly, which undergoes large-scale deformations during development.

BP 53.7 Fri 11:15 H 1058
Bridging from ionic to non-ionic thermophoresis — the smallest synthetic chemical nanomotors that have across the colloid, resulting in slip velocities at the particle surface, croparticles often makes use of local gradients that are established by macroscopic swimmers. Artificial means of realizing motion in microfluidic environments at the sub-mm scale is challenging. Moving building, powering, and operating structures that can navigate complex fluidic environments at the sub-mm scale is challenging. However, mechanisms that regulate the formation of veins and vascular architecture are largely unknown. In a growing leaf, in addition to genetic regulation, cell mechanics must also play an important role in forming veins. To what extent cell mechanics and the interplay between mechanics and biochemistry plays a role in vascular patterning is not well understood. Using a cell based model in which cells are polygons, here we describe the vascular development in early stages of growing leaf by a heuristic formula proposed by Piazza and attributed to hydrophobic effects, can be fully explained by the Seebeck effect: the temperature dependence of ionic thermophoresis is dominated by the temperature dependent thermophoresis of the small ions in solution. While this dependence is not yet fully known for H+ and OH-, the thermophoresis of peptide nucleic acid (PNA) with its pH dependent charge is described well across a wide range of pH with reasonable assumptions. These findings offer a new bridge from aqueous thermophoresis to none-aqueous solutions.

BP 53.8 Fri 11:30 H 1058
How to regulate droplet position in a heterogeneous chemical environment? — Spatial modulation of the cell mechanical properties based on cell mechanics and the interplay between mechanics and biochemistry plays a role in vascular patterning is not well understood. Using a cell based model in which cells are polygons, here we describe the vascular development in early stages of growing leaf by a heuristic formula proposed by Piazza and attributed to hydrophobic effects, can be fully explained by the Seebeck effect: the temperature dependence of ionic thermophoresis is dominated by the temperature dependent thermophoresis of the small ions in solution. While this dependence is not yet fully known for H+ and OH-, the thermophoresis of peptide nucleic acid (PNA) with its pH dependent charge is described well across a wide range of pH with reasonable assumptions. These findings offer a new bridge from aqueous thermophoresis to none-aqueous solutions.

BP 53.9 Fri 11:45 H 1058
Mechanical regulation of vein morphogenesis in plant leaves — The key idea, we introduce a tiling of the cellular network into triangles. This allows us to define the precise contribution of each of kind of cellular process to large-scale deformation. Additionally, our rigorous approach reveals subtle effects of correlated cellular motion, which constitute a novel source of large-scale tissue deformation. Finally, we introduce our new method on the wing of the fruit fly, which undergoes large-scale deformations during development.

BP 54.1 Fri 9:30 C 264
Invited Talk
From chemical nanomotors to biological microswimmers —
Building, powering, and operating structures that can navigate complex fluidic environments at the sub-mm scale is challenging. Moving through fluid environments at the scale of micro-organisms for instance presents a different set of challenges compared to those encountered by macroscopic swimmers. Artificial means of realizing motion in microparticles often makes use of local gradients that are established across the colloid, resulting in slip velocities at the particle surface, which in turn drives the motion. In its simplest form this can be realized with Janus-like colloids. I describe what, to the best of my knowledge, are the smallest synthetic chemical nanomotors that have been made and show that their active motion can be tracked with light scattering. Moving from enhanced diffusion to propulsion, I present recent results where colloidal nanopropellers can be moved in water by external magnetic fields similar to a bacterial flagellum and show how the motion of these structures can benefit from the complex rheology in biological media. Although strong Brownian forces dominate in water we achieve controlled propulsion in biological gels, which paves the way for applications inside biological media and the extracellular matrix. Finally, I present an example of a microscallop that does not move in water, but that swims in non-Newtonian liquids.

BP 54.2 Fri 10:00 C 264
Optothermal Manipulation of Plasmonic Nanoparticles in Viscous Solvents —
We present an all-optical approach to move and manipulate single plasmonic nanoparticles with high accuracy in viscous solvents.
Gold nanoparticles are subject to optical forces and heat generation upon irradiation with a focused laser beam. Tuning the laser wavelength with respect to the plasmon resonance frequency allows for switching between repulsive and attractive optical forces, which renders it possible to trap or push individual nanoparticles in two and three dimensions. At the same time, laser light can induce heat in the surrounding medium.

We explore how both effects can be employed to control nanoparticle movement by a combination of thermal gradients and optical forces and discuss further applications of this approach for nanolithography and nanoscale physics.

**BP 54.3 Fri 10:15 C 264**

**Dynamics of a carpet of self-propelled surfactant particles covering a liquid film — Andrei Pototsky, Uwe Thiele, and Holger Stark** — 1Department of Mathematics, Swinburne University of Technology, Hawthorn, Victoria, 3122, Australia — 2Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — 3Institut für Theoretische Physik, Technische Universität Berlin, 10623, Berlin, Germany

We consider a carpet of self-propelled surface-active particles that move along the liquid-gas interface of a liquid film on a solid substrate and whose swimming direction changes in time due to rotational diffusion and the inherent instability of these self-propelled insoluble surfactants on the stability of the film surface and show that depending on the strength of in-plane rotational diffusion and the absolute value of the in-plane velocity several instability modes can occur [1]. In particular, the rotational diffusion can have a stabilizing or destabilizing influence and may even suppress the instability entirely. In the limit of purely upwards swimming we recover the destabilisation described in the literature [2]. The results of the linear analysis are confirmed by fully nonlinear simulations of the complete continuum model and as well through a hybrid discrete self-propelled surfactant particles - continuous film model. [1] A. Pototsky, U. Thiele and H. Stark, Phys. Rev. E 90, 030401(R) (2014). [2] S. Alonso and A.S. Mikhailov, Phys. Rev. E 79, 061906 (2009).

**BP 54.4 Fri 10:30 C 264**

**Tangled Flagella: Importance in Bacterial Propulsion — Tapan Chandra Adhyanak and Holger Stark** — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

It has been well established that hydrodynamic interactions between flagella of peritrichous bacteria such as E. coli, leads to synchronization of rotation and bundling of those flagella [1,2]. Flagella are rotated at their bases by rotary motors embedded in the cell body. In response, the cell body has to rotate in the opposite sense such that total torque acting on the bacterium is zero. Often, such cell rotation causes flagella to tangle before they are synchronized completely. We show that tangling has a profound effect on the overall synchronization and that tangling has a profound effect on the swimming direction changes in time due to rotational diffusion and the absolute value of the in-plane velocity several instability modes can occur [1]. In particular, the rotational diffusion can have a stabilizing or destabilizing influence and may even suppress the instability entirely. In the limit of purely upwards swimming we recover the destabilisation described in the literature [2]. The results of the linear analysis are confirmed by fully nonlinear simulations of the complete continuum model and as well through a hybrid discrete self-propelled surfactant particles - continuous film model. [1] A. Pototsky, U. Thiele and H. Stark, Phys. Rev. E 90, 030401(R) (2014). [2] S. Alonso and A.S. Mikhailov, Phys. Rev. E 79, 061906 (2009).

**BP 54.5 Fri 10:45 C 264**

**Reorientation of passive Janus type swimmer in an external temperature profile — Andreas Frugulla and Frank Cichos** — University of Leipzig, department for experimental physics, Leipzig, Germany

Swimming on the micrometer level scale is dominated by omnipresent Brownian fluctuations and overwhelming viscous forces. Self-phoretic swimmers are an example how to overcome those limitations. Most of those particles are driven by phoretic surface flows generated by surface gradients. In the last decade many different phoretic swimming mechanisms have been proposed. When such self-propelled objects are starting to interact at higher densities, coherent collective motions are observed in which the swimmers align and form flocks, swarms or other complicated patterns. About the origin and details of these complex interactions only little is known. The lack of understanding is mostly due to the lack of control of such particles. Here we want to present a method which extends the existing phonon nudging algorithm to gather and collect a specific number of particles and study their interactions. The interactions themselves can be mediated through many different effects like changes, flow fields or through external profiles created by each active swimmer. The last mentioned interaction will be discussed in detail. An immobile gold colloid acts as an external heat source and mimics the temperature profile that an active swimmer would create in its surrounding. The motion of a passive Janus particle in this temperature field is investigated and the relative motion and alignment with respect to the heat source is quantified.

**BP 54.6 Fri 11:00 C 264**

**Thermophoretic Trapping of Single and Multiple Nano-Objects by Actively Controlled Temperature Fields — E. Braun and F. Cichos** — Molecular Nanophotonics, Fakultät für Physik und Geowissenschaften, Universität Leipzig, Deutschland

The understanding of nano-scale soft-matter science benefited enormously from the ability to study single molecules, such as DNA or proteins. In solution Brownian motion lets a molecule disappear quickly from the observation volume, which is why it is typically immobilized in a polymer matrix or by chemical interactions, generally accepted due to a lack of alternatives. However, this strongly changes the local physical and chemical properties. Here, we present an all-optical technique to trap single nano-objects in solution which exploits highly localized temperature fields. The so-called thermophoretic trap exploits thermophoretic interactions of a particle with a temperature gradient, which e.g., locally distorts the screening of the surface charges and by that induces a drift of the particle. In our approach the temperature field is generated by an optically heated gold nano-structure. Due to the small dimensions of the heat sources, even a small temperature increase introduces large temperature gradients causing a strong thermophoretic drift by which the motion of a Brownian particle can be manipulated. In our experiment an appropriate gold structure is heated locally by a focused laser beam with feedback to the Brownian particles position. The real-time control of the laser beam thereby allows for arbitrary effective trapping potentials for single and multiple particles.

**BP 54.7 Fri 11:15 C 264**

**Low-tech, high-throughput tracking of bacteria in 3D — Katja Taute, Sander Tans, and Tom Shimizu** — FOM Institute AMOLF, Science Park 102, Amsterdam 1098XG, The Netherlands

Many bacteria swim in liquids and execute complex motility patterns. The increasingly recognized diversity of motility strategies has sparked a growing interest in their characterization via 3D tracking. The only 3D tracking techniques thus far to have passed the benchmark of resolving the model bacterium E. coli's run-tumble motility suffer from being limited to single individuals [1] and/or are technically challenging and require specialized experimental setups [1,2,3].

Here we present a broadly applicable high-throughput 3D bacterial tracking technique which requires only a standard biological phase contrast microscope. We exploit the object's passive thermal relaxation due to a lack of alternatives. However, this strongly changes the local physical and chemical properties. Here, we present an all-optical technique to trap single nano-objects in solution which exploits highly localized temperature fields. The so-called thermophoretic trap exploits thermophoretic interactions of a particle with a temperature gradient, which e.g., locally distorts the screening of the surface charges and by that induces a drift of the particle. In our approach the temperature field is generated by an optically heated gold nano-structure. Due to the small dimensions of the heat sources, even a small temperature increase introduces large temperature gradients causing a strong thermophoretic drift by which the motion of a Brownian particle can be manipulated. In our experiment an appropriate gold structure is heated locally by a focused laser beam with feedback to the Brownian particles position. The real-time control of the laser beam thereby allows for arbitrary effective trapping potentials for single and multiple particles.

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Model selection and hypothesis testing for large-scale network models with overlapping groups

- Tiago P. Peixoto — Institut für Theoretische Physik, Universität Göttingen, Germany

The effort to understand network systems in increasing detail has resulted in a diversity of methods designed to extract their large-scale structure. Unfortunately, many of these methods yield diverging descriptions of the same network, making both the comparison and understanding of their results a difficult challenge. A possible solution to this outstanding issue is to shift the focus away from arbitrary methods, and move towards principled approaches based on statistical inference of generative models. In this talk we consider the comparison between a variety of generative models including features such as degree correction, where nodes with arbitrary degrees can belong to the same group, and community overlap, where nodes are allowed to belong to more than one group. Because such model variants possess an increased number of parameters, they become prone to overfitting. We present a method of model selection based on the minimum description length criterion and posterior odds ratios that is capable of fully accounting for the increased degrees of freedom of the larger models, and selects the best one according to the statistical evidence available in the data. In applying this method to many empirical datasets from different fields, we observe that community overlap is very often not supported by statistical evidence, and is selected as a better model only for a minority of them. On the other hand, we find that degree correction tends to be almost universally favored by the available data.

Breakdown of quantum transport in scale-free networks

- Nikolaj Kuvelis and Oliver Mülken — Uni-Freiburg, Deutschland

We apply the model of continuous time quantum walks (CTQW) to a subset of scale-free networks (SFN) containing solely trees. A quantity characterising the global transport for large time scales is introduced and, by means of estimating the dominant spectral degeneracy, calculated for given system size and branching strength. Taking the limit of infinite system size a phase transition resembling breakdown of transport is observed beyond a critical branching strength. All our analytic calculations are supported by Monte Carlo simulations and discussed.

Nonlinear elasticity of athermal networks: a critical phenomenon

- Abhinav Sharma, Albert Libup, Michael Shemin, Karin Jansen, Gise Koendrink, and Frederick Mackintosh — 1-1VU, Amsterdam, Netherlands — 2AMOLF, Amsterdam, Netherlands

Biopolymer networks exhibit highly interesting mechanical behavior. An instructive model system is that of a network composed of rope-like filaments–zero resistance to compression but finite resistance to stretching. For networks with connectivity below Maxwell point, there is no elastic modulus for small deformations. However, when networks are subjected to an external strain, stiffness emerges spontaneously beyond a critical strain. We demonstrate that the spontaneous emergence
of elasticity is analogous to a continuous phase transition. The critical point is not fixed but depends on the geometry of the underlying network. The elastic behavior near the critical point can be described analogously to that of Magnetization in ferromagnetic material near the Curie temperature. Surprisingly, the critical exponents are independent of the dimensionality and depend only on the average connectivity in the network. By including bending interactions in the rope network, we can capture the mechanical behavior of biologically relevant networks. Bending rigidity acts as a coupling constant analogous to the external magnetic field in a ferromagnetic system. We show that nonlinear mechanics of collagen are successfully captured by our framework of regarding nonlinear mechanics as a critical phenomenon.

BP 55.8 Fri 11:30 BH-N 128
Coarsening dynamics of transient networks in an experiment with dipolar hard spheres — Armin Korbé and Reinhard Richter
Experimentalphysik 5, Universität Bayreuth, D-95440 Bayreuth, Germany
Permanent magnetic dipoles may self-assemble to linear chains and rings, even without an externally applied magnetic field. This has been investigated for nano-sized particles in ferrofluids; see e.g. [1,2]. However, in this system the emerging structures and their dynamics are difficult to observe. Similar aggregates have also been observed in a mixture of glass beads and magnetized steel spheres, which are shaken in a vessel [3]. In the present contribution we focus on the formation of transient networks in this system, when quenching the amplitude of the vibrations [4]. We analyze the evolving networks by the number of spheres in a network cluster, its gyration radius, and its average shortest path length.


BP 55.9 Fri 11:45 BH-N 128
Exclusion processes on networks — Izaak Neri, Norbert Kern, and Andrea Parmeggiani
1 Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38 01187 Dresden Germany — 2 Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108 01307 Dresden — 3 Laboratoire Charles Coulomb UMR 5221 & CNRS, Universite Montpellier 2, F-34095, Montpellier, France
We present a study of exclusion processes on complex networks, as a paradigmatic model for transport subject to excluded volume interactions. Building on the phenomenology of a single segment and borrowing ideas from random networks we investigate the effect of connectivity on transport. In particular, we argue that the presence of disorder in the network crucially modifies the large scale transport features: disorder induces strong density heterogeneities in the network such that certain regions of the network are almost fully congested while other regions allow for free flow of matter.

BP 55.10 Fri 12:00 BH-N 128
Synchronization-Desynchronization Transitions in Complex Networks: An Interplay of Distributed Time Delay and Inhibitory Nodes — Carolin Wille, Judith Lehner, and Eckehard Schöll
1 Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — 2 Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany
We investigate the combined effects of distributed delay and the balance between excitatory and inhibitory nodes on the stability of synchronous oscillations in a network of coupled Stuart–Landau oscillators. To this end a network model is proposed for which the stability can be investigated analytically. It is found that beyond a critical inhibition ratio synchronization tends to be unstable. However, increasing distributional widths can counteract this trend leading to multiple resynchronization transitions at relatively high inhibition ratios. All studies are performed on two distribution types, a uniform distribution and a Gamma distribution.[1]


Friday
BP 55.11 Fri 12:15 BH-N 128
Efficient sampling of networks with high clustering — Rico Fischer, Jorge Leitao, Tiago Peixoto, and Eduardo Altmann
1 Max-Planck-Institut für Physik komplexer Systeme — 2 University of Bremen
The problem in network generation is to obtain networks which satisfy specified properties but that are otherwise random. Traditional Markov Chain Monte Carlo methods (like Metropolis-Hastings) can be used in this problem but often fail in important cases, e.g., they do not correctly sample random networks with high clustering coefficients due to a rough >> landscape, which typically leads to abrupt phase transitions, metastable states and hysteresis. In this talk we show how an efficient sampling of high-clustering networks is obtained using multicanonical Monte-Carlo methods. We characterize the efficiency of this method, we use it to investigate the phase transition methods, and we explore different applications.

BP 55.12 Fri 12:30 BH-N 128
Shape and scaling of spatially embedded transport networks — Robin de Regt and Christian von Ferber
1 Coventry University, UK
Real world transport networks are usually embedded in two- or three-dimensional space. Here, we explore the shape and scaling properties of these spatially embedded complex networks. The work presented we focus on the interplay of spatial embedding and scaling statistics. In particular, complex transport networks of public transport appear to show that spatial and scaling properties within these networks are closely correlated. To support our claim we have analysed a number of public transport networks in a number of large scale conglomerations.

BP 56: Aging in Physical and Biological Systems (focus session, joint DY/BP)
Physical aging is known from a number of complex systems such as spin glasses or materials like polymer glasses, colloids and gels. On the other hand, biological aging refers to the increase in mortality and the associated loss of functions with age that occurs (almost) universally across the kingdoms of life. This focus session aims to confront these different manifestations of aging in order to identify possible conceptual and methodological interrelations between two largely disjoint fields of research. (Organizers J. Krug and H. Meyer-Ortmanns)

Invited Talk
BP 56.1 Fri 9:30 BH-N 334
Demographic perspectives on the evolution of senescence — Annette Baudisch — University of Southern Denmark, Campusvej 55, 5230 Odense M
Senescence, the physiological decline that results in decreasing survival and/or reproduction with age, remains one of the most perplexing topics in biology. Most theories attempting to explain the evolution of senescence (i.e. antagonistic pleiotropy, mutation accumulation, disposable soma) were developed several decades ago. Confronted with empirical patterns of survival and reproduction, predictions of the theories do not hold. New theory is needed to shed light on the determinants of patterns of birth and death. At this point it might be feasible and instructive to broaden perspectives by cutting across disciplinary boundaries and seek for a general theory of determinants of birth and location: BH-N 334

Time: Friday 9:30–12:00

Location: BH-N 334
death patterns, i.e. life course trajectories, pertaining to animate or inanimate objects on any scale of observation.

**Invited Talk**

BP 56.2 Fri 10:00 BH-N 334

Biological mechanisms of aging — BJÖRN SCHUMACHER — CECAD Research Center, University of Cologne The Biology of aging has long been a descriptive research discipline. Only in the past 20 years mechanisms of aging have been uncovered through research in genetic model systems. A number of distinct an interconnected pathways that regulate longevity have been identified. However, the complexity of the aging process remains a challenge to modern aging research. Integration of quantitative data linking the age-dependent accumulation of harmful damage to macromolecules - particularly the genetic material - to the regulation of longevity assurance pathways have begun to unravel a more integrated and complete understanding the biological mechanisms of aging.

**Invited Talk**

BP 56.3 Fri 10:30 BH-N 334

Aging in out-of-equilibrium systems: an overview — JEAN-PHILIPPE BOUCHAUD — Capital Fund Management, 75007 Paris, France Aging is a particular type of out-of-equilibrium dynamics that is observed in a variety of systems, from glassy systems to atomic cooling and blinking dots, etc. I will review several distinct mechanisms that can lead to aging, discuss their theoretical underpinning and their experimental relevance.

**Invited Talk**

BP 56.4 Fri 11:00 BH-N 334

Aging in coarsening systems with non-algebraic growth laws — MICHEL PLEIMLING — Virginia Tech, Blacksburg, VA, USA Physical aging is generically encountered in systems far from equilibrium that evolve with slow dynamics. Well known examples can be found in structural glasses, spin glasses, magnetic systems, and colloids. Recent years have seen major breakthroughs in our understanding of aging processes in non-disordered systems characterized by an algebraic growth of the domains. Progress in understanding aging in systems with more complicated growth laws has been much slower though. After a brief introduction into the phenomenology of aging in simple coarsening systems, I discuss in this talk non-equilibrium relaxation and aging processes in systems characterized by a non-algebraic growth of the ordered domains. Disordered ferromagnets provide interesting examples where the relaxation process is dominated by a slow crossover from an algebraic-like regime at early times to the slower asymptotic growth that prevails for large times. In order to study aging processes deep inside an anomalously slow growth regime we turn to different versions of the ABC model where the biased exchanges of particles of different types yield domains that only grow logarithmically with time.

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BP 56.5 Fri 11:30 BH-N 334

Aging of Classical Oscillators during a Noise-Driven Migration of Oscillator Phases — HIILDEGARD MEYER-ORTMANNS and FLORIN IONITA — Jacobs University Bremen, 28759 Bremen We consider classical nonlinear oscillators like rotators and Kuramoto oscillators on hexagonal lattices of small or intermediate size. When the coupling between the elements is repulsive and the bonds are frustrated, we observe coexisting states, each one with its own basin of attraction. For special lattices sizes the multiplicity of stationary states gets extremely rich. When disorder is introduced into the system by additive or multiplicative Gaussian noise, we observe a noise-driven migration of oscillator phases in a rather rough potential landscape. Upon this migration, a multitude of different escape times from one metastable state to the next is generated. Based on these observations, it does not come as a surprise that the set of oscillators shows physical aging. Physical aging is characterized by nonexponential relaxation after a perturbation, breaking of time-translation invariance, and dynamical scaling. When our system of oscillators is quenched from the regime of a unique fixed point toward the regime of multistable limit-cycle solutions, the autocorrelation functions depend on the waiting time after the quench, so that time translation invariance is broken, and dynamical scaling is observed for a certain range of time scales. It is an open question as to whether physical aging as we have studied here, is also responsible for biological aging in these excitable or oscillatory systems in biological realizations.


BP 56.6 Fri 11:45 BH-N 334

Parametrization and interaction analysis of survival curves — IVAN G. SZENDRO1, RAHUL MARATHI2, YIDONG SHEN3, ADAM ANTEBR1, and JOACHIM KRUG3 — 1Institute for Theoretical Physics, University of Cologne, Germany — 2Department of Physics, IIT Delhi, India — 3Max Planck Institute for Biology of Ageing, Cologne, Germany A key signature of biological aging is the increase of mortality with age. Age-dependent mortality can be extracted from the survival curve, which monitors the surviving fraction of a population of individuals as a function of time. Experiments on longevity-related mutations and interventions in model organisms typically focus on mean life span only, thus neglecting much information contained in the shapes of survival curves. Here we present an exploratory study aimed at parametrizing experimental survival curves obtained for the nematode Caenorhabditis elegans. To this end, we fit survivorship data to models of varying complexity, including the classical Gompertz law as well as models based on reliability theory. We also analyze the multidimensional interactions between different interventions and mutations, using a published data set that contains all combinations of two interventions (dietary restriction and temperature) and two genetic mutations (daf-2 and clk-1).