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Fachverband Biologische Physik (BP)

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Overview of Invited Talks and Sessions

(Lecture Rooms: H 1028 and H 1058; 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** — Coline 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 Mukhortava, Andreas Hartmann, •Michael Schlierf
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 Blanchoin, •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

BP 52.1	Fri	9:30–10:00	H 1028	**Biophysics of light-activated ion transporters** — Arend Vogt, Jonas Wietek, •Peter Hegemann

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 Helmstädter
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 21.1–21.10	Tue	10:15–13:15	MA 001	**Complex Contagion Phenmomena (focus session, joint SOE/DY/BP)**
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 34.1–34.12	Wed	9:30–13:15	H 1028	**Statistical Physics of Biological Systems II (joint BP/DY/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/O)**
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

BP 1: Imaging

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

Invited Talk BP 1.1 Mon 9:30 H 1028

Light sheet-based fluorescence microscopy for quantitative biology — •Ernst 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, observed 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.

BP 1.2 Mon 10:00 H 1028

Reflected light-sheet microscopy reveals single molecules in Drosophila melanogaster embryo — •Ferdinand Greiss[1], Myrto Deligiannaki[2], Christophe Jung[2], Ulrike Gaul[2], and Dieter Braun[1] — [1]System Biophysics, Department of Physics, Ludwig Maximilians University, Amalienstr. 54, 80799 Munich, Germany — [2]Gene Center, Department of Biochemistry, Ludwig Maximilans University, Feodor-Lynen-Str. 25, 81377 Munich, Germany

Searching the growing field of light microscopy for dynamic high resolution imaging in vivo suggests total internal reflection microscopy (TIRF) as one of the most popular candidates. However, TIRF 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.

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 described by Gebhardt et al. (2013) and used it to study the epidermal barrier of Drosophila embryos.

Epidermal cells seal their intermembrane space by septate junctions, which impede free diffusion through the paracellular route. We were able to detect single 10 kDa Alexa647-conjugated Dextran diffusing in and around epidermal tissue. As discovered with ensemble measurements, mutants with disrupted septate junctions exhibit leaky epithelial barrier. We were able to confirm these findings with our optical setup on the single molecule level.

BP 1.3 Mon 10:15 H 1028

Single laser beam photothermal microscopy — •Andre Heber, Markus Selmke, Marco Braun, and Frank Cichos — 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 utilises two different laser beams at distinct wavelengths 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.

BP 1.4 Mon 10:30 H 1028

3D-Refractive Index Measurements of Single Cells by Optical Diffraction Tomography — •Paul Müller[1], Mirjam Schürmann[1], Christoph Faigle[1], Moritz Kreysing[2], and Jochen Guck[1] — [1]Biotechnology Center of the TU Dresden — [2]Max 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.

BP 1.5 Mon 10:45 H 1028

Wide-field fast frame-rate FLIM and simultaneous FCS for applications in molecular biology — •Csongor Keuer[1], Danilo Bronzi[2], Marco Vitali[1], Franco Zappa[2], Cornelia Junghans[1], Thomas Friedrich[1], and Franz-Josef Schmitt[1] — [1]Institute of Chemistry, Bioenergetics, TU Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany — [2]Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy

The application of a 64x32 SPAD-based CMOS image sensor for single molecule spectroscopy is presented. Fluorescence amplitudes and lifetimes are measured simultaneously with correlation of fluorescence singal for each pixel. The system is suitable to spatially resolve diffusion constants and concentrations of single molecules in total internal reflection (TIR) excitation of the sample. An image splitter has been added to simultaneously perform both FLIM and FCS of diffusing fluorophores in aqueous solution in two wavelength or polarization channels. The system is suitable for particle size measurement, fast concentration determination and imaging of molecular dynamic processes.

BP 1.6 Mon 11:00 H 1028

Label-free optical detection of single proteins — •Katharina König, Marek Piliarik, and Vahid 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 interferometric detection of the scattering (iSCAT) from a single protein. By combining this approach with microfluidics and functionalized surfaces, we are able to count single protein binding events and localize their positions with a precision of 5 nm. A wide-field detection arrangement and direct protein imaging capability make the method readily suitable for biomolecular analytics, outperforming previously reported label-free sensing approaches. We will show first emerging applications in ultra sensitive single-cell analysis.

15 min break

BP 1.7 Mon 11:30 H 1028

Helium Ion Microscopy of Biological Cells — •Natalie Frese[1], André Beyer[1], Matthias Schürmann[2], Barbara Kaltschmidt[2],

Christian Kaltschmidt[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, University of Bielefeld, 33615 Bielefeld, Germany — [2]Cell Biology, University of Bielefeld, 33615 Bielefeld, Germany

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.

BP 1.8 Mon 11:45 H 1028

PEEM and SEM of Magnetospirillum magnetotacticum's Magnetosome Chains — •Christoph Keutner[1], Alex von Bohlen[2], Ulf Berges[1], Philipp Espeter[1], Claus M. Schneider[3], and Carsten Westphal[1] — [1]DELTA/Experimentelle Physik I, TU Dortmund, Maria-Goeppert-Mayer-Straße 2, 44221 Dortmund, Germany — [2]ISAS Dortmund, Bunsen-Kirchhoff-Straße 11, 44139 Dortmund, Germany — [3]PGI-6, FZ Jülich, 52425 Jülich, Germany

Magnetotactic bacteria are of great interdisciplinary interest, since a vast field of applications from magnetic recording media to medical nanorobots is conceivable. A key feature for a further understanding is the detailed knowledge about the magnetosome chain within the bacteria.

Here, we present two preparation procedures of Magnetospirillum magnetotacticum suitable for UHV experiments. These allow us to preform photoemission electron microscopy (PEEM) on magnetotactic bacteria, for the first time. We show that PEEM combined with x-ray absorption spectra (XAS) can access the magnetic particles (magentosomes) within intact magnetotactic bacteria.

By combining scanning electron microscopy (SEM) with energy dispersive x-ray spectrometry (EDX), magnetosome chains of intact bacteria become directly visible through the cell envelope. Even single magnetosomes as individual parts of the chains can be imaged.

BP 1.9 Mon 12:00 H 1028

Visualization of subcellular temperature changes in living cells utilizing the nitrogen vacancy center — •Torsten Rendler, Zhiqin Chu, Andrea Zappe, and Joerg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart

For mammals which can maintain thermal homeostasis, temperature is vital to their life. Visualization of temperature change on subcellular organelles in living cells thus give a basic understanding of life science such as cell metabolism, cell division and gene expression. Despite the high impact to life science brought by such measurement, developing a precise and long term reliable thermometer in living cells has not been achieved. Although intracellular temperature gradients in the range of ~ kelveins in living cells have been found, it is still under debate if the existence of such temperature gradients on cellular level is reasonable. In our study, we use the nitrogen vacancy (NV), a color center in diamond, to monitor the temporal and spatial temperature change inside living cells. Embedded in nanometer sized diamond crystals, the NV centers becomes a localized sensor, capable of measuring the local temperature independently of their environment, i.e., pH, ionic strength and surrounding biomacromolecules. Our findings indicated that nanodiamonds with NV centers can serve as a nano-scaled thermometer in cellular thermal biology.

BP 1.10 Mon 12:15 H 1028

Three-dimensional orientation imaging of single fluorescent emitter transition dipoles — •Narain Karedla, Anna Chizhik, Ingo Gregor, Alexey Chizhik, and Jörg Enderlein — 3. Physikalisches Institut, Georg-August-Universität Göttingen

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.

BP 1.11 Mon 12:30 H 1028

High resolution surface charge mapping with a scanning ion-conductance microscope — •Lasse Hyldgaard Klausen, Thomas Fuhs, Flemming Besenbacher, and Mingdong Dong — Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark

Characterising the surface charge density (SCD) is important in interface and colloid science, and especially local variations in SCD of biological samples are of keen interest. The surface charge of lipid bilayers governs the uptake of charged particles and guides cell-cell interactions. As the electrostatic potential is screened by high physiological salt concentrations, direct probing of the potential can only be performed at a sub nanometre distance; therefore it is challenging to measure the local SCD under physiological conditions.

In this study we measure SCD using a scanning ion-conductance microscope (SICM) setup, where the electrolyte current through a nanopipette is monitored as the pipette is positioned in the vicinity of the sample. We investigate the current dependency of SCD and pipette potential using numerical solutions to Poisson and Nernst-Planck equations and characterise a complex system governed by a multitude of factors such as pipette size, geometry and charge. We then propose an imaging method and prove its feasibility by mapping the surface charge density of phase separated lipid bilayers with sub micrometre spatial resolution.

BP 1.12 Mon 12:45 H 1028

Propagation-based phase contrast tomography of neuronal tissues — •Mareike Töpperwien[1], Martin Krenkel[1], Jürgen Goldschmidt[2], and Tim Salditt[1] — [1]Institute for X-Ray Physics, Göttingen, Germany — [2]Leibniz Institute for Neurobiology, Magdeburg, Germany

In order to visualize the 3D native structure of neuronal tissues with cellular and sub-cellular resolution in macroscopically large volumes, hard x-ray tomography offers a unique potential beyond the current capabilities of histology. However, classical x-ray tomography based on absorption gives nearly no contrast for soft biological tissues. In order to visualize also non-absorbing or weakly absorbing structures, the much stronger phase shifts which the sample induces in a (partially) coherent wavefront can be exploited for contrast formation. During free space propagation behind the object, these phase shifts are converted to a measurable intensity image by interference of the disturbed wave fronts. Thus, the original phase distribution has to be reconstructed from the intensity images using suitable phase retrieval algorithms.

As proof-of-concept, in this work we present propagation-based x-ray phase contrast tomography of neuronal tissues. In specially dried samples, sub-cellular resolution in mm sized tissue volumes has been achieved yielding three dimensional renderings which are consistent with classical histology results. We also show that complementing the synchrotron radiation results, a compact laboratory setup with a high brilliance liquid-metal microfocus source can be used.

BP 2: Neurophysics I

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

BP 2.1 Mon 9:30 H 1058

The vertebrate retina as an optical image processor — •Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

The neuronal processing capabilities of the vertebrate retina are increasingly well understood. These processes are thought to be initiated by the detection of light by the photoreceptors as projected by the lens. However, recent findings show that cells inside the light path give rise to fine changes in these projected images prior to the detection event. Using the concept of modulation transfer function analysis, we firstly describe the neuronal retina as a frequency domain, optical image processor. Based on direct measurements we discuss to which extend demodulation of transmitted image frequencies must be understood as the result of simple contrast loss due to scattering. We further analyze transmitted light fields for newly generated image frequencies, and discuss these in relation to the retina's optical architecture and possible benefits for vision under low light conditions.

BP 2.2 Mon 9:45 H 1058

General Anaesthesia: From experiments to theory — •Axel Hutt — 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 microscopic scale of single synapses and the macroscopic scale of electroencephalogram (EEG) and Local Field 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 features in EEG.

BP 2.3 Mon 10:00 H 1058

Up and down states in top-down input may be advantageous to the transmission of information about weak signals — •Felix Droste and Benjamin Lindner — HU Berlin & Bernstein Center for Computational Neuroscience Berlin, Berlin, Germany

How a single neuron transmits information about a sensory stimulus is heavily dependent on the state of the embedding network. This allows higher cortical areas, providing so-called top-down input, to influence the processing of a bottom-up signal. Cortical networks may be in asynchronous-irregular states, where the population firing rate is roughly constant in time. In this case, analytical approaches to signal transmission are well established. However, the firing rate may also be time dependent. It may, for instance, jump between so-called up and down states (observed under anesthesia, during sleep, or quiet wakefulness). While the effect of such input on information transmission has been studied in experiments, theoretical approaches have so far been lacking.

Here, we model up/down input to a leaky integrate-and-fire neuron by dichotomous noise, a simple stochastic two-state process. We derive exact results for the spike train power spectrum and the susceptibility for pure two-state input and expand this to incorporate additional fluctuations around the states, which take into account the shot-noise nature of the input. This allows us to compare signal transmission with an asynchronous-irregular background to that in the presence of up/down state input. We find that if the overall input firing rate is low, up/down states may be beneficial for information transmission.

BP 2.4 Mon 10:15 H 1058

How does addition, deletion, or shifting of spikes by intrinsic noise affect signal transmission in spiking neurons? — •Sergej Voronenko[1,2], Wilhelm Stannat[1,3], and Benjamin Lindner[1,2] — [1]Bernstein Center for Computational Neuroscience, Berlin, Germany — [2]Humboldt University, Berlin, Germany — [3]TU Berlin, Berlin, Germany

We study analytically how different effects of intrinsic noise on the output of a spiking neuron influence signal transmission. To this end, we consider populations of neurons driven by a strong common time-dependent signal, where each neuron is subject to independent intrinsic noise. In this setup the intrinsic noise degrades the transmission of information by single neurons. On the population level, however, the intrinsic noise can lead to enhancement of the information transmission, an effect known as suprathreshold stochastic resonance. The strength and the robustness of the stochastic resonance effect is determined by whether the output spikes of the single neurons are shifted by the intrinsic noise, or whether the intrinsic noise adds and deletes output spikes. Our investigation is one of the first analytical studies of the transmission of information by neurons with highly correlated input.

BP 2.5 Mon 10:30 H 1058

Information filtering by partial synchronous spikes in a neural population — •Alexandra Kruscha — Bernstein Center for Computational Neuroscience, Berlin, 10115, Germany — Institute for Physics, Humboldt-Universität zu Berlin, Berlin, 12489, Germany

Synchronous firing of neurons is a prominent feature in many brain areas. Here, we are interested in the information transmission by the synchronous spiking output of a noisy neuronal population, which receives a common time-dependent sensory stimulus. Experimental and theoretical work revealed that synchronous spikes encode preferentially fast components of the stimulus, i.e. synchrony acts as an information filter. In these studies a rather strict measure of synchrony was used: all neurons in the population have to fire within a short time window. Here, we generalize the definition of the synchronous output, for which only a certain fraction γ of the population has to fire in synchrony. We present an analytical approach to characterize the information transfer in dependence of this fraction and the population size, by deriving the cross-correlation and the coherence function between the stimulus and the partial synchronous output. We show that there is a critical synchrony fraction, namely the probability at which a single neuron spikes within the predefined time window, which maximizes the information transmission of the synchronous output. At this value, the partial synchronous output acts as a low-pass filter, whereas deviations from this critical fraction lead to a more and more pronounced band-pass filtering effect. We confirm our analytical findings by numerical simulations for the leaky integrate-and-fire neuron.

BP 2.6 Mon 10:45 H 1058

Synthetic Neuronal Networks on Glass Using Topological and Chemical Cues — •Andreas Schlegel[1], Aune Koitmäe[1], Paul Gwozdz[1], Jann Harberts[1], Christian Heusinger[1], Gabriele Loers[2], and Robert H. Blick[1] — [1]Center for Hybrid Nanostructures (CHYN) and Institute of Nanostructure and Solid State Physics, University of Hamburg, Germany — [2]Center for Molecular Neurobiology Hamburg, University Medical Center Hamburg-Eppendorf, 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 $\sim 20\,\mu$m) and channels (width $\sim 4\,\mu$m, length $30 - 200\,\mu$m). The distance between the lines varies between 10 and 200 μm. The depth of the structures is $4\,\mu$m. 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.

BP 2.7 Mon 11:00 H 1058

Spatiotemporal imaging of neurotransmitter release using near infrared fluorescent carbon nanotube probes — •Sebastian Kruss — Institut für Physikalische Chemie / Universität Göttingen

Neurotransmitters are central for chemical communication between (neuronal) cells. So far there are no analytical tools available to

spatially detect or image neurotransmitters. Therefore, the chemical events in synapses and neural circuits remain largely unexplored. Optical nanoscaled 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 those 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 cells.

15 min break

BP 2.8 Mon 11:30 H 1058

Probing a quantum mechanical model of olfaction in insects — Marco Paoli[1,2], Elisa Rigosi[1,2], Gianfranco Anfora[3], Giorgio Vallortigara[1], Renzo Antolini[1,4], and •Albrecht Haase[1,4] — [1]Center of Mind/Brain Sciences, University of Trento, Rovereto, Italy — [2]BIOtech center, University of Trento, Trento, Italy — [3]Research and Innovation Centre, Fondazione Edmund Mach, S.Michelle all'Adige, Italy — [4]Department 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 odorants. Here we present first *in vivo* functional imaging experiments in the honeybee brain showing evidence for the bees' ability to distinguish isotopes by smell. A possible correlation of these results with the odorants' vibrational spectra is discussed.

BP 2.9 Mon 11:45 H 1058

Dynamic changes in network synchrony reveal resting-state functional networks — •Vesna Vuksanovic[1,2] and Philipp Hövel[1,2] — [1]Institute für Theoretische Physik, Technische Universität Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Humboldt-Universität zu Berlin, Germany

Experimental studies of the human brain activity at rest i.e. without any overt-directed behavior have revealed patterns of correlated activity, so called resting-state networks. The neural mechanisms contributing to the formation of these networks are largely unknown. We use modeling approach to interpret these experimental findings, looking at the brain as the dynamical system. We characterize brain network dynamical properties by synchrony and variability in synchrony. We demonstrate that functional brain interactions may arise from the network dynamics which allow flexible changes between different network configurations. We show that these changes reflect almost periodic alternations between network synchronized and desynchronized state.

BP 2.10 Mon 12:00 H 1058

Discrimination, correlation and prediction of collective neural responses to natural sounds in the auditory midbrain — •Dominika Lyzwa[1,2] and Michael Herrmann[2] — [1]Dept. Nonlinear Dynamics, MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Perception, Action and Behavior, School of Informatics, University of Edinburgh, U.K.

The main structure in the auditory midbrain, the inferior colliculus (IC) is the central converging station for all sound information and important for processing complex sounds, such as speech. How complex sounds are encoded by groups of neurons across the IC is an open question. In order to better understand the processing of this nucleus, we investigated the separability of multi-unit responses. To explore the spatial extent of the neural representation, we computed noise correlations between neural groups across the IC. 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 while presenting 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-units yielded improved discrimination over an individual unit, but temporal correlations between the units did not improve discrimination. The findings suggest that encoding of vocalizations in the mammalian inferior colliculus is shaped by the input and organization of receptive fields and not by neural interactions within this nucleus.

BP 2.11 Mon 12:15 H 1058

anomalous transport in complex dendrites - geometrical considerations — m reza shaebani, •anne e hafner, and ludger santen — Department of Theoretical Physics, Saarland University, Saarbrucken, Germany

Dendritic spines, which are small membranous protrusions emerging from the dendrites, serve as the main recipients of exitatory inputs in the mammalian brain. The spines undergo dynamic structural changes, which is regulated by neuronal activity and is believed to be a cellular basis of neural functions such as cognition, memory, and learning. The density, morphology, and spatial distribution of spines vary at different cortical areas or due to neurodegenerative diseases or aging. Morphological changes of spines influences the transport characteristics of ions and other molecules in dendrites, since they are 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 morphological properties. Here we analytically study a diffusive motion composed of two 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.

BP 2.12 Mon 12:30 H 1058

The effects of positive interspike interval correlations on neuronal information filtering properties. — •Sven Blankenburg[1,2] and Benjamin Lindner[1,2] — [1]Department of Physics Humboldt University Berlin, Germany — [2]Bernstein 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.

BP 2.13 Mon 12:45 H 1058

Nonlinear population dynamics for finite-size spiking neural networks with adaptation – Non-Gaussian fluctuations and information filtering — •Tilo Schwalger, Moritz Deger, and Wulfram Gerstner — 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 approach 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 mean field theory and a quasi-renewal approximation [1,2], we present 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 information filtering by coupled populations of adapting neurons [2].

References: [1] R. Naud, W. Gerstner, PLoS Comp. Biol. (2012); [2] M. Deger, T. Schwalger, R. Naud, W. Gerstner, Phys. Rev. E (2014)

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

Time: Monday 9:30–12:15 Location: BH-N 243

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 Hebisch, Erwin Frey, and •Madeleine Opitz — Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany

Spreading of species into uncolonized territory is a fundamental ecological process in the evolution and maintenance of biological diversity. Although interactions between species have experimentally been identified as major determinants of species coexistence in spatially extended populations, their role in spatially expanding populations is largely unknown. Here, we address the roles of resource and interference 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 despite 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 initial 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 Ritterskamp and Bernd Blasius — ICBM, University Oldenburg, Germany

Food webs encode feeding interactions of ecological communities, originating from an intricate interplay of evolutionary and ecological processes. This dynamic can be described by evolutionary food web models, 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 dynamics in space.

Here, we go beyond traditional approaches and develop an evolutionary food web model in a two dimensional niche space, where the additional niche axis might describe a spatial coordinate or an environmental variable. Using numerical simulations, we investigate population dynamics, evolutionary behaviour and the emerging community structure in space. The model is able to produce both static and dynamic 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 niche-dimension 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. Allhoff and Barbara Drossel — TU Darmstadt, Germany

We analyze an evolutionary food web model where each species is characterized 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 thus gives insights into how the functional diversity changes during the initial network buildup 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 Hartich, Andre C. Barato, and Udo Seifert — II. Institut für Theoretische Physik, Stuttgart, Germany

We study theoretical models inspired by the *E. coli* sensory network, using the framework of stochastic thermodynamics for bipartite systems [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 conditional Shannon entropy reduction, characterizing the learning of the internal process about the external process, is bound by the thermodynamic entropy production [2]. This approach allows for the definition of an informational efficiency that can be used to study cellular information 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 dissipation inside the cell can only be obtained if the external process compensates for it.

[1] DH, ACB and US, J. Stat. Mech., P02016 (2014)
[2] ACB, DH and US, New J. Phys. **16**, 103024 (2014)

BP 3.5 Mon 10:45 BH-N 243

Tackling your free energy estimates with pyfeat — •Antonia Mey, Christoph Wehmeyer, Fabian Paul, Hao Wu, and Frank Noé — 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 often 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 sampling).

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 simulation. 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 straight forward usability makes comparing different estimation method applied to the same input data trivial.

Generally, any multi-ensemble simulation can be used for the analysis ranging from all-atom protein molecular dynamics simulations to simulations of condensed matter systems. Pyfeat is available for download 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 curvature — •Sina Sadeghi, 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

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.

BP 3.7 Mon 11:30 BH-N 243

DNA denaturation transition: environmental effects on scaling — •Christian von Ferber[1] and Yurij Holovatch[2] — [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.

BP 3.8 Mon 11:45 BH-N 243

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 thermodynamics 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 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.

Using a 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

BP 3.9 Mon 12:00 BH-N 243

Simple association-dissociation-aging process: recursive solution — •Thomas Niedermayer 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 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.

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

Time: Monday 9:30–12:45 Location: C 130

BP 4.1 Mon 9:30 C 130

Disclination lines at homogeneous and heterogeneous colloids immersed in a chiral liquid crystal — •Sergej Schlotthauer[1], Michael Melle[1], Carol K. Hall[2], Enrique Diaz-Herrera[3], and Martin Scheon[1,2] — [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 colloid in a choleteric 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 colloid relative to the cholesteric helix.

BP 4.2 Mon 9:45 C 130

Anisometry versus anisotropy in systems of colloidal magnetic cubes — •Joe Donaldson[1] and Sofia Kantorovich[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Ural Federal University, Lenin av. 51, 620083, Ekaterinburg, Russia

Contemporary colloid 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] orientated 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.

BP 4.3 Mon 10:00 C 130

Active microrheology of a nematic Liquid crystal — •Tillmann Stieger[1], Andrés Córdoba[2], Marco G. Mazza[3], Juan J. de Pablo[2], and Martin Schoen[1] — [1]Technische Universität Berlin — [2]University of Chicago — [3]MPIDS Göttingen

The knowledge of rheological properties of soft matter is of great importance for a variety of applications such as lubricants or the reduction of friction. The rheology of materials becomes particularly relevant if systems are miniaturized to the nanometer length scale at which physical properties of soft matter are altered significantly from their microscopic bulk properties. The focus of this work are 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.

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 faiencerie, L1511 Luxemburg

I present computational results on the compression of a hard sphere liquid into the solid phase in finite time.
I will discuss the properties 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[1,2], Fangfang Chu[1,2], Matthias Ballauff[1,2], and Joachim Dzubiella[1,2] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Humboldt-Universität zu 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[1], Markus Franke[2], Thomas Palberg[3], and •Hans Joachim Schöpe[4] — [1]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [2]DB Systel GmbH, Weilburger Straße 22 B4.14, 60326 Frankfurt a. Main — [3]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — [4]Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

Metastable fluids exhibit heterogeneous dynamics as well as heterogeneous structure [1]. These dynamical and structural heterogeneities play an important role in the understanding of the glass transition and crystallization. Simulations suggest that these heterogeneities in dynamics and structure are linked, but the direct experimental proof is still lacking [2]. Using space- and time-resolved dynamic light scattering and time-resolved multi angle static light scattering [3], we study the dynamics and structure in a model system of colloidal hard spheres during crystallization and vitrification. For the first time, direct correlation between the temporal evolution of the dynamical heterogeneities and the structural heterogeneities was obtained from an analysis of the subensemble resolved particle dynamics and the evolution of the static structure factor.

[1] L. Berthier and G. Biroli, Rev.s of Mod. Phys., 83, (2011,[2] T. Kawasaki and H. Tanaka, JPCM, 22 (2010),[3] M. Franke, S. Golde and H.J. Schöpe, Soft Matter 10, 5380 (2014)

15 min. break

BP 4.7 Mon 11:15 C 130

Dense Colloidal Suspensions in Microfluidic Flow — •Philipp Kanehl and Holger 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 collision 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.

[1] D. Semwogererea and E. R. Weeks, Phys. Fluids, 20, (2008).
[2] A. I. Campbell and M. D. Haw, Soft Matter 6, (2010).

BP 4.8 Mon 11:30 C 130

Rheological study of anisometric pigment particle suspensions — •Yong Geng, Alexey Eremin, and Ralf Stannarius — Otto-von-Guericke-Universität Magdeburg, FNW/IEP/ANP, Postfach 4120, 39016 Magdeburg, 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.

1. Eremin, Alexey, et al., Adv. Funct. Materials 21.3 (2011): 556-564.

BP 4.9 Mon 11:45 C 130

Structure analysis of stable and metastable hard sphere fluids by confocal microscopy — Achim Lederer[1] and •Hans Joachim Schöpe[2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudingerweg 7, 55128 Mainz, Germany — [2]Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

The structural properties of the metastable melt play a key role in the understanding of the glass transition and crystal nucleation. Using laser scanning confocal microscopy we study the structure of stable and metastable colloidal hard sphere fluids. The used system was characterized with extreme care to allow a meaningful comparison with theory and simulation. While the Percus-Yevick (PY) approximation works quite perfectly for stable fluids at moderate volume fractions, it starts to fail for volume fractions larger than 0.45 approaching the freezing transition at 0.494. Strong deviation can be observed in metastable fluids: In the pair correlation function g(r) the experimental data display a significant higher principal peak and a different shape in the higher order peaks than the PY-approximation. In the static structure factor S(q) the data display a split in the second structure factor maximum suggesting a local short range crystalline like order. An analysis on the particle level reveals the existence of clusters with higher bond orientation order (q6(i)q6*(j)), although the overall hexagonal order of the ensemble does not increase.

BP 4.10 Mon 12:00 C 130

Effects of shear and walls on the diffusion of colloids in microchannels — •somnath ghosh, frieder mugele, and michel duits — Physics of Complex Fluids group, MESA+ institute, University of Twente PO Box 217, 7500 AE Enschede, The Netherlands

Colloidal suspensions flowing through micro-channels were studied for the effects of both shear flow and the proximity of walls on the particles* self-diffusion. Use of hydrostatic pressure to pump micron-sized silica spheres dispersed in water-glycerol through poly (dimethylsiloxane) channels with a cross section of 30x24 micron, allowed variation

of the Péclet number(Pé) 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 Pé>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 Wirner[1], Christian Scholz[1], and •Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

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

Isobutyric 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 isobutyric 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 seperation of water and isobutyric 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.

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

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

BP 5.1 Mon 9:30 C 243

Iron Oxide Nancube Monolayers at the Air/Water Interface: Self-Organization on Nano- and Mikroscale — •Heiko Ahrens[1], Sarah Mehdizadeh Taheri[2], Thomas Ortmann[1], Andreas Gröning[1], Stephan Förster[2], and Christiane A. Helm[1] — [1]Physik, Uni Greifswald, 17487 Greifswald, Germany — [2]Physikalische Chemie I, Uni Bayreuth, 95440 Bayreuth, Germany

Monodisperse Cubic Iron Oxide nano particles (5-8 nm) covered in oleic acid form stable films on the air water interface. Isotherms exhibit a plateau at 18 - 20 mN/m, then the pressure increases steeply. At zero surface pressure, Brewster angle microscopy(BAM)shows micrometer sized domains consisting of nanocubes immersed in a matrix of excess oleic acid. These small domains show Brownian motion. Then linear and mesh-like rigid domains (size 100 *m) are observed. The 5.5nm nanocubes form a homogenous monolayer in the plateau region, on further pressure increase large (100 *m) homogenous domains of bi- and even multilayer appear. The films of the larger 8 nm nanocubes remain heterogeneous at all surface pressures. Large (100 *m) patches of oleic acid monolayers coexist with medium sized (50*m) domains of particle monolayer and small domains (10 *m) of bi- and multilayers. All aggregation is irreversible.

These observations are confirmed by X-ray reflectivity and Grazing Incidence X-ray diffraction.

BP 5.2 Mon 9:45 C 243

ZnO nanoparticle stabilization - How much is necessary? — •Torben Schindler[1], Tilo Schmutzler[1], Wei Lin[2], Doris Segets[2], Wolfgang Peukert[2], and Tobias Unruh[1] — [1]Lehrstuhl für Kristallographie und Strukturphysik, Friedrich-Alexander-Universität Erlangen Nürnberg, Staudtstr. 3, 91058 Erlangen — [2]Lehrstuhl für Feststoff- und Grenzflächenverfahrenstechnik, Friedrich-Alexander-Universität Erlangen Nürnberg, Cauerstr. 4, 91058 Erlangen

The stabilization of small nanoparticles is of highest importance for their use in different applications. For these applications the stabilizer used in the synthesis is often exchanged by different species which offer the possibility of e.g. light harvesting for solar cells. However, the amount of stabilizer needed in the first place was seldomly addressed in the literature. In the case of solution processed ZnO nanoparticles acetate is often used as primary stabilizer. However, by washing of the samples it was observed that the nanoparticles become unstable and show strong agglomeration after three washing cycles. We investigated the changes in the stabilizing acetate layer by the combination of small angle X-ray and neutron scattering (SAXS&SANS). Initially the shell incorporates about 10% of the total acetate. This factor is clearly reduced in the washed samples which show still stability against agglomeration. Thus only a small amount of acetate is actually needed to stabilize the nanoparticles. In addition to these results the effect of first ligand exchange reactions using different amounts of catechol will be presented.

BP 5.3 Mon 10:00 C 243

A Toolbox to Connect the Physicochemical Properties of GNPs 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, e.g. surface charge.

To circumvent these problems, we present a toolbox of GNPs with a defined protein corona.[1,2] This defined protein corona enables the GNPs to meet the first requirement for biological applications: high colloidal stability in the presence of salt, other proteins and over a large range of pH values. A toolbox of more than 10 proteins and different purification procedures allow the exceptional chance of tailoring the physicochemical properties of nanoparticles, such as surface charge, colloidal stability and responsiveness.

1Chanana, M.; Correa-Duarte, M. A.; Liz-Marzan, L. M., Small 2011, 7 (18), 2650-2660.

2Chanana, M.; Gil, P. R.; Correa-Duarte, M. A.; Liz-Marzan, L. M.; Parak, W. J., Angewandte Chemie-International Edition 2013, 52 (15), 4179-4183.

BP 5.4 Mon 10:15 C 243

Electrochemical growth of ZnO nanostructures for biosensing applications — •Raluca - Ancuta Suciu, Nivedita Yumnam, and 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 nanorods grown via electrochemical deposition on Au covered flexible PET (polyethylene terepthalate) substrate. The size and distance of ZnO nanostructures can be effectively controlled by tuning the electrochemical deposition parameters. Furthermore, self-assembled monolayer (SAM) of 1-octadecanethiol has been applied on Au to tune the nucleation density of ZnO. Application of SAM prevents overly dense growth of ZnO and instead allows ZnO to electrochemically grow through the pinholes in the SAM. To realize a capacitive sensor ad-

ditional Au finger contacts have been fabricated using optical lithography. The sensor operation is verified by detection of Streptavidine biomolecules.

BP 5.5 Mon 10:30 C 243

In situ Study of Spray-deposited Gold Nanoparticles Assemblies on Polymer Substrates Using GISAXS — •Peng Zhang[1], Koyiloth v. Sarathlal[1], Santoro Gonzalo[1], Nipam Shah[2], Guangsu Huang[3], and Stephan v. Roth[1] — [1]Deutsches Elektronen Synchrotron, Notkestr. 85,22607 Hamburg — [2]Fachbereichs Maschinenbau und Wirtschaft, Fachhochschule Lübeck, 23562 Lübeck — [3]College of Polymer Science and Engineering, State Key Laboratory of Polymer Materials Engineering, Sichuan University, Chengdu 610065, China

The assembly of the nanoparticles from the solution still remains challenging, namely inhomogeneous material dispersion for example, coffee-stain-like or clumps of particles is observed1. To get designed nanocomposite in thin films, controlling the solution evaporation and promoting the ordering of nanoparticles on the templated substrates is a smart and feasible choice. Spray deposition is one of the desirable techniques to manipulate solvent evaporation by atomizing the solution2,3. Here we present our recent in situ studies on the directed assembly of spray deposited gold nanoparticles on patterned substrates. By manipulating the assembly process, we find that the well-ordered gold nanoparticles show enhanced optical properties. These findings are attractive for the applications such as solar cells and antireflection coating. [1] Yunker et al. Nature 476, 308 (2011); [2] Al-Hussein et al. Langmuir 29, 2490 (2013); [3]Herzog et al. Langmuir 29, 11260 (2013).

Invited Talk BP 5.6 Mon 10:45 C 243

Functional Nanocomposites: Disordered media with a cooperative macroscopic action — •Mady Elbahri — Nanochemistry and Nanoengineering, Institute for Materials Science,Faculty of Engineering, Christian-Albrechts-University Kiel, Germany

So far, research on polymer based nanocomposites mostly centered on structural composites where little attempt was made to precisely control the nanostructure. During the last years, however, there has been increasing interest in functional nanocomposites due to novel applications ranging from sensors and plasmonics through stretchable electronics and smart coatings to energy conversion and human health. In this context the concept of a disordered "glassy" nanocomposite with a cooperative macroscopic action has not been suggested so far. The present talk aims at introducing a particularly promising new class of functional optical materials based on closely spaced ultrafine nanoparticles acting as "artificial molecules" embedded in a polymeric host where the unique properties arise from the strong and cooperative near field coupling between neighbouring nanoparticles. This gives rise to coherent cooperative action thus determining the macroscopic properties.

15 min. break

BP 5.7 Mon 11:30 C 243

Self-assembly of nanoparticles in block copolymer nanotemplates — •Manfred Stamm[1,2], Andreij Horechyy[1], and Bhandu Nandan[3] — [1]Leibniz-Institut für Polymerforschung Dresden — [2]Technische Universität Dresden — [3]Indian Institute of Technology, Delhi

Nanotemplates generated by microphase segregation of diblock copolymers can be used for directed self-assembly of nanoparticles. There are several routes possible where functional nanoparticles are either added to the copolymer solution prior to film formation and then preferentially migrate to one of the phases or where the nanoparticles are added after copolymer nanotemplate formation and then show preferential adsorption to one of the phases. In both cases ordered nanoparticle arrays are obtained and by combination of the two approaches dual structures /1/ may be formed. With hexagonal structures and removal of the majority phase, nanorods are generated /2/. Under certain conditions helical arrangements of nanoparticles inside the cylinders are observed /3/ which are due to dense packing in confined geometry. Copolymer nanotemplates thus provide an interesting tool for generation of ordered nanoparticle structures. We acknowledge funding by DFG. /1/ Adv.Fun.Mater. 23 (2013) 483-90; /2/ J.Mater.Chem. 22 (2012) 25102-7; /3/ Angew. Chem. Int. Ed. 53 (2014) 1-5.

BP 5.8 Mon 11:45 C 243

Insulin capped gold nanoparticles-polymer brush composites — •Muriel Rovira Esteva, Zuleyha Yenice, Stephanie Christau, Stefan Wellert, and Regine von Klitzing — Stranski Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, 10623 Berlin, Germany

Polymer brushes are polymers grafted to a surface by one end, with a density high enough to induce the polymer chains to 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 affect the behavior of the composite is of high scientific and technological significance.

Gold nanoparticles capped with sodium citrate are often used in these composites, but they pose a series of instability problems. In this work, monodisperse gold nanoparticles with sodium citrate and tannic acid cappings were synthesized, and their capping was replaced by insulin, adapting a method by M. Chanana et al. The higher stability against strong pH variations of the insulin capped particles was confirmed with UV-Vis. Incorporation of particles with different cappings into brushes with different geometries allowed to obtain a variety of polymer brush-gold nanoparticle composites, and the effect of the geometrical parameters on the brush-nanoparticle interactions was then explored using a number of techniques, such as AFM and reflectometry.

BP 5.9 Mon 12:00 C 243

Drug delivery to cancer cells by nanodiamonds — •Anna Ermakova[1], Yuzhou Wu[2], Boris Naydenov[1], Tanja Weil[2], and Fedor Jelezko[1] — [1]Institute of Quantum Optics, University Ulm, Ulm, Germany — [2]Institute 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 precise drug delivery to cancer cells with the exception 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.Siegel et al,CA Cancer J Clin,63(2013) [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)

BP 5.10 Mon 12:15 C 243

Metal nanopattering using block copolymers: Differences between ionic and atomic metal selectivity — •Ezzeldin Metwalli[1], Yuan Yao[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg

Metal nano-patterns with a particular structural symmetry, characteristic length scale and periodicity are of growing interest, e.g. for photonic applications and high-density memory devices. The characteristic metal affinity towards the minority block of the self-assembled block copolymer (BC) templates plays an essential role to fabricate highly-order and well-defined metal nanopatterns [1]. Though, ions of metal are highly selective towards the ionic polymer block, the metal atoms show an opposite behavior, an extreme selectivity towards the neutral block. A simple explanation based on like-dissolves-like is ruled out. Experiments are performed by depositing gold in its atomic state on several homopolymer and block copolymer films with DC magnetron sputtering. At time resolution of 15 milliseconds, the nucleation/growth kinetics of gold nanoparticles on the polymer films is monitored using in-situ GISAXS. An extreme selectivity of the metal

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 — •Martin 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 Polysorbate 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[1], Henrich Frielinghaus[1], Zhenyu Di[1], Marie-Sousai Appavou[1], Alessandra Luchini[2], Luigi Paduano[2], Alice Klapper[3], Oleg Petracic[3], Peter Müller-Buschbaum[4], and Dieter Richter[1] — [1]JCNS@FRMII, Lichtenbergstrasse 1, 85747 Garching — [2]University of Naples, Federico II, Dipartimento di Scienze Chimiche, Via Cinthia, 80126 Naples,Italy — [3]JCNS-2, Forschungszentrum Jülich GmbH, 52425 Jülich — [4]TU 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 Location: MA 001

BP 6.1 Mon 12:15 MA 001

How mutational networks shape evolutionary processes — •Henning Siemen, 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[1], Theo Geisel[2], and Frank Stollmeier[2] — [1]ETH Zurich — [2]MPI 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 imbalanced 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-Wiebke Harder[1,2] and Jens Christian Claussen[2,1] — [1]Institut für Neuro- und Bioinformatik, Universität zu Lübeck — [2]Computational 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.

[1] C. Kamp PLoS Comput Biol 6 e1000984 (2010)
[2] M. Müller-Linow, C. Marr, M.-T. Hütt, Phys. Rev. E 74 026112 (2006)
[3] J.C. Claussen, J. Math. Phys. 49 062701 (2009)
[4] J. Nagler and J.C. Claussen Phys. Rev. E 71 067103 (2005)
[5] J.C. Claussen, in: Online Encyclopedia of Integer Sequences, entries http://oeis.org/A138276 and http://oeis.org/A138277 (2008)

BP 6.4 Mon 13:00 MA 001

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

Coupling 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.

BP 7: Superresolution Optical Microscopy (focus session)

Time: Monday 14:30–17:15 Location: H 1028

Invited Talk BP 7.1 Mon 14:30 H 1028

Super-resolution imaging of small, fast moving cellular structures — •Alexander Rohrbach — Lab for Bio- and Nano-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 biophysical transport processes at the periphery of macrophages. 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 Schoen[1], Susanna Früh[1], Jonas Ries[2], and Viola Vogel[1] — [1]ETH Zurich, Zurich, Switzerland — [2]European 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-termini 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 Cremer[1,2,3], Aleksander Szczurek[1], Hyun Keun Lee[1,3], Kirti Prakash[1,2], and Udo Birk[1,3] — [1]Institute of Molecular Biology (IMB), D-55128 Mainz/Germany — [2]Institute for Pharmacy and Molecular Biotechnology (IPMB), University Heidelberg & Kirchhoff-Institute for Physics (KIP), D-69120 Heidelberg/Germany — [3]Department 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-limit*). 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).

BP 7.4 Mon 15:30 H 1028

Recent Advances in Pattern Matching based Multi-Species FLIM Analysis — •Felix Koberling[1], Benedikt Krämer[1], Thomas Niehörster[2], Anna Löschberger[2], Marcelle König[1], Paja Reisch[1], Matthias Patting[1], Ingo Gregor[3], Markus Sauer[2], and Rainer Erdmann[1] — [1]PicoQuant GmbH, Rudower Chaussee 29, 12489 Berlin, Germany, info@picoquant.com — [2]Julius-Maximilians-University Wuerzburg, Germany, Department of Biotechnology & Biophysics, Am Hubland, 97074 Wuerzburg, Germany — [3]Georg-August-University Göttingen, 3rd Institute of Physics, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

A pattern matching based fluorescence decay analysis is a successful alternative to multi-exponential decay fitting and to the phasor analysis approach. We describe the complex single pixel decay with a linear combination of reference decays (patterns) and calculate analytically the individual amplitudes for the reference patterns followed by a re-iteration with MLE fitting. This procedure is now further accelerated by a purely analytical vector projection based method. We will compare the different approaches for multi-species FLIM analysis and present latest application examples also combining spectral and lifetime information for a multidimensional fluorescence pattern analysis.

15 min break

BP 7.5 Mon 16:00 H 1028

Superresolution with Transient Binding: Getting all the Photons — •Philip Tinnefeld — Institut für Physikalische & Theoretische Chemie, TU Braunschweig, Germany

The resolution of localization based superresolution microscopy is intricately connected to the number of photons detected from a single molecule per localization event. We developed DNA PAINT, a super-resolution technique with single-molecule switching induced by transient binding of a short labeled oligonucleotide to structures labeled with a complementary nucleic acid strand. Because no photophysical dark-states are involved, the maximum number of photons can be extracted from each fluorescent dye. With DNA PAINT, we resolved two distinct locations (docking strands) at a distance of 6 nm on DNA origami nanostructures. Besides resolution, DNA PAINT offers exquisite multiplexing capabilities without inducing chromatic aberrations. Just by using different sequences, different structures can be imaged. As the number of detectable photons is ultimately connected to the photostability of fluorescent dyes we will also present a new single-protectant mechanism that represents an advancement over the established ROXS-concept for photostabilization and blinking.

BP 7.6 Mon 16:15 H 1028

Optical nanoscopy with self-healing fluorophores — Jasper H. M. van der Velde, Jingyi Huang, Andreas Herrmann, and •Thorben Cordes — Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands

Customized buffer cocktails are so far the method of choice to facilitate photoswitching and to enhance signal stability for various implementations of optical super-resolution microscopy - a strategy that is not applicable for live-cell imaging.

In this contribution, we tested organic fluorophores with intramolecular photostabilization in STED-type microscopy to improve spatial and temporal resolution without using buffer additives. To obtain fluorophore-photostabilizer conjugates we use a recently published synthesis strategy based on unnatural amino acids. We explored the photostability and achievable spatial resolution of single ATTO647N-labelled oligonucleotides in STED imaging. We further tested KK114-conjugates for antibody labelling and STED imaging of the nuclear pore complex with the aim to increase the number of possible subsequent STED images. Finally, KK114-, Bodipy-Fl, and RhodamineB-derivatives were tested in STED-FCS. Our results show that intramolecular photostabilization is a simple and effective method to increase the photostability of dyes used for STED to achieve high spatial and temporal resolution. Strikingly, ATTO647N-photostabilizer conjugates allowed to generate single-molecule fluorescent time traces with excitation and STED-laser turned on, something that could so

far not be achieved with standard fluorophores.

BP 7.7 Mon 16:30 H 1028

Cryo-Fluorescence Microscopy of Single Molecules — •Weixing Li, Simon Stein, Ingo Gregor, and Joerg Enderlein — DPI, Georg-August-University Goettingen, Germany

The super-resolution fluorescence localization microscopy methods such as Stochastic Optical Reconstruction Microscopy (STORM), Photoactivation Localization Microscopy (PALM), or Ground State Depletion Imaging (GSDIM), routinely achieve a lateral image resolution of ~ 30 nm. This resolution is directly related to the number of photons emitted from a single fluorescent molecule and roughly scales with the invers 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.

BP 7.8 Mon 16:45 H 1028

Optimizing STED Performance — •Marcelle Koenig, Rhys Dowler, Benedikt Kraemer, Felix Koberling, Sebastian Tannert, Matthias Patting, and Rainer Erdmann — PicoQuant GmbH, Rudower Chaussee 29, 12489 Berlin, Germany, info@picoquant.com

Stimulated Emisson Depletion (STED) microscopy is becoming a standard technique in biological imaging, reaching an optical resolution far below 100*nm. The improvement in optical resolution can be achieved with different optical tools and data acquisition, as well as data processing workflows. These have a significant influence not only on the optical resolution itself but also on the general applicability of the technique for specific labels, specimen and phenomena to be studied. We present results based on a confocal microscope which was upgraded with an EASYDOnut phaseplate to convert the STED laser beam into the required donut-shaped focal spot while leaving the co-aligned excitation beam unaffected [1]. On the way towards suitable imaging conditions, various experimental modalities to minimize irreversible photobleaching and to improve photon statistics will be discussed. Different analysis methods based upon the arrival times of photons have also been compared in order to sharpen the images and to suppress unwanted contributions in addition to spectral filtering. Multilabel STED with only one depletion wavelength can be achieved by employing spectral as well as temporal information which act as a fingerprint for individual dyes. Pattern Matching analysis allows for a fast and simple separation of the different fluorescent labels.

BP 7.9 Mon 17:00 H 1028

A Scanning Cavity Microscope — •Matthias Mader[1,2], Jakob Reichel[3], Theodor W. Hänsch[1,2], and David Hunger[1,2] — [1]Ludiwgs-Maximilans-Universität München, Fakultät für Physik, Schellingstraße 4, 80799 München — [2]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching — [3]Laboratoire Kastler Brossel, ENS/UPMC-Paris 6/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 microcavity 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 nm^2, 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].

[1] D. Hunger, T. Steinmetz, Y. Colombe, C. Deutsch, T. W. Hänsch and J. Reichel, New J. Phys. 12, pp. 065038 (2010)

[2] M. Mader, J. Reichel, T. W. Hänsch and D. Hunger, arXiv preprint arXiv:1411.7180 (2014)

BP 8: Neurophysics II

Time: Monday 14:30–17:00 Location: H 1058

BP 8.1 Mon 14:30 H 1058

Born to be critical: Spontaneous activity in early cortex and its role in shaping sensory representations — •Bettina Hein[1], Klaus Neuschwander[1], David E. Whitney[2], Gordon B. Smith[2], David Fitzpatrick[2], and Matthias Kaschube[1] — [1]Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany — [2]Max 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 a single trial basis in chronic recordings 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 organization of the orientation preference map, several days prior to the time when this map was evoked by visual stimulation. We conclude that early spontaneous activity patterns exhibit a rich dynamics and an orderly columnar structure that forms the basis for building sensory evoked representations during cortical development.

BP 8.2 Mon 14:45 H 1058

Input spike trains suppress chaos in balanced target circuits — •Rainer Engelken, Michael Monteforte, and Fred Wolf — MPI for Dynamics and Self-Organization, Bernstein Center for Comp. Neurosc., Göottingen, Germany

A longstanding hypothesis claims that structured input in neural circuits enhances reliability of spiking responses. While studies in single neurons well support this hypothesis [Mainen, Sejnowski 1995] the impact of input structure on the dynamics of recurrent networks is not well understood. Studies in rate chaotic networks suggest a suppression of chaos by structured input [Molgedey 1992], but in spiking input, this has not yet been thoroughly analyzed. Previous studies of the dynamic stability of the balanced state used a constant external input [v.Vreeswijk 1996; Monteforte 2010] or white noise [Lajoie 2013, 2014].

We generalize the analysis of dynamical stability for balanced networks driven by input spike trains. An analytical expression for the Jacobian enables us to calculate the full Lyapunov spectrum. We solved the dynamics in numerically exact event-based simulations and calculated Lyapunov spectra, entropy production rate and attractor dimension. We examined the transition from constant to stochastic input in various scenarios.We find a suppression of chaos by input spike trains. We also find that both independent bursty input spike trains and common input more strongly reduces chaos in spiking networks. Our study extends studies of chaotic rate models [Molgedey et al. 1992] to spiking neuron models and opens a novel avenue to study the role of sensory streams in shaping the dynamics of large networks.

BP 8.3 Mon 15:00 H 1058

A Frequency-resolved Mutual Information Rate — •Davide Bernardi[1,2] and Benjamin Lindner[1,2] — [1]Bernstein Center for Computational Neuroscience, Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik

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 juxtacellular stimulation — Experiment and theory — •Jens Doose[1,2], Guy Doron[1,2], Michael Brecht[1,2], and Benjamin Lindner[1,2] — [1]Bernstein Center for Computational Neuroscience — [2]Humboldt University of Berlin, 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 for reproducing spike times of pyramidal cells under noisy current stimulation in vitro.

BP 8.5 Mon 15:30 H 1058

Synaptic unreliability facilitates information transmission in balanced cortical populations — •Leon A. Gatys[1], Alexander S. Ecker[1], Tatjana Tchumatchenko[2], and Matthias Bethge[1] — [1]Centre for Integrative Neuroscience and Institute for Theoretical Physics, Tuebingen, Germany — [2]Max 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 central question how neural systems can afford 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 Fromme[1], Andreas Neef[2,3], and Christoph F. Schmidt[1] — [1]Faculty for Physics, George August University, Goettingen, Germany — [2]Bernstein Center for Computational Neuroscience, Goettingen, Germany — [3]MPI for Dynamics and Self-Organization, Goettingen, 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 Levina[1,2,3], Theo Geisel[1,3], and Viola Priesemann[1,3] — [1]BCCN Göttingen, Germany — [2]MPI MIS, Leipzig, Germany — [3]MPI 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. When testing 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 Wilting[1], Theo Geisel[1,2], and Viola Priesemann[1,2] — [1]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]BCCN, 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 ϵ , 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 ϵ 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 to infer ϵ fail, we have developed a novel approach based on the autocorrelation function that for the first time allows to robustly infer ϵ even under subsampling. Importantly, our method generalizes to autoregressive processes with both additive and multiplicative noise, making it widely applicable. We demonstrate that our method correctly estimates ϵ 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 ($\epsilon = 0.95$)

BP 8.9 Mon 16:45 H 1058

Self-consistent spectra in recurrent spiking networks — •Stefan Wieland[1,2] and Benjamin Lindner[1,2] — [1]Bernstein Center for Computational Neuroscience Berlin, Germany — [2]Humboldt 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: Biomaterials and Biopolymers I (joint BP/CPP)

Time: Monday 14:30–17:15 Location: EB 202

BP 9.1 Mon 14:30 EB 202

Determination of Conformational Entropy of Fully and Partially Folded Conformations of Holo- and Apomyoglobin — •Andreas Stadler[1], Marek Koza[2], and Jörg Fitter[3,4] — [1]Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Institut Laue-Langevin, CS 20156, 38042 Grenoble, France — [3]Institute of Complex Systems (ICS-5): Molecular Biophysics, Forschungszentrum Jülich GmbH, 52425 Jülich — [4]I. Physikalisches Institut (IA), AG Biophysik, RWTH Aachen, Sommerfeldstrasse 14, 52074 Aachen

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 ΔSconf 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 ΔS obtained from thermodynamic parameters. The observed difference between ΔS and ΔSconf was attributed to the entropy difference ΔShydr 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 Gensler[1], Christian Eidamshaus[2], Arthur Galstyan[2], Ernst-Walter Knapp[2], Hans-Ulrich Reissig[2], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt-Universität zu Berlin — [2]Institute 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 off-rates. The 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 into 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 — Lukas Galla[1], •Andreas J. Meyer[1], Andre Spiering[1], Andy Sischka[1], Michael Mayer[2], Adam R. Hall[3], Peter Reimann[1], and Dario Anselmetti[1] — [1]University of Bielefeld, Germany — [2]University of Michigan, USA — [3]Wake 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.

[1] L. Galla, A. J. Meyer, A. Spiering, A. Sischka, M. Mayer, A. R. Hall, P. Reimann, and D. Anselmetti (2014). Hydrodynamic slip on DNA observed by optical tweezers-controlled translocation experiments with solid-state and lipid-coated nanopores. Nano Letters, 14(7), 4176-4182.

BP 9.5 Mon 15:30 EB 202

How to escape the maze — •Teresa Behl[1], Felix Höfling[2], and Thomas Franosch[3] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität, München — [2]Max Planck Institute for Intelligent Systems, Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart — [3]Institut 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.

15 min break

BP 9.6 Mon 16:00 EB 202

Theory on linear viscoelasticity of a cytoskeletal network — •Tetsuya Hiraiwa and Roland 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 a 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 Schuldt[1,2], Jessica Lorenz[2], Jörg Schnauss[1], Tina Händler[1], Martin Glaser[1], Josef A. Käs[1], and David M. Smith[2] — [1]University of Leipzig, Soft Matter Physics Division, Leipzig, Germany — [2]Fraunhofer 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 emplyoing 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 Helbing[1], Robert Schulze[1], Dominik Hering[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science (CMS), Otto-Schott-Institute of Materials Research (OSIM), Friedrich Schiller University Jena, Jena, Germany — [2]Clemenshospital Münster, Münster, Germany

The biological performance of materials is mostly determined by protein adsorption at the biomaterials surface. Nanostructured surfaces 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 αC-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 Lutz[1], Vance Jaeger[2], Jim Pfaendtner[2], Mischa Bonn[1], and Tobias Weidner[1] — [1]Max-Planck-Institute for Polymer Science, Mainz — [2]University 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 simulation techniques 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. — Jean-Baptiste Forien[1], •Claudia Fleck[2], Peter Fratzl[3], and Paul Zaslansky[1] — [1]Julius Wolff Institut, Berlin, Germany — [2]Technical University, Berlin, Germany — [3]Max 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 orientated 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 Location: C 130

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 — •Sebastian 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 Israelachvilli: $f(x)=-A*e^{(-x/\xi)}*\cos(2\pi(x-\Delta x)/\lambda)$, with f the force as a function of x, the separation. The Amplitude A describes the strength of the particle interaction, the decay length ξ is a measure of how fast the order decays and the wavelength λ 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

deviations in A, λ and ξ 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 Fery — Physical Chemistry II, University of Bayreuth, 95447, Germany

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.

[1] C. Hanske et al., Langmuir, 2012, 28, 16745-16750. [2] C. Hanske et al., Nano Letters, 2014, DOI:10.1021/nl502776s. [3] M. Tebbe et al., submitted.

BP 10.4 Mon 15:45 C 130

Linking intermolecular interactions, microstructure, and macroscopic rheology in protein suspensions — •Alessio Zaccone[1], Miriam Siebenbürger[2], Henning Winter[3], Frank Schreiber[4], and Matthias Ballauff[2] — [1]Physics-Department, Technische Universität München — [2]Helmholtz-Zentrum Berlin für Materialien und Energie — [3]University of Massachusetts Amherst — [4]Applied 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 Philipp[1], Ralitsa Aleksandrova[2], Ulrich Müller[2], Jan K. Krüger[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — [2]Université du Luxembourg, LPM, Luxembourg, Luxembourg

The phase separation of thermo-responsive solutions is known to strongly affect the volume expansion behaviour and the elastic properties, being directly coupled to the macroscopic order parameter [1-3]. On the molecular scale, massive changes in H-bond and hydrophobic interactions, and in structure govern the demixing process. However, the relationship between the molecular and macroscopic order parameters is poorly understood for such complex segregating solutions. We contribute to the clarification of this problem by first following the diffusion behaviour of the hydration water across the phase transition of model aqueous poly(N-isopropylacrylamide) solutions using quasi-elastic neutron scattering [2]. By probing the molecular bond polarisabilities, we adopt an alternative, highly revealing perspective on the changes in molecular interactions and in structure happening within dilute to concentrated phase-separating solutions [1, 3]. [1] M. Philipp, et al., Soft Matter 10, 7297-7305 (2014), [2] M. Philipp, et al., J. Phys. Chem. B 118, 4253-4260 (2014), [3] R. Aleksandrova, et al., Langmuir 30, 11792-11801 (2014)

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[1], Martine Philipp[1], Joseph Adelsberger[1], Sebastian Jaksch[1], Anatoly V. Berezkin[1], Dersy M. Lugo[2], Walter Richtering[2], Isabelle Grillo[3], Anna Miasnikova[4], André Laschewsky[4], Peter Müller-Buschbaum[1], and •Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching — [2]RWTH Aachen University, Institut für Physikalische Chemie — [3]Institut Laue-Langevin, Grenoble, France — [4]Universität 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 polystyrene-*b*-poly(N-isopropylacrylamide) (PS-*b*-PNIPAM) diblock copolymers and (ii) PNIPAM homopolymers in D_2O 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.

1. Kyriakos et al., *Macromolecules* **47**, 6867 (2014)

BP 10.7 Mon 16:30 C 130

Cation-activated attractive patches to control protein interactions — •Felix Roosen-Runge[1], Fajun Zhang[2], Frank Schreiber[2], and Roland Roth[3] — [1]Institut Laue-Langevin, Grenoble, France — [2]Institut für Angewandte Physik, Universität Tübingen — [3]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 different pathways of crystallization [1,3]. The good agreement between theory and experiments indicates that protein-cation solutions represent a natural model system for patchy particles. 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.

[1] F. Roosen-Runge, F. Zhang et al. *Sci. Rep.* 4 (2014) 7016
[2] F. Zhang, A. Sauter et al. *J. Appl. Cryst.* 44 (2011) 755
[3] F. Zhang, R. Roth et al. *Soft Matter* 8 (2012) 1313

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 deformation field in the polymer gel. The 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 wavy structure with higher number of buckles. A higher magnetic field strength and a lower modulus of gel matrix lead to higher amplitude of the buckling. The deformation field around a deformed 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.

15 min. break

BP 10.9 Mon 17:15 C 130

Environmentally compatible microemulsion at solid surfaces: Wetting behavior and extraction properties — •Salomé Vargas Ruiz[1], Christoph Schulreich[2], Ramasia Sreich[2], Martin Jung[3], Regine von Klizing[1], Thomas Hellweg[2], and Stefan Wellert[1] — [1]Stranski Laboratory, TU Berlin, Str. d. 17 juni 124, 10623 Berlin, Germany — [2]Physical Chemistry III, University Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany. — [3]Armed Forces Scientific Institute for NBC Protection, Humboldtstraße 1, 29633 Munster, 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 nerves agents, pesticides). The main advantage of microemulsions relies on their capability to degradate 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 we evaluated their ability to extract 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.

BP 10.10 Mon 17:30 C 130

Supramolecular structure of pure and mixed monohydroxy alcohols — •Thomas Büning[1], Christian Sternemann[1], Sebastian Peter Bierwirth[1], Catalin Gainaru[1], Jennifer Bolle[1], Michael Paulus[1], Christoph J. Sahle[2], Roland Böhmer[1], and Metin Tolan[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]European Synchrotron Radiation Facility (ESRF), F-38000 Grenoble, France

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 MA mixtures. Here, the first 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 respect to 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).

BP 10.11 Mon 17:45 C 130

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

MD-simulations are a powerful tool to investigate microscopic processes in complex systems as ionic liquids. The interactions between the cation and the anion are only weak but in the case of adding lithium to an ionic liquid the anions strongly interact with this small lithium ion. The role of the cation on this interaction was never investigated.

Here, we compare the cations 1-ethyl-3-methylimidazolium with N-metyhl-N-propylpyrrolidium and as counterion bis-(trifluoromethanesulfonyl)-imide was used. Both cations differ in size and viscosity but on the microscopic scale only a comparison for pure ionic liquids is published. We performed MD-simulations for the two ionic liquids doped with lithium salts at different temperatures and different oxygen polarizations. The change of the TFSI oxygen polarization was necessary due to new DFT calculations that predicts the Li^+ - Ntf_2 binding energy more accurate. We observed a dramatic influence of the polarization on structural properties while the dynamics are only slightly affected. The comparison of the cations shows only small differences for the lithium ion coordination.

BP 10.12 Mon 18:00 C 130

A systematic study of the influence of trivalent metal ions on phase behaviour in protein solutions — •Olga Matsarskaia[1], Michal Braun[1], Andrea Sauter[1], Marcell Wolf[1], Roland Roth[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Institut 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 crystallisation. 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 ($YbCl_3$, YCl_3, $GdCl_3$, $CeCl_3$ and $LaCl_3$). 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 Yb^{3+} leads to the largest LLPS area, Ce^{3+} features the smallest one. La^{3+}, the largest cation studied, induces RC, but does not lead to LLPS at all. The findings thus indicate that the size of cations present in the environment of a protein influences the strength of protein-cation interactions and therefore plays an important role in phase transitions of the protein.

[1] Zhang et al (2008). Phys. Rev. Lett., 101(14), 148101; [2] Zhang et al (2012). Soft Matter, 8, 1313-1316.

BP 10.13 Mon 18:15 C 130

New relaxation process for water in electric fields — •Zoran Ilič[1], David M. Smith[2,3], and Ana-Sunčana Smith[1,3] — [1]Institut für Theoretische Physik and Cluster of Excellence: Engineering of Advanced Materials, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]Computer Chemie Centrum, FAU Erlangen-Nürnberg, Erlangen, Germany — [3]Ruđer Bošković Institute, Zagreb, Croatia

Despite a heavily increasing number of electrochemical applications, theoretical and experimental studies of solvent shear properties in the presence of electric fields are almost non-existent. Here we study the shear viscosity of water by performing extensive MD simulations using the GROMACS software package as a function of the electric field strength which breaks the otherwise isotropic nature of the solvent. The shear viscosity is related to the autocorrelation function (ACF) of the off-diagonal elements of the pressure tensor by the Green-Kubo relation. The value of the shear viscosity is determined from the plateau value of the time integral of the ACF or, alternatively, by exploiting the Kohlrausch fit curve of the ACF using a uniform 2-step (fast plus slow) relaxation function. Apart from the fact that the two approaches show an excellent agreement, we find that the field decreases the component of the shear viscosity perpendicular to itself and increases the components which are parallel. Importantly, the field induces an additional slow relaxation process (decoupled from the fast relaxation) only in the parallel direction, increasing by about tenfold the total relaxation time with respect to the perpendicular direction. Furthermore, the overall water shear viscosity increases slightly with the field strength.

BP 10.14 Mon 18:30 C 130

Excess entropy scaling for the segmental and global dynamics of polyethylene melts — •Evangelos Voyiatzis, Michael Böhm, and Florian Müller-Plathe — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center of Smart Interfaces, Technische Universität Darmstadt, Alarich-Weiss-Strasse 4, D-64287 Darmstadt, Germany

The range of validity of the Rosenfeld and Dzugutov excess entropy scaling laws is analyzed for linear polyethylene chains. We consider two segmental dynamical quantities, the bond and the torsional relaxation times, and two global ones, the chain diffusion coefficient and the viscosity. The excess entropy is approximated by either a series expansion of the entropy in terms of the pair correlation function or by an equation of state for polymers. For all temperatures and chain lengths considered, the two excess entropy estimates are linearly correlated. The scaled segmental relaxation times fall into a non-linear master curve. For a fixed chain length, the reduced diffusion coefficient and viscosity scale linearly with the excess entropy. An empirical reduction to a chain length independent master curve is accessible for both quantities. The Dzugutov scheme predicts an increased value of the scaled diffusion coefficient 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

Do Macroscopic Properties of Nanocomposites Require Glassy Layers? — Klaus Nusser and •Gerald J. Schneider — Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science & Institute of Complex Systems, 52425 Jülich, Germany

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 microscopic 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 Scheler — 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 nanoparticles coated with thin films 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 tube diameter. The choice of compact stars represents a model system of nanocomposites without polymer-particle adsorption. The 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 inversed 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).

BP 11.4 Mon 15:45 C 243

Polymer/metal hybrids: Adhesion behaviour and polymer dynamics before and after corrosion treatment — •Marieke Füllbrandt[1,2], Andreas Schönhals[2], and Regine von Klitzing[1] — [1]Technische Universitaet Berlin, Str. des 17. Juni 124, 10623 Berlin — [2]BAM Bundesanstalt fuer Materialforschung und -pruefung, Unter den Eichen 87, 12205 Berlin

Polymer/metal hybrids are of high interest for example in lightweight constructions used in the automotive industry. They combine a high functional integration with a lower weight compared to pure metal parts. The joining of these dissimilar materials without using additional material is a central challenge. In a first step, the metal/polymer interface is characterized with regard to the adhesion behaviour on a macro- and microscopic length scale using contact angle (CA) measurements and colloidal probe atomic force microscopy. The latter method determines the adhesion force and energy which can be analysed and related to a work of adhesion per area. The effect of a (sub)micrometre scale roughness is considered using the Rabinovich approach. With CA measurements the surface energy of the solids is determined using the Owens-Wendt-Rabel-Kaelble method and further be related to the corresponding work of adhesion per area. In a second step, the influence of a corrosion treatment on the adhesion behaviour is investigated. Complementary, broadband dielectric spectroscopy measurements in a wide frequency (0.01 Hz to 1 MHz) and temperature range (-120 to 180 °C) are performed in order to characterize the polymer dynamics in bulk and at the metal interface before and after treatment.

BP 11.5 Mon 16:00 C 243

Organic inorganic hybrid PU-POSS networks: A multi-length-scale investigation of morphology and a multi-time-scale investigation of dynamics — •Konstantinos N. Raftopoulos[1,2], Stefanos Koutsoumpis[3], Malgorzata Jancia[2], Konstantinos Kyriakos[1], Edyta Hebda[2], Christine M. Papadakis[1], Krzysztof Pielichowski[2], and Polycarpos Pissis[3] — [1]TU München, Physik-Department, Fachgebiet Physik weicher Materie, Garching — [2]Cracow University of Technology, Department of Chemistry and Technology of Polymers, Poland — [3]National Technical University of Athens, Department of Physics, Greece

Polyhedral oligomeric silsesquioxanes (POSS) bridge the gap between nanoparticles and conventional chemical reagents. A wide variety of organic, ligands bind on a sub-nm siliceous core, and allow it to participate as a nanobuilding block on the very structure of the macromolecular chain. Here, octa-OH functional moieties crosslink a phase separated polyurethane. On the basis of X-ray diffraction in a wide q-range covering both WAXS and SAXS and atomic force microscopy we show that POSS reside in the soft phase, and the hard microdomains become progressively thinner with increasing POSS content. The segmental dynamics of the soft phase slow down as a result of both crosslinking and diminishing microphase separation, as evidenced by differential scanning calorimetry and broadband dielectric spectroscopy. Interestingly, all the effects show a step-like behavior between 4 and 6 wt% of POSS, possibly as a result of a percolation of the POSS crosslinked phase.

BP 11.6 Mon 16:15 C 243

Nanomechanical Investigation of Rubber-modified Epoxy Resins — •Lisa Maria Uiberlacker and Sabine Hild — Institute of Polymer Science, Johannes Kepler University, 4040 Linz, Austria

Epoxy resins have a broad application scope due to the wide range of properties which can be easily modified by mixing various basic components - e.g. to modify the toughness of epoxy resins rubber auxiliaries are added.

This study focused on epoxy mixtures based on a bisphenol A diglycidyl ether cured with diethyltoluenediamine with various amounts of nitrile rubber. Both, morphology and the mechanical properties of these two phase systems were examined with scanning force microscopy (SFM).

In SFM phase images the epoxy phase was clearly distinguished from the rubber phase. The nitrile rubber formed spherical domains in the epoxy matrix. Phase separation occurred also in the rubber matrix. Mechanical properties of both phases were quantified by nanoindentation experiments. In addition, the influence of different amounts of rubber additive on the toughness of the epoxy matrix was examined.

15 min. break

BP 11.7 Mon 16:45 C 243

Matryoshka-Doll-like Shish-Kebab Nanocomposite: Nanohybrid Shish-Kebabs within Nanofiber Shish-Kebabs — •Matthias M.L. Arras[1], Richard Jana[1], Christian Grasl[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science (CMS), Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Germany — [2]Center for Medical Physics and Biomedical Engineering, Medical University of Vienna, Austria

The shish-kebab morphology in semi-crystalline polymer fibers is a key to the outstanding properties of polymer fibers. Here, we present the creation of a two-level hierarchical fiber structure by combining two recent artificial shish-kebab nanostructures: The nanohybrid shish-kebab (NHSK), i.e., a carbon nanotube (CNT) overgrown by polymer kebabs and the nanofiber shish-kebab (NFSK), i.e., an electrospun nanofiber decorated by larger lamellae crystals. We tested the hypothesis that during electrospinning of a CNT/polymer solution the NHSK can form directly and that the resulting fibers can be used to subsequently create the NFSK. The resulting nanocomposite was analyzed by transmission and scanning electron microscopy and revealed the successful creation of both the NHSK and the NFSK. Thus, for the first time, we demonstrated the creation of the NHSK morphology during electrospinning. The two-level hierarchical nanocomposite is a proof of principle that the shish-kebab morphology can be extended from the nanoscale to the macroscale which may contribute to future high strength nanocomposites.

BP 11.8 Mon 17:00 C 243

Structural changes of diisocyanates covalently attached to the semiconducting carbon nanotube — •Mariana Kozlowska[1], Jakub Goclon[2], and Pawel Rodziewicz[1] — [1]Institute of Chemistry, University of Bialystok, Poland — [2]Interdisziplinäres Centrum für Molekulare Materialien(ICMM) und Computer-Chemie-Centrum (CCC), Department Chemie und Pharmazie,Friedrich–Alexander–Universität Erlangen–Nürnberg

Reinforced polymers are of a great interest since the individual properties of the initial materials can be combined, resulting in a new hybrid material with better properties. Carbon nanotubes are popular polymer filler and reinforcing agent. They enhance the mechanical strength and corrosion resistance.

We performed first-principles DFT calculations of the covalent and noncovalent sidewall functionalization of metallic (6,0) and semiconducting (10,0) single-walled carbon nanotubes (SWCNTs) via the attachment of two aromatic diisocyanates: 4,4'-methylene diphenyl diisocyanate (MDI) and toluene-2,4-diisocyanate (TDI).

In this work, we focus on the structural rearrangements of the diisocyanates molecules covalently attached to the SWCNT(10,0) surface at the finite temperature, using the Car-Parrinello molecular dynamics (CP-MD) scheme.

Mariana Kozlowska is a beneficiary of the project Scholarships for PhD students of Podlaskie Voivodeship. The project is co-financed by European Social Fund, Polish Government and Podlaskie Voivodeship.

BP 11.9 Mon 17:15 C 243

Formation of anisotropic gold nanoparticles with different 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

Au 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 synthesize various 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 UV-Vis spectroscopy, SAXS and TEM to understand indirectly the formation mechanism of such particles.

[1] C.J. Murphy et al., J. Phys. Chem B. 2005, 109, 13857-13870.

BP 11.10 Mon 17:30 C 243

Local Chemical Characterization of Nanoporous Materials with Atom Probe Tomography — •Carsten Nowak, Philipp Sauerbier, and Björn Pfeiffer — Georg-August-Universität Göttingen, Insitute for Materials Physics, Göttingen, Germany

Because of their high surface-to-volume-ratio and their chemical activity, nanoparticles and nanoporous materials receive 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 nanoporous gold 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.

BP 11.11 Mon 17:45 C 243

Semiconductor Nanocrystal Blinking monitored via Fast Spectrally and Intensity Resolved Single Molecule Spectroscopy — •Clemens Göhler, Cornelius Krasselt, and Christian von Borczyskowski — Fakultät für Naturwissenschaften, TU Chemnitz, D-09126 Chemnitz

Colloidal CdSe Semiconductor Nanocrystals (NCs) are promising candidates for improving different applications, e.g. in photovoltaics or sensoring, due to their size-dependend optical and spectroscopic properties. With techniques from Single Molecule Spectroscopy, we avoid ensemble-averaging and investigate these characteristics on individual NCs. On that level, luminscence intermittency (so called blinking) is observable, for which the underlying mechanisms are yet not fully understood.

To contribute, we applied Change-Point-Analysis to time-correlated single-photon counts from single NC photoluminescence (PL) emission, which allows resolving discrete PL intensity levels [1]. In addition, we splitted the PL-signal with a dichroic beamsplitter towards two detectors. By combining these techniques, we were able to examine spectral diffusion within the single NC PL on a μs-timescale and to correlate that to the fluctuating emission intensity. The results are in agreement with blinking models based on a multiple recombination-center approach.

[1] Schmidt, R., Krasselt, C., Göhler, C., & von Borczyskowski, C. (2014). *ACS nano*, *8*(4), 3506-3521.

BP 11.12 Mon 18:00 C 243

Interrelation of fluorescence and morphology of molecular aggregate structures — •Mohammadreza Bahrami[1], Tamam Bohamud[1], Clemens Schindler[1], Lukas Rathje[1], Hannes Hartmann[1], J.A.A.W Elemans[2], Ingo Barke[1], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics, 18051 Rostock, Germany — [2]Radboud 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 excitons. 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 nanostructures in the vicinity of molecule aggregates, and address the role of these metal systems as local sources of electromagnetic fields.

[1] Wenqi Zheng, et al., Dyes and Pigments 77 (2008) 153e157 [2] M.J.J. Coenen, et al., Phys. Chem. Chem. Phys. 15, 12451 (2013)

BP 11.13 Mon 18:15 C 243

Electric detection of ortho and para water in fullerene cages — •Benno Meier, Salvatore Mamone, Javier Alonso-Valdesueiro, Maria Concistrè, Andrea Krachmalnicoff, Richard J. Whitby, 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.

BP 11.14 Mon 18:30 C 243

Effective mechanical properties of graphene obtained by computational mechanical tests — •Markus A. Hartmann[1], Melanie Todt[2], and Franz G. Rammerstorfer[2] — [1]Institute of Physics, Montanuniversität Leoben, 8700 Leoben, Austria — [2]ILSB, 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 of 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 large than 5 nm.

[1] Holec et al., Phys. Rev. B 81, 235403 (2010)
[2] Hartmann et al., Europhys. Lett. 103, 68004 (2013)

BP 12: Evolutionary Game Theory I (joint SOE/BP/DY)

Time: Monday 15:00–15:45 Location: MA 001

BP 12.1 Mon 15:00 MA 001

Dynamics of human behaviour in prisoner dilemma games — •Martin Spanknebel and Klaus Pawelzik — Institute for Theoretical Physics, University of Bremen, Germany

When playing simple games humans sometimes fail to achieve maximally possible earnings, which is often considered to reflect 'irrationality'. Such behaviour has been attributed to accessory objectives or emotional biases. For instance, recently humans were found to cooperate far less than required for optimizing mean payoff when playing prisoner dilemma games against extortion strategies. But against generous strategies humans performed to optimise their behaviour properly. Here we propose an alternative explanation based on preference shifts towards choices that proved more rewarding in the immediate past. This 'melioration' is found to account for human behaviour in prisoner dilemma games with opponents exhibiting different degrees of extortion and generosity. In particular, melioration explains reduced cooperation in extortion and high cooperation in generous games and reproduces the broad distributions of choice rates in ensembles of players. These results indicate that the alleged irrationality of human behaviour could be the consequence of elementary learning mechanisms and not necessarily involves auxiliary motives.

BP 12.2 Mon 15:15 MA 001

When do microscopic assumptions determine the outcome in evolutionary game dynamics? — •Bin Wu[1], Bebedikt Bauer[1], Tobias Galla[2], and Arne Traulsen[1] — [1]Department of Evolutionary Theory, Max Planck Institute for Evolutionary Biology, Ploen, Germany — [2]Theoretical Physics, School of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, United Kingdom

The modelling of evolutionary game dynamics in finite populations requires microscopic processes that determine how strategies spread. The exact details of these processes are often chosen without much further consideration. Different types of microscopic models, including in particular fitness-based selection rules and imitation-based dynamics, are often used as if they were interchangeable. We challenge this view and investigate how robust these choices on the micro-level really are. Focusing on a key macroscopic quantity, the probability for a single mutant to take over a population of wild-type individuals, we show that there is a unique pair of a fitness- based process and an imitation process leading to identical outcomes for arbitrary games and for all intensities of selection. This highlights the perils of making arbitrary choices at the micro-level without regard of the consequences at the macro-level.

BP 12.3 Mon 15:30 MA 001

Social particles. On the common roots of aggression, altruism, co-operation and grouping — •Karl Kalveram — Tu Darmstadt and Uni Duesseldorf

We are accustomed of the strange outcome of the interaction of particles: particles that annihilate if meeting each other and/or re-emerge from vacuum. Some attract and some refute others. Their overall demeanor, however, is, temporal stationarity presumed, only describable statistically, and governed by equations proposed by Schroedinger or Heisenberg. Now we look at another type of particles interacting, too, with randomly varying outcomes. Their properties, however, can change over time, some rules of which being formulated first by Darwin. Here I present a mathematical formalism describing behavior and evolution of a selection called 'social particles'.

The formalism considers population dynamics as dependent on the particles' average birth and death rate, the average outcome of social interactions as influencing this ratio, and the reproduction ratio (birth

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

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) — •Stephan Kramer, Anthony de Vries, Nathan Cook, Donna Arndt-Jovin, and Thomas Jovin — Labor f. Zelluläre Dynamik, Max-Planck-Institut f. biophysikalische Chemie, Am Faßberg 11, 37077 Göttingen

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 mm^2. 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 30×30 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 analyze the recorded images concurrent to the acquisition so that after a first scan of the total area only those tiles are 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.

[1] W. Caarls et al., Minimizing light exposure with the programmable array microscope, J. Microscopy **241**, 101 – 110 (2010)

[2] P. De Beule et al. Generation-3 programmable array microscope with digital micro-mirror device. SPIE proceedings (2011)

BP 13.2 Mon 17:30 Poster A

Wide Field Detection and Imaging of Atomic Spins using Nitrogen-Vacancy Centers — •Florestan Ziem, Philipp Scheiger, Helmut Fedder, and Jörg Wrachtrup — 3. Physikalisches 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 sample volumes, directing the focus at novel sensors. Here, we show how nitrogen-vacancy centers in diamond hosts allow the detection of small ensembles of electronic [1,2] and nuclear [3,4] spins at ambient conditions by optically detected magnetic resonance. In a wide field microscope, parallel magnetic detection and imaging on the microscale are demonstrated.

[1] Steinert, S. *et al.* Magnetic spin imaging under ambient conditions with sub-cellular resolution. Nat. Commun. **4**, 1607 (2013).

[2] Ziem, F. C., *et al.* Highly sensitive detection of physiological spins in a microfluidic device. Nano Lett. **13**, 4093 (2013).

[3] Mamin, H. J. *et al.* Nanoscale Nuclear Magnetic Resonance with a Nitrogen-Vacancy Spin Sensor. Science **339**, 557 (2013).

[4] Staudacher, T. *et al.* Nuclear Magnetic Resonance Spectroscopy on a (5-Nanometer)^3 Sample Volume. Science **339**, 561 (2013).

BP 13.3 Mon 17:30 Poster A

X-ray waveguide optics for nanoscale phase contrast tomography — •Martin Krenkel[1], Andrea Markus[2], Matthias Bartels[1], Christian Dullin[2], Frauke Alves[2], and Tim Salditt[1] — [1]Institute for x-ray physics, University Göttingen, Germany — [2]University 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.

To reduce beam inhomogeneities and to fulfill the theoretical assumptions needed for proper reconstruction, we use a divergent x-ray waveguide beam geometry at the synchrotron. Thus, the magnification can be easily tuned by placing the sample at different defocus distances. Due to the small Fresnel numbers in this geometry the measured images are of holographic nature which poses a challenge in phase retrieval. With nearly mono modal x-ray beams resolutions down to 23 nm are achieved. We demonstrate this technique on soft hydrated mouse lung tissue yielding 3D reconstructions for a large field of view and region of interest zoom tomography. To further improve the imaging scheme, we develop new reconstruction algorithms that impose minimal restrictions to the objects, based on an optimized measurements or on using an intrinsic consistency constraint of different tomographic projections.

BP 13.4 Mon 17:30 Poster A

Calibration of the diffusion coefficients of the FCS standard Rhodamine 6G in aqueous solutions — •Günter Majer — MPI for Intelligent Systems, Stuttgart, Germany

Precise diffusion measurements of rhodamine 6G (Rh6G) dissolved in D_2O 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 Rh6G concentrations, a water suppression PFG-NMR sequence was applied. The temperature and concentration dependent diffusion coefficients of Rh6G can be used as calibration references in fluorescence correlation spectroscopy (FCS). Besides measuring the diffusivity of Rh6G, the diffusion coefficient of the solvent in the same system could be determined in parallel by PFG-NMR as the resonances of water and Rh6G are well separated in the ^{1}H NMR spectrum. The isotope effect of the solvent on the diffusion coefficient is determined by FCS measurements on Rh6G dissolved in both D_2O and H_2O.

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 biomineralised 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 biomineralise 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 gryphiswaldense* MSR-1 cells using confocal laser scanning microscopy. From these measurements, we conclude that the biomineralisation of iron nanoparticles in MTB 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.

BP 13.6 Mon 17:30 Poster A

Embedding of flagellate Trypanosoma brucei for single-molecule microscopy — •Marius Glogger[1], Simone Stichler[2], Jörg Tessmar[2], Jürgen Groll[2], Markus Engstler[1], and Susanne Fenz[1] — [1]Biocenter: Cell and Developmental Biology, University of Würzburg, Würzburg, Germany — [2]Department of Functional Materials in Medicine and Dentistry, University of Würzburg, Würzburg, Germany

The uniflagellate protozoa Trypanosoma brucei are the causal agents of African sleeping sickness. High-resolution microscopy of trypanosoma 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 require 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 hydrogel 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

In situ nanoscale imaging of chromosome oscillations in living yeast cells — •Natalja Strelnikova[1], Vasily Zaburdaev[2], Nora Sauter[1], Manuel Guizar Sicairos[3], Ana Diaz[3], Petrina Delivani[4], Mariola Chacon[4], Iva Tolic-Norrelykke[4,5], and Thomas Pfohl[1] — [1]Department of Chemistry, University of Basel, Switzerland — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [5]Division of Molecular Biology, Institute Rudjer Boskovic, 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 chromatin 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 fission 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 Schachoff, Alice Abend, 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 fluorescent probes and hampered by their photophysical processes such as bleaching and blinking. Recently, photothermal microscopy, which is based on the absorption of light, has been pushed to a new level of sensitivity allowing even the detection of single molecules. The technique employs the conversion of optical energy into heat by an absorbing non-fluorescent species. The released heat has been shown to create a nano-lens deflecting a focused probe laser in a microscopy setup. Gold nano particles down to 5 nm in size exhibit large absorption cross sections and high photo stability and, thus, deliver intense and stable optical signals in photothermal microscopy with large signal to noise ratios even in heterogeneous environments. Since this method is highly sensitive to the absorbing species and non invasive, we recently startet to implement photothermal detection and correlation spectroscopy in living cells to study local dynamics in biological samples. Further, we aim to use gold nano particles as single nano heat sources in cells 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 Schürmann[1], Paul Müller[1], Moritz Kreysing[2], and Jochen Guck[1] — [1]Biotechnology Center, TU-Dresden, Tatzberg 47/49, 01307 Dresden, Germany — [2]Max 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 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 LP_{11} 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

GPU-based statistical multi-resolution estimators for image reconstruction — •Jan Lebert[1], Johannes Hagemann[2], and Stephan Kramer[3] — [1]G. A. U. Göttingen, Fakultät f. Physik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Institut f. Röntgenphysik, G. A. U. Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [3]Max-Planck-Institut f. biophysikalische Chemie, Am Faßberg 11, 37077 Göttingen

We present two implementations of Dykstra's projection algorithm on NVIDIA's compute unified device architecture (CUDA). Dykstra's algorithm 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 preprocessing 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 — •Ingmar Schoen — ETH Zurich, 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 Cramer-Rao lower bounds (CRLBs) that were in general anisotropic and depended on emitter intensity and position. We performed simulations to benchmark the extent to which different analysis procedures reached these ideal CRLBs. The accumulation of noise from several images accounted for the worse localization precision in image subtraction. Propagation of fitting errors compromised the CRLBs in sequential fitting using fixed parameters. 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 depended critically on the exact bleaching kinetics and was correctly 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.

BP 13.12 Mon 17:30 Poster A

Parallelizing super-resolution optical fluctuation imaging (SOFI) — •Bartosz Kohnke[1], Stephan Kramer[1], Johannes Hagemann[2], and Suzunosuke Nagaoka[3] — [1]Max-Planck-Institut f. biophysikalische Chemie, Am Faßberg 11, 37077 Göttingen —

[2]Institut F. Röntgenphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [3]Institut f. Informatik, Universität Göttingen, Goldschmidtstraße 7, 37077 Göttingen

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 compute 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].

[1] Dertinger et al., PNAS Vol. 106, No. 52, pp. 22287 (2009)
[2] SciPAL: Expression Templates and Composition Closure Objects for High Performance Computational Physics with CUDA and OpenMP, S. C. Kramer and J. Hagemann, ACM TOPC (to appear).
[3] https://code.google.com/p/scipal/

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 Stein, 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.

The visual fidelity of SOFI, however, is limited by the finite size of the camera's pixel grid. We present a new approach for creating sub-pixel resolution images which is completely artifact-free and straightforward to implement, keeping the simplicity of the original algorithm.

Furthermore 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

SIM microscopy to investigate lipofuscine granules in retinal pigment epithelial cells — •Florian Schock[1,2,3,4], Gerrit Best[1,2,4], Nil Celik[2], Alena Bakulina[5,9], Saadettin Sel[2], Udo Birk[1,3], Rainer Heintzmann[6,7,10], Jürgen Hesser[5,9], Stefan Dithmar[2,8], and Christoph Cremer[1,3,4] — [1]Kirchhoff Institute for Physics, University of Heidelberg — [2]Department of Ophthalmology, University-Hospital Heidelberg — [3]Institute of Molecular Biology, University of Mainz — [4]Institute of Pharmacy and Molecular Biotechnology, University of Heidelberg — [5]Experimenatal Radiation Oncology, University Medical Center Mannheim, University of Heidelberg — [6]Institute for Physical Chemistry and Abbe Center of Photonics, University of Jena — [7]Leibniz Institute of Photonic Technology — [8]Department of Ophthalmology, Hospital Wiesbaden — [9]Institute for Scientific Computation, University of Heidelberg — [10]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 lipofuscine granules inside the retinal pigment epithelial cells (RPE cells). Here we demonstrate that the super-resolution technique "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 lipofuscine granules and intra-granule regions.

BP 13.15 Mon 17:30 Poster A

Image Scanning Microscopy — •Jörg Enderlein — 3. Physikalisches Institut, Georg-August-Universität Göttingen

Recent years have seen an explosion in new advanced and super-resolution methods in fluorescence microscopy, which have culminated in the Nobel Prize in Chemistry for 2014. One of the early methods of these techniques was structured illumination microscopy (SIM), which combines wide-field imaging with a structured illumination for doubling the resolution of a wide-field microscope. An alternative approach is image scanning microscopy (ISM), which combines a conventional confocal laser scanning microscope with a wide-field imaging detector. Although the idea was theoretically proposed by Colin Sheppard already in 1988, its first successful realization was only achieved in 2010. Since then, a whole flood of modifications and implementations of this idea have been published, and by now, even the first commercial implementation of ISM (Airy Scan Microscope by Carl Zeiss Jena) is available. I will present the working principle of ISM and its several implementations and applications.

BP 14: Posters: Neurophysics

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

BP 14.1 Mon 17:30 Poster A

Frequency modulated signal transmission in neurons — •Tim Herfurth and Tatjana Tchumatchenko — Max Planck Institute for Brain Research, Max-von-Laue-Str. 4, 60438 Frankfurt/M

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 have been treated as additive noise. Alternatively, amplitude modulations of the noise by the signal have been proposed, effectively coding in the variance channel. In this work we suggest and present closed form expressions for another kind of signal modulation: frequency modulation (FM). Here, the signal modulates the noise by linear frequency modulation. The concept is well known, e.g. from communication techniques. However, we present a representation that incorporates arbitrary forms of input signals and noise, define a signal-to-noise ratio and show consequences for statistics and mutual information of the FM channel.

BP 14.2 Mon 17:30 Poster A

Activity propagation in feed-forward neuronal networks described by reaction-diffusion like equations — •Dmytro Grytskyy[1], Markus Diesmann[1,2], and Moritz Helias[1] — [1]INM6&IAS6, Juelich Research Centre and JARA, Jülich, Germany — [2]Medical Faculty, RWTH Aachen, 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 K nearest neighbor coupling in diffusion approximation to obtain equations for the activity evolution from layer to layer. The equations are similar but not identical to those describing reaction-diffusion systems. We develop an appropriate solution scheme also applicable to generalized systems with several synapse or neuron types. We obtain 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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BP 14.3 Mon 17:30 Poster A

Mechanotransduction in the pentamere organ of the Drosophila larva — •Achintya Prahlad[1], Ben Warren[2], Mar-

tin Göpfert[2], and Christoph Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität, Göttingen — [2]Schwann-Schleiden Research Centre, Georg-August-Universität, Göttingen

The fruit fly Drosophila melanogaster uses mechanosensation for several purposes. One class of specialized organs are the chordotonal organs, such as the antennal auditory organ of the adult, and the larval pentamere organ (or lch5). The sensory neurons at the core of these organs have one dendrite, which terminates in a cilium. The cilia are believed to be the main mechanotransducers. The lch5 organ aids in locomotion by giving feedback to the central nervous system. We focus on this organ because its sensory neurons are well accessible to manipulation under the microscope.

Some molecular and anatomical aspects of these organs have been studied. However, an understanding of the internal transduction mechanics and the manner in which membrane channels are activated upon deflection of the cilium is still elusive. We are using a preparation of the larva under buffer solution that allows us to directly contact the sensory neurons of the lch5 after removing 2-3 layers of muscles. Our approach is to provide controlled mechanical stimuli to the cilia and measure the mechanical and electrical response.

BP 14.4 Mon 17:30 Poster A

Stochastic thermodynamics of biological information processing — •Sebastian Goldt and Udo 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.

1 U. Seifert, Rep. Prog. Phys. **75**, 126001 (2012).

2 A. C. Barato and U. Seifert, Phys. Rev. Lett. **112**, 090601 (2014).

BP 14.5 Mon 17:30 Poster A

An objective function for Hebbian self-stabilizing neural plasticity rules — •Rodrigo Echeveste and Claudius Gros — Institute for Theoretical Physiscs, Goethe University Frankfurt, Germany

Objective functions provide a useful framework for the formulation of guiding principles in dynamical systems. In the case of information processing systems, such as neural networks, these guiding principles can be formulated in terms of information theoretical measures with respect to the input and output probability distributions. In the present work, a guiding principle for neural plasticity is formulated in terms of an objective function defined as the Fisher information with respect to an operator that we denote as the synaptic flux[1]. By minimization of this objective function, we obtain synaptic plasticity rules that both account for Hebbian/anti-Hebbian learning and are self-limiting to avoid unbounded weight growth.

As an application, the non-linear bars problem[2] is studied, in which each neuron is presented with a grid of inputs, depicting the superposition of a random set of bars. We show that, under the here presented rules, the neurons are able to learn single bars or points (the independent components of the input), even when these are never presented in isolation.

[1] Echeveste, R., & Gros, C. (2014). Generating functionals for computational intelligence: The Fisher information as an objective function for self-limiting Hebbian learning rules. Front. Robot. AI, 1, 1.

[2] Földiak, P. (1990). Forming sparse representations by local anti-Hebbian learning. Biological cybernetics, 64(2), 165-170.

BP 14.6 Mon 17:30 Poster A

Patterning and Interfacing of Biological Neural Networks — •Norman Shepheard[1,2], Stefan Niehörster[1], Matthias Schürmann[3], Savio Fabretti[1], Barbara Kaltschmidt[3], Christian Kaltschmidt[3], Ulrich Rückert[2], Elisabetta Chicca[4], and Andy Thomas[1] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Cognitronics and Sensor Systems, Bielefeld University, Germany — [3]Cell Biology, Bielefeld University, Germany — [4]Neuromorphic Behaving Systems, Bielefeld University, Germany

The scale of neural networks reaches from large structures such as the whole human nervous system down to small single neurone networks. To examine the small types of single neurone networks we use a bottom up approach, which consist of two important parts. The first part is the pattern of the cell adhesion layer. The second part is the interface to the network.

To achieve self grown networks we produce an adhesion layer stack made of (3-aminopropyl)triethoxysilane (APTES), glutaraldehyde and poly-lysine. This adhesion layer is patterned via the uv-lithographic "lift-off" technique. The hyppocampal mouse neurones are cultured on top of the adhesion layer. Our results show that the neurones adhere to the poly-lysine and aligning themselves with the pattern. The adhesion pattern is designed to fit to the electrode layout of a multi electrode array, which interfaces the networks.

BP 14.7 Mon 17:30 Poster A

Can compartmentalization explain fast population coding? — •David Hofmann[1,2], Andreas Neef[1,2], and Fred Wolf[1,2] — [1]Max Planck Institut für Dynamik und Selbstorganisation, Göttingen — [2]Bernstein Center for Computational Neuroscience, Göttingen

Cortical neurons, driven by noisy current injections, change their firing rate within 1 ms of a small step in the current average. This sets the speed of cortical information processing. Theoretical and experimental evidence points at the rapidness of the action potential (AP) onset as the key determinant of the fast neuronal response. However, the biophysical basis of this onset rapidness is unclear and a matter of current debate.

Recently, a minimal multi-compartment model was presented that produces a rapid onset in the somatic AP waveform (Brette *PloS Comp. Neuro.* 2013). This occurs by electric decoupling of the soma from the site of AP initiation (compartmentalization).

Here we investigate whether the electric decoupling mechanism can also explain the fast neural response. Specifically, we tested whether the model reproduces two robust experimental observations, a) the high cut-off frequency of the dynamic gain function in the range of 200 Hz b) the increasing cut-off frequency for increasing input current correlation time which is called the Brunel effect.

We find that the gain function is dominated by a single pole low pass filter around the membrane time constant independent of the electric decoupling. Hence, the model is not able to explain fast population responses. In addition, the model does not display a Brunel effect.

BP 14.8 Mon 17:30 Poster A

Computer generated holography for optogenetic modulation of neural network activity in vitro — •Manuel Schottdorf[1,2], Hecke Schrobsdorff[1], Walter Stühmer[2] und Fred Wolf[1] — [1]MPI für Dynamik und Selbst-Organisation, Göttingen — [2]MPI für Experimentelle Medizin, Göttingen

A randomly plated culture of neurons resembles to some extend *in-vivo* neural tissue in structural features, activity and development [Chiappalone et al. 2006, Huettner & Baughman 1986, Cohen et al. 2008] and has been used for various studies of learning, memory, plasticity, connectivity, and information processing. The activity of neurons in a culture can be measured with multi-electrode arrays. However, providing the cell culture with precise and spatially complex input patters is limited, most obviously by current diffusion from the electrodes.
Here, we address this problem using holography [Golan et al. 2009]. A laser and a spatial light modulator, assembled in the beam path of an inverted microscope, are used to generate holographic interference patterns in the object plane. These precise and spatially complex patterns excite a cell culture of optogenetically modified cortical neurons of a rat. The neural responses are monitored with a multielectrode array.
We present a performance assessment of our setup. We show that cultured neurons react well to external stimuli and we present some preliminary results on the modulations in network activity by the spatially complex optical excitation.

BP 14.9 Mon 17:30 Poster A

Switching dynamics in subnetworks of spiking neural networks — •Fereshteh Lagzi and Stefan Rotter — Bernstein Cen-

ter Freiburg and Faculty of Biology, Freiburg, Germany

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[1,2], Viola Priesemann[3], and Jochen Triesch[1] — [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 excitable systems subject to colored noise — Jannis Schuecker[1], Markus Diesmann[1,2], and •Moritz Helias[1] — [1]Institute of Neuroscience and Medicine (INM-6) and Institute for Advanced Simulation (IAS-6), Jülich Research Centre and JARA — [2]Medical Faculty, RWTH Aachen University

Many phenomena in nature are described by excitable 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 excitable units.

[1] Klosek MM, Hagan PS. J Math Phys 1998, 39:931-953
[2] Doering CR, Hagan PS, Levermore CD. PRL 1987, 59:2129-2132
[3] Schuecker J, Diesmann M, Helias, M. 2014, arXiv:1411.0432

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

BP 14.12 Mon 17:30 Poster A

Die E8-Gruppe, eine Theorien zum Verständnis des Gehirns. — •Sadler Norbert — Wasserburger Str. 25a: 85540 Haar

Wird das Gehirn als ein komplexes, kollektives System aufgefasst, kann durch Anwendung der Exzeptionellen E8-Gruppe, der Explorativen Faktorenanalyse und Methoden der Statistischen Physik eine neue Theorie zum Verständnis des Gehirns gefunden werden. Für das Human Brain Projekt kann die E8-Gruppe die Grundlage für ein neues Simulationsmodell des Gehirns dienen.

Die Algebren der E8-Gruppen Simulation:

(Träger-Matrix;453060**2)x(Anz.Verknüpf.2**22)=8.61x10**17

In der Simulation erhält jedes der 8.9x10**10 Neuronen des Gehirns eine Identität, die synaptischen Verknüpfungen, die spezifischen Sinnesmodalitäten, die gemessenen Reizintensitäten und die Entropie der Reizstärken bzw. den Energieumsatz des Gehirns.

Das Simulationsmodell:

(453060**2)x(e**Ry(13.6eV))/(QCD)x(log(QCD)))=E8xlog(QCD)

Ry=13.6eV, das photo-elektrische Intensitätszunahme-Quant zur Registrierung eines Sinnenreizes und QCD =0.192 die Starke Wechselwirkung und Intensität der spez. Sinnenreize. Die spezifischen Sinnarten, Modalitäten sind Vielfache des Intensitätszunahme-Quants.

Weitere Information:www.cosmology-harmonices-mundi.com

BP 15: Posters: Multi-cellular systems

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

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, Kaushikaram Subramanian, Eugene Myers, and Moritz Kreysing — 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 PCR 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 model tissue — •Damir Vurnek[1], Sara Kaliman[1], Carina Wollnik[2], Florian Rehfeldt[2], and Ana-Sunčana Smith[1] — [1]Theoretical Physics I, FAU Erlangen — [2]3rd institute Phyiscs-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, mm^2 to cm^2 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

and the center at relatively high densities. We characterize the osmolyte/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 osmolarity brings added features to tissue cooperativity and nuclei elongations show differences in the stress forces for different applied osmolytes.

BP 15.3 Mon 17:30 Poster A

Transporting Dpp in the fly wing: A theoretical analysis. — •Daniel Aguilar-Hidalgo[1], Maria Romanova-Michailidi[2], Marcos González-Gaitán[2], and Frank Jülicher[1] — [1]Max Panck Institute for the Physics of Complex Systems, Dresden, Germany — [2]University 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 growth factors stimulating cell and tissue growth. 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. We analyze the dynamical properties of two proposed transport mechanisms for Dpp in the wing: (i) a model of effective diffusion by trancytocis 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 Rademaker[1], Julia Dölger[1,3], Johannes Liesche[2], Alexander Schulz[2], and Tomas Bohr[1] — [1]Technical University of Denmark — [2]University of Copenhagen, Denmark — [3]Technische 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). We 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 [Dölger 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 are 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 Bock[1], Hitoshi Morita[2], Carl-Philipp Heisenberg[2], and Guillaume Salbreux[1] — [1]MPI-PKS, Dresden, Germany — [2]ISTA, 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 establish the shape of organisms. Here we ask how flows during Zebrafish dome formation can be understood quantitatively by describing embryonic tissues as a fluid, active material.

In early Zebrafish morphogenesis, approximately 25% of the embryo volume is occupied by the blastoderm, 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 1, 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 compared nuclei trajectories in different embryos. 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 rounding correlates with the orientation of cell division axes.

[1] R. Fickentscher, P. Struntz & M. Weiss, Biophys. J, 105 (2013)

BP 15.7 Mon 17:30 Poster A

Growth Dynamics of MDCK II Clusters on Elastic Substrates — •Philipp Linke[1], Carina Wollnik[1], Sara Kaliman[2], Damir Vurnek[2], Ana-Sunčana Smith[2], and Florian Rehfeldt[1] — [1]Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — [2]Institute 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 cluster monolayer after a short time. 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 which hampers long-term observations. We have designed and constructed a fully automated single-plane illumination microscope (SPIM) for imaging embryos of the nematode Caenorhabditis elegans in the early stages of development [1]. The combination of rapid widefield detection with optical sectioning and reduced bleaching allows for long-term, three-dimensional imaging of living specimen with a high spatio-temporal resolution. Using our SPIM setup, we have quantified cell movement and arrangment 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 embryogenetic events on several length scales, i.e. it is hence well suited to examine dynamic pattern formation in organismal biology.

[1] R. Fickentscher, P. Struntz & M. Weiss, Biophys. J. 105, 1805 (2013)

BP 15.9 Mon 17:30 Poster A

A computational model of tumor growth based on large scale vascular networks — Michael Welter[1], •Thierry Fredrich[1], Heiko Rieger[1], and Herbert Rinneberg[2] — [1]Saarland University — [2]PTB 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 there, 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 like MVD, 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 linelike 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.

[1] Gödde and Kurz, [2] Preziosi, [3] Welter and Rieger, [4] Rinneberg

BP 15.10 Mon 17:30 Poster A

Mechanistic models of carcinogenesis: Radiation-induced risk of lung cancer in the Mayak workers — •Sascha Zöllner[1], Mikhail Sokolnikov[2], and Markus Eidemüller[1] — [1]Helmholtz Zentrum München, Institute of Radiation Protection (Germany) — [2]Southern 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 Käs — Soft Matter Physics (PMW), Leipzig University, Germany

During tumor development epithelial cells undergo a remarkable carcinogenetic 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 relationship has not been thoroughly investigated. We aim to classify the significance of Vimentin as a counteracting 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 Tumorigenesis — •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 preneoplastic dynamics from a systematical 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 arrest, aging, 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 tumor 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.

BP 16: Posters: Cell adhesion, mechanics and migration

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

BP 16.1 Mon 17:30 Poster A

Real-time deformability cytometry - a theoretical and experimental analysis — •Alexander Mietke[1,2,3], Oliver Otto[3], Salvatore Girardo[3], Philipp Rosendahl[3], Anna Taubenberger[3], Elke Ulbricht[3], Stefan Golfier[3], Jochen Guck[3], and Elisabeth Fischer-Friedrich[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Strasse 38, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstrasse 108, Dresden, Germany — [3]Biotechnology Center, TU Dresden, Tatzberg 47/49, 01307 Dresden, Germany

Cell stiffness is a sensitive indicator of physiological and pathological changes in cells with many potential applications in biology and medicine. A new method, Real-Time Deformability Cytometry (RT-DC), probes cell stiffness at high throughput by exposing cells to a shear flow in a microfluidic channel allowing for mechanical phenotyping based on single cell deformability. However, observed deformations of cells in the channel are not only determined by cell stiffness, but also depend on flow speed and cell size relative to channel size. Here, we disentangle mutual contributions of cell size, flow speed and cell stiffness to cell deformation by a theoretical analysis in terms of hydrodynamics and linear elasticity theory. Performing RT-DC experiments on both, model spheres of known elasticity and biological cells, we demonstrate that our analytical model predicts the deformation inside the channel and allows for quantification of cell mechanical parameters making cell stiffness accessible in high-throughput measurements.

BP 16.2 Mon 17:30 Poster A

Dynamics of blood platelet spreading on elastic substrates — •Aishwarya Paknikar[1], Rabea Sandmann[1], Noam Nisenholz[2], Assaf Zemel[2], and Sarah Köster[1] — [1]1Institute for X-Ray Physics, Georg-August-Universität Göttingen, Germany — [2]2Institute of Dental Sciences and Fritz Haber Center for Molecular Dynamics, Hebrew University of Jerusalem, Israel

Platelets, essential for repairing of damaged blood vessels spread at the site of injury and impressively rearrange their acto-myosin cytoskele-

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 (Esub in the physiological range of 1-100 kPa) polyacrylamide (PAA) gels. We observe that the final platelet spread area increases with increasing values of Esub and 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 Hartung[1], Morgan Delarue[2], and Oskar Hallatschek[1,2] — [1]MPI DS, Göttingen, Germany — [2]UC 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 microbes this can lead for instance to biofouling [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.

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BP 16.4 Mon 17:30 Poster A

Spreading and force generation of blood platelet dynamics on soft and structured substrates — •Jana Hanke, Rabea 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 influences of these cues, we perform 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 maintained, platelets show an adaptation of spreading to the underlying substrate. By following cellular protrusions over time, we find that the number of filopodia influences the adaptation to the substrate suggesting that the pathways of spreading (via filopodia/lamellipodia) influences how well the platelets can cope with the underlying substrate. In order to study stiffness dependent force generation, we perform time-resolved Traction Force Microscopy (TFM). As blood platelets are much smaller than 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 Meyer[1], Felix Segerer[2], Joachim Rädler[2], and Florian Rehfeldt[1] — [1]3rd Institute of Physics - Biophysics, Georg-August University, Göttingen, Germany — [2]Faculty 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 are 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 life 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 Feulner, Julian Steinwachs, Christoph Mark, Ben Fabry, and Claus Metzner — Biophysics Group, Univ. of Erlangen-Nürnberg

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. We 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 statistics as the training data. Strikingly, 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 — •Chii Jou Chan[1,2], Wenhong Li[2], Jana Scholze[2], Mirjam Schürmann[2], and Jochen Guck[1,2] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, UK — [2]Biotechnology 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 microfluidic optical stretcher. We find that isolated nuclei swell under uniaxial stress 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 Kress — Department of Physics, University of Bayreuth, Bayreuth, Germany

In the process of phagocytosis, cells internalize micrometer-sized objects like bacteria and dead cells, thus being a main function of innate immunity. After the detection of foreign particles, the membrane starts to wrap around the phagocytic target. 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 dynamics of the major regulators. Using the technique of 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 microm-

eters. 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[1], Ulla Nolte[1], Susanne Rappl[1], Michael Beil[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University — [2]Department 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 substrates is 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 Steps of Bacterial Biofilm Formation: Dynamic and Molecular Principles of Surface Based Cell Motility and Mechano-Sensing — •Nora Sauter[1,2], Matteo Sangermani[3], Urs Jenal[2,3], and Thomas Pfohl[1,2] — [1]Department of Chemistry, Universität Basel — [2]Swiss Nanoscience Institute, Universität Basel — [3]Biozentrum, Universität Basel

We use a microfluidic-based optical tweezers set-up to probe the initial steps 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 approaching and adhesion characteristics of Caulobacter to different surfaces - colloid 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[1], Susanne Steeger[1], Stefan Hansen[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Heinrich-Heine-Universität Düsseldorf, Deutschland — [2]Univ.-HNO-Klinik Düsseldorf, Deutschland

In this contribution we report on measurements of the mechanoelastic 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 Youngs modulus in the Hertz model we take 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 appearence.

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. Successive steps $\vec{u}_t$ of the cell's trajectory can locally be described as a discrete persistent random walk, with $\vec{u}_t = q\vec{u}_{t-1} + a\vec{\epsilon}_t$, however, the persistence q and the migratory activity a change over longer timescales. These superstatistical changes can in turn be described by another stochastic process $(q(t), a(t))$, 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 with and without fibronectin coating, and in 3D collagen matrices. The resulting joint distribution and temporal correlations of the superstatistical parameters show distinct and characteristic features depending on the dimensionality and adhesiveness of the environment.

BP 16.13 Mon 17:30 Poster A

Mechano-sensing of cells on elastic substrates — •Galina Kudryasheva and Florian Rehfeldt — 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 microenvironment. 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 actomyosin 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 mechano-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 nanometer precision at a microsecond timescale 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

Analyzing the influence of external shear stress on cellular force generation with cell traction force microscopy — •Maja Gulic[1], Thomas Kerst[1], Manfred Frick[2], Anita Ignatius[3], and Kay-E. Gottschalk[1] — [1]Institute for Experimental Physics, Ulm, Germany — [2]Institute of General Physiology, Ulm, Germany — [3]Institute of Orthopaedic Research and Biomechanics, Ulm, Germany

External shear stress influences cell properties like cell shape or migration. Important components of the cell migration machinery are integrins, the actin cytoskeleton and messenger proteins. Connection of these components leads to assembly of focal adhesions and thus generation of traction forces. Using cell traction force microscopy we have the possibility to examine these forces under different conditions.

We fabricated polydimethylsiloxane micropost arrays via photolithography. Measuring the deflection of a micropost during cell adhesion made it possible to calculate the cellular force. We examined various cell lines, with and without applied shear stress. The AT I like rat epithelial cell line R3/1 and the adenocarcinomic human alveolar epithelial cell line A549, as an in vitro model for a AT II cell, were used in our experiments. Applying shear stress simulates the negative effects of pulmonary diseases whereupon liquid occlusions in the lung might produce fluid wall shear stress during breathing. In addition we examined the osteocyte-like cell line MLO-Y4. Osteocytes are known to react to fluid shear stress occurring in the canalicular system in bones. In vitro studies showed e.g. upregulation of cell proliferation after inducing shear stress.

BP 16.16 Mon 17:30 Poster A

Early cell adhesion on hydrogels with graded stiffness and ligand affinity — •Christina Müller and Tilo Pompe — Universität Leipzig, Institut für Biochemie, Johannisallee 21-23, 04103 Leipzig

Mechanotransduction is known as one control mechanism for several basic cell functions, like proliferation, differentiation and cell death. For a better understanding of mechanotransduction, we investigated early cell adhesion on hydrogels with an independent variation of substrate stiffness and affinity of adhesion ligands to the hydrogel surface. Thin film coatings of maleic acid copolymers on top of polyacrylamide hydrogel layers were fabricated to tune protein binding to the hydrogel surface. The stiffness of the hydrogel was modulated between 2.5 kPa and 9 kPa. Human umbilical vein endothelial cells were monitored during the first two hours of cell adhesion by time-resolved cell traction force microscopy. Three different regimes of traction force generation were found. In the first regime (R0) cells spread fast, but traction forces were negligibly small. In the second regime (R1) spreading slowed down and traction forces increased until they saturated in the last regime (R2). The force curve characteristics, for instance the slope in R1 and the saturation force in R2 were substrate-dependent. From 2.5 kPa to 5 kPa both parameters showed a tremendous increase and leveled off for 9 kPa hydrogels. For the two polymer coatings an offset in the averaged forces additive to the stiffness dependence could be observed in positive correlation to protein affinity to the substrate surface. These results can be interpreted as a superposition of conservative and dissipative processes in cell adhesion.

BP 16.17 Mon 17:30 Poster A

Examining the influence of size and shape of a particle on phagocytic uptake — Iris Kuntz, •Rebecca Michiels, and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Köhler-Allee 102, 79110 Freiburg, Germany

Phagocytosis is the process of a cell engulfing and uptaking a particle. This 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 16.18 Mon 17:30 Poster A

Examining the influence of size and shape of a particle on phagocytic uptake — Iris Kuntz, •Rebecca Michiels, and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Köhler-Allee 102, 79110 Freiburg, Germany

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

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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 Grannemann[1], Ann-Christin Moritzer[1], Helene Schellenberg[1], Astrid Kassner[2], Volker Walhorn[1], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Biophysics, Bielefeld University,Germany — [2]Heart and Diabetes Center NRW, Bad Oeynhausen,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 to ARVC [2,3]. Both proteins 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. The measurements were performed with skin fibroblasts, which serve 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 exposes an explicit gender dimorphism we also investigated the impact of testosterone on the elasticity.

BP 16.20 Mon 17:30 Poster A

Model-based traction force microscopy reveals differential tension in cellular actin bundles — •Christoph A Brand[1,2], Jérôme RD Soiné[1,2], Jonathan Stricker[3], Patrick W Oakes[3], Margaret L Gardel[3], and Ulrich S Schwarz[2] — [1]These authors contributed equally — [2]Institute for Theoretical Physics and BioQuant, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [3]Institute for Biophysical Dynamics, Department of Physics, and The James Franck Institute, University of Chicago, Chicago, IL 60637, USA

Animal tissue cells continuously probe the mechanical properties of their environment, with dramatic consequences for cell adhesion, migration, differentiation and fate. Cellular forces originate mainly from the actomyosin system and are transmitted to the extracellular space via focal adhesions. A method called traction force microscopy has been developed to quantify these forces from the deformation of soft elastic substrates and to correlate them with observable structures of the cytoskeleton. For strongly adherent cells, major force generators are actin stress fibers, which have further been classified into different subtypes. However, the reconstruction of traction fields in this context is an ill-posed problem, which requires the use of regularization techniques. We present a new type of traction force microscopy that abolishes the need for regularization and allows us to directly estimate internal cell forces using a biophysical model for cell contractility. We use this method to demonstrate that ventral stress fibers are typically under higher tension than transverse arcs or dorsal stress fibers.

BP 16.21 Mon 17:30 Poster A

Mechanically tunable biomimetic hyaluronic acid based hydrogels — •Frederike Derksen and Florian Rehfeldt — 3rd Institute of Physics - Biophysics, Georg-August-University, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Mechanical properties of the microenvironment of cells, e.g. matrix elasticity, influence many aspects of cell behavior including morphology, motility and even more complex processes such as differentiation. Therefore, it is important to design and characterize hydrogels for cell culture that resemble the in vivo environment of cells. Cross-linked hyaluronic acid (HA) matrices offer an alternative to conventionally used polyacrylamide hydrogels as HA is biocompatible and therefore

not toxic for cells. Using different thiol modifications of HA, we prepare hydrogels with a well-defined elasticity in the physiologically relevant range of E = 0.1 kPa to 100 kPa, which is much softer than glass or tissue culture plastic. Another advantage is the possibility of preparing 3D culture environments by embedding cells during hydrogel polymerization. Gelation kinetics of the hydrogels were investigated by rheology using oscillatory deformation tests. Both the storage modulus G' as well as the loss modulus G" were measured in order to analyze the viscoelastic properties of the cross-linked hydrogels.

BP 16.22 Mon 17:30 Poster A

Symmetry breaking motility of Flavobacterium johnsoniae — •HsuanYi Chen — Department of Physics, National Central University, Taoyuan, Taiwan

A Flavobacterium johnsoniae moves on a substrate by processive adhesive proteins which are distributed in a close-loop track. Even in a homogeneous medium, the bacterium nevertheless breaks the front-rear symmetry and shows directional movement. I will show that at sufficiently high adhesive protein speed, the distribution of closed bonds between the proteins and the substrate has a bifurcation that leads to a directional movement for the bacterium. Such mechanism has the advantage that the bacterium can tune the adhesive protein speed to detect small gradient of nutrient or toxin in the environment.

BP 16.23 Mon 17:30 Poster A

Alteration of rolling adhesion in aged monocytes. — •Samira Khalaji[1], Lisa Zondler[2], Jochen Weishaupt[2], Veselin Grozdanove[2], Karin Danzer[2], Ulla Nolte[1], and Kay-E Gottschalk[1] — [1]Institut für Experimentelle Physik, Universität Ulm, Ulm, Germany — [2]Klinik für Neurologie , Universitätsklinikum Ulm, Ulm, Germany

Aging is associated with a deterioration in immune function. Consequently susceptibility to inflammation and degenerative age-related diseases are 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 artery walls is an important early step in the development of atherosclerotic lesions. The adhesion of monocytes often takes place at positions with exposed collagen. To study the effect of age on monocyte rolling and adhesion, 'human aged monocyte' (isolated from 8 individuals >48 years old) were compared to 'human young monocytes' (Isolated from 8 individuals 25-36 year old). We measured the adhesion rate and rolling velocity of monocytes on collagen coated microfluidic flow chambers at a shear stress of 0.6 dynes/cm2. The function of cells were compared additionally by their ability to be activated by lipopolysaccharide. Our results shows a significantly higher number of firmly adhered aged monocyte compared to the young monocytes (P=0.022) in LPS stimulated monocytes. This study shows that aging is associated with alterations in monocytes function, which may have beneficial implications for the development of studies regarding age-related diseases.

BP 16.24 Mon 17:30 Poster A

Microtubule-based intracellular transport: a liquid crystal approach — •Marco Linke[1,2], Vytaute Starkuviene-Erfle[2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University — [2]BioQuant, Heidelberg University

Mammalian cells show great variability in cell shape and intracellular structure when grown on planar cell culture substrates with homogeneous protein coating. Therefore micropatterns are increasingly used to normalize their shape and structure, but a quantitative understanding of the resulting cellular organization is missing. In order to investigate the consequences for microtubule-based transport, here we model the microtubule cytoskeleton as a nematic liquid crystal and minimize the free energy functional considering biologically plausible boundary conditions. The resulting nematic director configuration describes the preferred transport direction inside the cell and is used to simulate vesicle transport from the cell periphery towards the perinuclear region. We compare the simulation results to experimental measurements of internalized integrin and investigate changes in the distributions caused by RNAi mediated knockdown of genes that are responsible for the regulation of endocytosis and intracellular transport.

BP 16.25 Mon 17:30 Poster A

Viscoelastic mechanics of non-adhering cells — •Samaneh Rezvani Boroujeni, Abhinav Sharma, and Christoph F. Schmidt — 3rd Institute of Physics - Biophysics, Georg-August-Universität Göttingen, Germany

Cells sense their micro-environment through biochemical and mechanical interactions. They can respond to biochemical and mechanical stimuli by undergoing shape- and possibly volume-changes. To understand such responses, one needs a quantitative model for the mechanical properties of a cell. The key components in determining the mechanical response of a cell are the viscoelastic properties of the actomyosin cortex, effective surface tension, and the osmotic pressure. We probe suspended rounded-up cells by active and passive microrheology and construct a model to describe the roles of the various components.

BP 16.26 Mon 17:30 Poster A

Cell response to lateral constraints — •Andreas Müller and Tilo 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 as 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.

[1] Müller, A., Meyer, J., Paumer, T., Pompe, T. Cytoskeletal Transition in Patterned Cells Correlates with Interfacial Energy Model. Soft Matter, 2014, 10, 2444-2452.

BP 16.27 Mon 17:30 Poster A

Cellular mechanics at the onset of phagocytosis — •Konrad Berghoff, Steve Keller, and Holger Kress — Department of Physics, University of Bayreuth, Universitätsstr. 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 consistent of 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 mechanics 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 bead and cell. We also hypothesize that 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 the role of zipper-like 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 Brownian dynamics 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 loading. The adhesive strength or lifetime of receptor-ligand bond cluster depends on the density of knobs, external loading, and the mean number of receptors per knob. We also simulated the capture efficiency of

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. During phagocytosis invaders larger than a few hundred nanometers are internalized by macrophages followed by lysosome fusion and digestion. A key part of this maturation process is the phagosomal transport from the cell membrane to the perinuclear region. While on average, phagosomes are transported to this region, individual phagosomes undergo complex motion which frequently consists of directed transport with interjacent phases of putative random motion. Up to now it is largely unknown what determines these high phagosome to phagosome variations of the individual transport paths. Natural differences between these phagosomes in vivo are their size and shape as well as the position, where the first contact to the cell membrane and the subsequent engulfment occurs. To investigate these naturally occurring phagosome variations systematically, we move IgG-coupled polystyrene beads with different diameters to well-defined positions at the cell membrane of J774 macrophages by using holographic optical tweezers. By tracking the bead motion during and after internalisation, we are able to characterize the transport of individual phagosomes. Preliminary results indicate that larger particles move faster and in a more persistent way towards the perinuclear region whereas smaller particles move slower with more interjacent phases of random motion.

BP 16.30 Mon 17:30 Poster A

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

Gliding motility is a form of movement observed in unicellular organisms 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, gliding is occasionally arrested by large, stationary adhesion patches. In order to investigate the stochastic dynamics of gliding motility, we derive a model for a propulsion mechanism based on the cooperation of multiple, actively displaced adhesion bonds. We study the dynamic regimes of gliding motility emerging from the binding characteristics of the adhesion bonds, which are described either as slip bonds or catch bonds, and from the effective processivity and force-velocity relation characterizing the displacement of the adhesion bonds. In order to assess the role of flexibility of the cell body, we study the motion of elastically coupled, stiff segments of the basic model.

BP 16.31 Mon 17:30 Poster A

Model analysis of P-Selectin-mediated leukocyte rolling — •Mats Moskopp[1], Andreas Deussen[1], Triantafyllos Chavakis[2], and Peter Dieterich[1] — [1]Institut für Physiologie, TU Dresden, Germany — [2]Klinische Pathobiochemie, TU Dresden, Germany

Invasion of leukocytes from the blood stream into tissue proceeds as coordinated sequence called leukocyte adhesion cascade and is indispensable for an efficient immune response. Numerous proteins realize interactions between leukocytes and vessel covering endothelial cells allowing rolling, adhesion, crawling and transmigration towards the tissue. In this study we observe P-Selectin-mediated rolling of THP1 myelomyonocytic cells in flow chambers where coating densities of P-Selectin are varied. Cell contours are extracted automatically by image-segmentation. The resulting positions of THP1 cells show a mean drift superimposed by intermittent fluctuations. Assuming that these fluctuations result from the properties of the bonds allows to assess their biomechanical properties. Therefore, we construct a simplified biomechanical model incorporating coupling to fluid shear stress, viscoelastic behavior of bonds, force-dependent rupture kinetics, and variations of receptor and ligand densities. Simulations of artificial position data are performed to extract the corresponding biomechanical parameters with Bayesian data analysis. This approach unveils the possibilities and limitations of parameter extraction from position curves and is further applied to experimental data. In summary, the combination of experiments and modeling allows the estimation of biomechanical properties at the nano-scale from observations of the whole cell.

BP 16.32 Mon 17:30 Poster A

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

It is nowadays widely acknowledged that mechanical cues are as important 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 modulus E . While the differentiation process takes several days, the acto-myosin cytoskeleton organisation shows significant differences within the first 24 hours after plating. We investigate the mechanical properties of the nucleus by atomic force microscopy and fluorescence microscopy and demonstrate the impact of substrate elasticity E on nuclear morphology via acto-myosin stress fibres. Elucidating the mechanical coupling of the cytoskeleton and the nucleus might reveal a direct mechanical pathway that alters gene transcription and might impact adult stem cell differentiation.

BP 16.33 Mon 17:30 Poster A

Complex thermorheology of cells — •Enrico Warmt, Sebastian Schmidt, Tobias Kiessling, Anatol Fritsch, Roland Stange, and Josef Käs — Universität Leipzig Faculty of Physics and Earth Sciences, Leipzig, Germany

Temperature has a reliable and nearly instantaneous influence on mechanical responses of cells. We measured thermorheological behaviour of eight common cell types within physiologically relevant temperatures 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, albeit cells with complex temperature responses do not fit the model. These results reveal broad insights into thermally sensitive stress-strain relations of various cell types.

BP 17: Posters: Protein structure and dynamics

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

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, the grid points can be 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 pKA and redox 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 insight into the local deformation during helix formation as a function of chain length (16 to 23 residues). Finally, the method is used to fold the 50-residue-long major pVIII coat protein (fd coat) of the filamentous fd bacteriophage. The results show excellent agreement with experimental structures and atomistic simulations in implicit membrane, demonstrating that such a protocol can serve as a starting point for better-refined atomistic simulations in a multiscale framework.

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 — •Sepideh Sknadary[1], Martin Hussels[1], Thomas Renger[2], Frank Müh[2], Athina zouni[3], Alfred Meixner[1], and Marc Brecht[1,4] — [1]Universität Tübingen, IPTC and Lisa + Center, Tübingen, Germany — [2]Johannes Kepler Universität, Institut für Theoretische Physik, Linz, Austria — [3]Humboldt-Universität zu Berlin, Berlin, Germany. — [4]Zurich University of Applied Science Winterthur (ZHAW), Winterthur, Switzerland

Photosystem II (PSII) is the membrane protein complex of higher plants, green algae and cyanobacteria that uses solar energy to catalyze the electron transfer from water to plastoquinone. The PSII core complex (PSIIcc) is composed of the two intrinsic antenna protein subunits; CP43 and CP47, coordinating 13 chlorophyll a (Chl) a 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 Lesch[1], Vasileios A. Tatsis[1], Andreas Heuer[1], Christian Holm[2], and Jens Smiatek[2] — [1]Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster — [2]Institut für Computerphysik, Universität Stuttgart

Ionic liquids are considered as environmentally friendly compared to organic compounds. Furthermore, they have an ionic character which leads to interesting solvation properties.

We present molecular dynamics simulations of the protein 2GB1 in explicit water and doped with the ionic liquid 1-ethyl-3-methylimidazolium acetate (4.55 mol/l). The solvation of the protein as well as the solvent's structure induced from the protein were investigated on the atomistic scale. The protein is stabilized by the ionic liquid because of specific interactions.

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 depends strongly on the type of coordinates, use of internal coordinates like dihedral angles (dPCA[1]) instead of cartesian atomic coordinates often provides higher resolution, especially for large-amplitude motion e.g. found in folding systems[2]. In contrast to dihedral angles which mainly reflect the behaviour of neighbouring residues in a protein, distances between pairs of atoms also contain information about residues further apart in the primary sequence.

We employ and classify different types of PCA for dimension reduction by quantities based on information theory and on their structural resolution. 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.

[1] Y. Mu, P. H. Nguyen, and G. Stock, Proteins **2005**, *58*, 45.

[2] F. Sittel, A. Jain and G. Stock, J. Chem. Phys. **2014**, *141*, 014111.

BP 17.6 Mon 17:30 Poster A

Insoluble proteins in presence of salt: a computational study — •Patrick Kreissl 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 solvation behavior.

BP 17.7 Mon 17:30 Poster A

Multivalent interaction of hemagglutinin with sialic acid as studied by scanning force microscopy and force spectroscopy — •Valentin Reiter[1], Manuel Gensler[1], Sumati Bhatia[2], Luis Cuellar[2], Daniel Lauster[3], Rainer Haag[2], An-

dreas Herrmann[2], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt-Universität zu Berlin — [2]Institute of Chemistry & Biochemistry, Freie Universität Berlin — [3]Department of Biology, Humboldt-Universität zu Berlin

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 scanning force microscope (SFM) can be used to directly probe the bond strength of single and multiple HA - SA - interactions. SFM 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 disaccharide groups — •anand narayanan krishnamoorthy[1], jens smiatek[2], and christian holm[3] — [1]Institute for Computational Physics,University of Stuttgart — [2]Institute for Computational Physics,University of Stuttgart — [3]Institute 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 AFGP 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 — •Sina Zendehroud, Bernhard Reuter, and 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

Apolipoprotein A1 adsorption at solid/liquid and liquid/air-interfaces — •Susanne Dogan[1], Irena Kiesel[1,2], Matthias Kampmann[1,3,4], Kolja Mende[1], Florian J. Wirkert[1], Michael Paulus[1], Christian Sternemann[1], and Tolan Metin[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Institut Laue-Langevin, 38000 Grenoble, France — [3]DESY, D-22603 Hamburg, Germany — [4]Department 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 DPPA 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 — •João R. Robalo and 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 analogues. 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 — •Sadra Kashef Ol Gheta and 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 < phosphonate, 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 — •Björn Bastian and 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 a few selected system coordinates up to long simulation times 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-

scape without the requirement of input data being correctly Boltzmann weighted. Here, we present an algorithm that can treat full second-order Langevin equations in several dimensions due to more stable estimators. As proof of principle, we demonstrate the recovery of the stochastic fields for a test model.

[1] Schaudinnus N, Rzepiela AJ, Hegger R, Stock G. Data driven Langevin modeling of biomolecular dynamics. J. Chem. Phys. 138, 204106 (2013).

BP 17.14 Mon 17:30 Poster A

Biomolecules at gold-water interfaces: the role of the metal polarization — •Isidro Lorenzo[1], Hadi RAmezani-Dakhel[2], Hendrik Heinz[2], and Marialore Sulpizi[1] — [1]Johannes Gutenberg University Mainz, Staudinger Weg 7 55099 Mainz — [2]Departament of Polymer Engineering, University of Akron, Ohio 44325

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 contribution we aim to provide a characterization of different peptides / gold interactions at a molecular level in order to explain and interpret 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 theory (DFT) calculations are also discussed. Results for aminoacids and nucleic acids nano assembly different gold surfaces are presented.

[1] V. Humblot, A. Tejeda, J. Landousi, A. Vallee, A. Naitabdi, A. Taleb, C.-M. Pradier. Surface Science 2014, 628, 24-29.

[2] Heinz H, Vaia RA, Farmer BL, Naik RR J. Phys. Chem. C 2008, 112, 17281 17290; Heinz H, Farmer BL, Pandey RB, Slocik JM, Patnaik SS, Pachter R, Naik RR. J. Am. Chem. Soc. 2009, 131, 9704-9714

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[1], Nicolas Thewes[1], Thomas Faidt[1], Christian Kreis[2], and Karin Jacobs[1] — [1]Saarland University, Experimental Physics, 66041 Saarbrücken, Germany — [2]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 investigate 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 misfold in bigger amounts it results in serious health impairments like neurodegenerative diseases (i.e. Alzheimer's and prion diseases). In this context the question of the effect of 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 induced a transition from a beta-sheet into a helix conformation. Also the effect of an spatial temperature gradient on a proteinlike designed heteropolymer 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[1,2] and Patrick Huber[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbruecken — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, D-21073 Hamburg

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 pore wall and protein 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 readily 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 Willoweit, Nico Herder, Luisa Sauthof, Neslihan Tavraz, Franz-Josef 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 *Rp*BphP2 (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 Y258F 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

Dielectric relaxation spectroscopy of solvated ubiquitin [1] has shown the sensitivity of the direct current to conformational sampling. Experimentally, 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.

[1] Ban et al. Angew. Chem. Int Ed., 50(48):11437-11440, 2011.
[2] S. C. Kramer and J. Hagemann, ACM TOPC (to appear), https://code.google.com/p/scipal/

BP 17.20 Mon 17:30 Poster A

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 four oxidizing equivalents needed for O-O bond formation at the reaction center, a Mn_4Ca-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 Y_Z. 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 Q_A, 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 multienzyme complexes.

BP 17.22 Mon 17:30 Poster A

Free Energy Decomposition: A Model System with Focus on Entropic Contributions of Water — •Jonas Landsgesell and Jens Smiatek — 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 entropy changes by using internal 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.

BP 18: Membranes and vesicles I (joint BP/CPP)

Time: Tuesday 9:30–12:30 Location: H 1028

Invited Talk BP 18.1 Tue 9:30 H 1028

Multifaceted BAR-domain proteins to shape cell membranes — Coline Prévost[1], Mijo Simunovic[1,2], Henri-François Renard[1], Emma Evergren[3], Harvey McMahon[3], Ludger Johannes[1], Jacques Prost[1], Andrew Callan-Jones[4], and •Patricia Bassereau[1] — [1]Institut Curie, Paris, France — [2]University of Chicago, USA — [3]MRC, Cambridge, UK — [4]University Paris-Diderot, France

Cell plasma membranes are highly deformable and are strongly curved upon membrane trafficking or during cell motility. BAR-domain proteins with their intrinsically curved shape and their interaction with the actin cytoskeleton are involved in many of these processes.We have used in vitro experiments to study the interaction of BAR-domain proteins with curved membranes for understanding how inverted-BAR domain proteins such as IRSp53 are involved in the generation of filopodia and how the BAR-domain protein endophilin A2 can scission tubules induced by Shiga toxin internalization. We have pulled membrane nanotubes of controlled curvature from Giant Unilamellar Vesicles (GUVs) using optical tweezers and micropipette aspiration. With this approach coupled to theoretical modeling, we have evidenced for IRSp53 a protein phase separation along the nanotube occurring at low protein density for weakly curved membranes. It can explain the in vivo local clustering of the protein, a primary step in filopodia generation that precedes the recruitment of other partners. We have also shown that endophilin A2 scaffolds and stabilizes tubes in static conditions but induces scission when the tube is dynamically extended.

BP 18.2 Tue 10:00 H 1028

Measuring the composition-curvature coupling in binary lipid membranes by computer simulations — •Israel Abraham Barragán Vidal and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

This manuscript contributes to the field of biophysics, in particular, the formation of local composition inhomogeneities in model membranes (rafts). We present a simple phenomenological model to describe the effective coupling between curvature and composition in a two-component lipid bilayer. Beside the elastic contribution to the free energy and an intrinsic coupling between curvature and composition, our model also includes contributions from a composition- and curvature-dependent free energy of mixing.

Using an implicit-solvent model we extract the intrinsic composition-curvature coupling from computer simulations with planar and highly curved cylindrical bilayers. Beside the effective curvature-composition coupling, our computational strategy offers an alternative to obtain the spontaneous curvature from moments of the stress profile across a bilayer membrane. We expect this strategy will find further applications.

BP 18.3 Tue 10:15 H 1028

New Strategy to Study a Single SNARE Mediated Membrane Fusion Event — •Jose Nabor Vargas[1], Kewin Howan[2], Andrea Gohlke[2,4], Ralf Seemann[1,3], Jean-Baptiste Fleury[1], and Frederic Pincet[2,4] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Laboratoire de Physique Statistique, Ecole Normale Supérieure, 75005 Paris, France — [3]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [4]Department of Cell Biology, School of Medicine, Yale University, CT 06520 New Haven, USA

We present an approach to explore the properties of a single SNARE mediated membrane fusion event in a microfluidic chip. In a first step, a single free standing lipid membrane is generated at a defined position with the Droplet Interface Bilayer technique (DiB). In a second step, we inject a solution of divalent cations (Calcium, Ca2+) and small unilamellar vesicles functionalized with T-SNARE proteins (T-SUVs) around the planar membrane using a volume controlled flow. The presence of calcium mediates the direct fusion of the vesicles with the planar membrane, which is incorporating the proteins into the membrane. In a third step, we remove the calcium and the T-SUVs with a buffer solution. After this washing step, a solution of small unilamellar vesicles functionalized with V-SNARE proteins (V-SUVs) is injected around the planar membrane. And finally, we study single fusion event with good optical and electrical access.

BP 18.4 Tue 10:30 H 1028

Mechanics of the cell membrane coupled to the actomyosin cortex — •Jochen A. M. Schneider and Guillaume Salbreux — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

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

Using Markov state models to obtain free energies of (de)mixing — •Djurre H. de Jong and Andreas Heuer — 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.

15 min break

BP 18.6 Tue 11:15 H 1028

The Mechanism of Phagocytosis: Two Stages of Engulfment — •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 fractional engulfment as a function of time and demonstrate that phagocytosis occurs in two distinct stages. During the first stage, engulfment 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 explains why 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 Beta — 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 — •Patrick Paul[1], Nina Hobi[2,3], Susanne Rappl[1], Thomas Haller[3], Manfred Frick[2], and Kay E. Gottschalk[1] — [1]Institute of Experimental Physics, Ulm University, Ulm, Germany — [2]Institute of General Physiology, Ulm University, Ulm, Germany — [3]Department of Physiology and Medical Physics, Division of Respiratory Cell Physiology, Medical University of Innsbruck, Innsbruck, Austria

Type II pneumocytes produce and secrete pulmonary surfactant into the alveoli of the lung. Surfactants lower the surface tension between the air-liquid interface within the alveoli. Surfactant consists of multilayers of lipids, mainly phosphatidylcholine, and specific, embedded surfactant proteins (SP-B and SP-C). Physiological studies demonstrated that these proteins play a major role in the stability of the surfactant [1]. However, the precise nature and exact structure of how these proteins are arranged within the lipids is yet unknown.

Hence, we imaged the structure of SP-B and SP-C assembly within a single-lipidlayer surfactant with single molecule force spectroscopy.

Reference: [1] Jesús Pérez-Gil, Structure of pulmonary surfactant membranes and films: The role of proteins and lipid-protein interactions, 2008, Biochimica et Biophysica Acta 1778, 1676-1695

BP 18.9 Tue 12:00 H 1028

Local viscosities near plasma membranes of living cells — •Felix Jünger and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Georges-Koehler-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 γ changes strongly with the distance to the interface. In our work we use photonic force microscopy (PFM) to investigate how γ changes when an optically trapped 1μm 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 Λ(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 Λ(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[1], Vladimir Kreslavski[2], Galina N. Schirshikova[2], Csongor Keuer[1], Sergei K. Zharmukhamedov[2], Suleyman I. Allakhverdiev[2], and Thomas Friedrich[1] — [1]Institute of Chemistry, Bioenergetics, TU Berlin, Berlin, Germany — [2]Institute of Basic Biological Problems, RAS, Pushchino, Moscow Region, Russia

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 naphthalene (Naph), a lipophilic PAH, was studied 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 as well as swelling of thylakoids and distortion of cell plasma membranes. It could be shown that Naph treated leaves of Arabidopsis thaliana show enhanced DCF fluorescence in the thylakoid membrane. 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 Location: H 1058

Invited Talk BP 19.1 Tue 9:30 H 1058

Emerging social behaviour during aggregation in Dictyostelium discoideum — Giovanna De Palo[1], Darvin Yi[2], Thomas Gregor[2], and •Robert Endres[1] — [1]Department of Life Sciences, Imperial College London, UK — [2]Joseph 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

Adaption of fluid flow in the slime mold *Physarum polycephalum* — •Karen Alim, Gabriel Amselem, François Peaudecerf, Anne Pringle, and Michael Brenner — 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 *P. 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 individuals network growth and adaptation.

BP 19.3 Tue 10:15 H 1058

Foraging in the Slime Mold Physarum polycephalum — •Jonghyun Lee, Christina Oettmeier, and Hans-Günther Döbereiner — 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 is dependent on environmental conditions and life stage. We find oscillating microplasmodia 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 microplasmodia. The number of satellites forming out of a spherical patch of single microplasmodia 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 Pönisch[1], Christoph Weber[1], Khaled Alzurqa[2], Hadi Nasrollahi[2], Nicolas Biais[2], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Brooklyn 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 are mediated by type IV pili, 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 Ehrig[1], Cécile M. Bidan[2], Philip Kollmannsberger[3], Peter Fratzl[1], and John W. C. Dunlop[1] — [1]Max Planck Institute of Colloids and Interfaces, Germany — [2]Université Joseph Fourier, Grenoble, France — [3]Laboratory 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 from 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 design 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 Kaliman[1], Carina Wollnik[2], Damir Vurnek[1], Florian Rehfeldt[2], and Ana-Sunčana Smith[1] — [1]Institut fur Theoretische Physik, FAU, Erlangen — [2]3rd Institute of Physics-Biophysics, Uni Gottingen

Tissue growth is a complex and indisputably important process but

despite all the effort in past decades mechanism remains unclear. As model system for such study we have chosen MDCK II cell line seeded on polyacrylamide gels or glass substrates. In most common scenario cluster of cells forms radial monolayers with very dense bulk surrounded by a low density ring of a moving and proliferating edge. To elucidate the mechanism behind compartmentalization to bulk and edge we have simulated cluster growth with Voronoi tessellation model. In the simulation we use measured area growth of the cluster, proliferation rates and speed distribution inside the cluster. Our aim is to distinguish passive from active mechanism during epithelial tissue development. Furthermore, we answer is organization of cells in the tissue random. To do so we compare various morphological parameters of real tissue with randomly distributed mono-disperse and poly-disperse circles and ellipses. We find that elongation and size distribution of nuclei predetermines cell shapes and correlations in the tissue. Lastly, we write free energy functional as a sum of morphological and elastic term and prove that tissue minimizes energy as it approaches steady state density and undergoes phase transition at intermediate densities when surface tension of cell membrane starts to play a role.

BP 19.7 Tue 11:30 H 1058

Hydrodynamic theory of developing epithelia — •Marko Popovic[1], Raphael Etournay[2], Matthias Merkel[1], Amitabha Nandi[1], Frank Jülicher[1], Suzanne Eaton[2], and Guillaume Salbreux[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

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 rearrange their neighbors, 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.

BP 19.8 Tue 11:45 H 1058

Dynamics and precision of mouse neural tube patterning — •Marcin Zagórski[1], Anna Kicheva[2], Gašper Tkačik[1], James Briscoe[2], and Tobias Bollenbach[1] — [1]Institute of Science and Technology (IST) Austria, Klosterneuburg — [2]Medical Research Council (MRC), National Institute for Medical Research, London, UK

Early in vertebrate development, different neuronal subtypes are generated from neural progenitor cells arrayed along the dorsal-ventral axis of the neural tube. This pattern of neural progenitors is established by morphogens - signaling molecules secreted by cells in restricted source regions at the tissue boundaries. In the neural tube, the morphogens Shh and BMP form opposing concentration profiles which provide positional information to cells and induce the expression of target genes, such as Nkx6.1 and Pax3, at defined positions. It is not understood how the two morphogen signals and the regulatory interactions between target genes together determine the target gene pattern. To address this issue, we measured the two signaling gradients. We quantified the positional information available to the cells with both direct and Gaussian approximation techniques. Early in development, positional information is high, enabling patterning at a precision of three cell diameters; after 20h, however, precision declines significantly in the middle region. Still, after 30h, the expression boundary between Pax3 and Nkx6.1 is precisely specified in the middle. These results suggest that cells in the central neural tube integrate positional information from two opposing morphogen gradients early in development to achieve precise target gene boundary positions at later stages.

BP 19.9 Tue 12:00 H 1058

Robust balance of stochastic stem cell fate through revesible differentiation — •Philip Greulich[1] and Benjamin D. Simons[1,2] — [1]TCM Group, Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Gurdon Institute, University of Cambridge, Cambridge, UK

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 stay constant over time, i.e. proliferation and differentiation of stem cells must be perfectly balanced (homeostasis). Otherwise, tissues degenerate or dysplastic lesions develop, which can evolve into cancer. In recent years studies have shown that in many mammalian tissues the stem cell fate (stem cell duplication vs. differentiation) is decided stochastically, with equal chances for gain (duplication) and loss of stem cells (differentiation). Nonetheless, the mechanism to maintain the balance in cell fate outcomes remains largely unknown.

Here I present a non-equilibrium stochastic model for cell fate dynamics, where balance of cell fate outcomes follows automatically from two properties of the cells: (i) the cells' potential to reversibly differentiate independent from cell divisions, (ii) their ability to sense and respond to mechanical cues. The model is able to accurately reproduce experimental cell lineage data of living tissues and, remarkably, shows a high robustness towards failure of regulatory pathways. This mechanism 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.

BP 19.10 Tue 12:15 H 1058

Optical Modulation Transfer by the Vertebrate Retina — •Kaushikaram Subramanian[1], Zuzanna Blaszczak[2], Matthäus Mittasch[1], Alfonso Garcia Ulloa[1], Jochen Guck[3], and Moritz Kreysing[1] — [1]The Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [3]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.

BP 19.11 Tue 12:30 H 1058

Experiments and Model: Buckling instability of Regenerating Tissues — •Benjamin Friedrich[3], Hans Kubitschke[2], and Claus Fütterer[1] — [1]Translational Centre of Regenerative Medicine, Leipzig and Biophysical Tools GmbH, Leipzig, Germany — [2]Experimentalphysik I, Universität leipzig, Leipzig, Germany — [3]Max-Planck Institut für die Physik komplexer Systeme, Dresden, Germany

We propose tissue toroids as an ideal minimal model geometry to quantitatively study regeneration, morphogenesis and wound healing. It minimizes nutrient depletion effects which can even lead to necrosis. We report experiments with *Hydra vulgaris* epithelium revealing that tissue rings fold by an original mechanism. This is accompanied by a highly self-organized acto-myosin string spanning along the inner side of the toroid. This folding initiates a transition to a spherical shape and the full regeneration of viable organism. We propose a minimal theoretical description that conceptualizes this mechanical transition in terms of a buckling instability of the tissue torus driven by active mechanical forces. We predict a critical contractility threshold, in agreement with our experimental observations. This versatile model system allows to study and understand morphological transitions in a well defined minimal set-up.

BP 20: Microswimmers, Active Liquids II (joint DY/BP/CPP)

Time: Tuesday 9:30–12:30 Location: BH-N 128

BP 20.1 Tue 9:30 BH-N 128

Trapping of active particles in inhomogeneous systems — •Martin P. Magiera, Kevin Schröer, and Lothar Brendel — Fakultät für Physik, Universität Duisburg-Essen

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 tumble rates of bacteria or inhomogeneous drive of men-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 larger agglomerates generated by dynamical clustering [Fily and Marchetti, PRL **108**, 235702] and pinned to the passivity region.

BP 20.2 Tue 9:45 BH-N 128

Statistics of passive tracers in an active fluid — •Levke Ortlieb[1], Matthias Mussler[1], Christian Wagner[1], Thomas John[1], Philippe Peyla[2], and Salima Rafaï[2] — [1]Universität des Saarlandes — [2]Université Joseph Fourier - CNRS - LIPHY, Grenoble

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 swims as a puller. 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.

BP 20.3 Tue 10:00 BH-N 128

Characterization of Swimming Bacillus Subtilis — •Javad Najafi[1], Thomas John[1], Gert Bange[2], and Christian Wagner[1] — [1]Experimental Physics, Saarland University, D-66123 Saarbruecken, Germany — [2]LOEWE 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 the swimming behavior and efficiency. We study wild type strain of bacillus subtilis as a model system to unravel a few fundamental questions on swimming behavior of bacteria. Our microorganism is a peritrichous bacterium with about 25 flagella, and uses run and tumble strategy to explore its surrounding. Using dark field microscopy and tracking of single cell movements, we calculate statistics of swimming velocity, running and tumbling times, turning angles, diffusion coefficients and the temporal auto-correlations in changes of swimming directions. In further steps, we will investigate the influence of number of flagella on genetically engineered bacillus subtilus in aforementioned quantities.

BP 20.4 Tue 10:15 BH-N 128

Non-linear dynamics of self-organized ciliary beats — •pablo sartori and frank julicher — Max Planck Institute for the Physics of Complex Systems. Noethnitzer Strasse 38 , 01187, Dresden, Germany.

The dynamic bending of cilia is driven by forces generated by dynein motor proteins. These forces slide adjacent microtubule doublets within the cilium. 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 cilium, which are regulated by local strains such as sliding or cuvature. 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 regulation, 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.

BP 20.5 Tue 10:30 BH-N 128

Simulation of a microswimmer consisting of a four bead ring — •Hendrik Ender and Jan Kierfeld — Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund

Bead-spring structures undergoing cyclic shape changes in a viscous liquid can serve as model systems for artificial microswimmers. Closed ring-like bead-spring models can propel by cyclic shape changes, for example, induced by cyclic expansion and contraction of springs. Using multi-particle collision dynamics, we simulate a four-bead swimmer model in which the spheres are linked into a square-shaped ring structure. We show that cyclic changes of linker lengths give rise to a net swimming motion. The model can be generalized by including more beads into the ring structure and represents the first step towards the simulation of bigger ring or spherical swimmers, which propel by cyclic swelling and shrinking.

BP 20.6 Tue 10:45 BH-N 128

Spontaneous chiral symmetry breaking in model bacterial suspensions — Rebekka E. Breier[1], Robin L. B. Selinger[2], Giovanni Ciccotti[3,4], Stephan Herminghaus[1], and •Marco G. Mazza[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany — [2]Chemical Physics Interdisciplinary Program, Liquid Crystal Institute, Kent State University, Kent, OH, USA — [3]Department of Physics, University of Rome "La Sapienza", P.le A. Moro 5, 00185 Rome, Italy — [4]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

Chiral symmetry breaking 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 stable (or long-lived metastable) collective states that exhibit chiral organization although the interactions are achiral. We elucidate under which conditions these chiral states will emerge and grow to large scales. We also study a related equilibrium model that clarifies the role of orientational fluctuations.

15 min. break

BP 20.7 Tue 11:15 BH-N 128

Velocity distributions in active Brownian suspensions — •Zahra Mokhtari and Annette Zippelius — Institute for Theoretical Physics, Georg-August University of Goettingen

We study numerically a model of self-propelled polar disks in suspension. The active particles interact via hard-core elastic interactions and are driven 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 furthermore 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.

BP 20.8 Tue 11:30 BH-N 128

Experimental setup for 3D tracking of artificial active microswimmers — •Gunnar Klös, Carsten Krüger, Corinna C. Maass, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

During solubilisation in an aqueous surfactant solution well above the critical micelle solution, droplets of nematic liquid crystal show self-propelled swimming, driven by a Marangoni flow at the droplet interface [1]. These active pusher-type swimmers provide a potential physical model-system for micro-bioswimmers. We expect dimensional confinement to have a significant impact on their dynamics [2].

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.

[1] S. Herminghaus et al., Soft Matter **10**, 7008 (2014). [2] E. Lauga et al., Biophys. J. **90**, 400 (2006). [3] J. Huisken et al., Science **305**, 1007 (2004).

BP 20.9 Tue 11:45 BH-N 128

Liquid crystal droplets as artificial microswimmers — Carsten Krüger, Gunnar Klös, Chenyu Jin, Corinna 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 confinements, the collective behavior, and the influence of the nematic or isotropic state of the mesogenic droplets.

[1] S. Herminghaus, C. C. Maass, C. Krüger, S. Thutupalli, L. Goehring, and C. Bahr, Soft Matter **10**, 7008 (2014).

BP 20.10 Tue 12:00 BH-N 128

3D-tracking reveals how sperm find the egg — Jan F. Jikeli[1], Luis Alvarez[1], •Benjamin M. Friedrich[2], and Laurence Wilson[3] — [1]CAESAR, Bonn, Germany — [2]MPI PKS, Dresden, Germany — [3]University of York, York, UK

Sperm cells are guided to the egg by chemical cues in a process termed chemotaxis. We have previously put forward a theory of how sampling a concentration gradient along helical paths allows sperm of marine species to steer up-gradient [1]. Now, high-speed tracking in three space dimensions allows to probe sperm navigation live. 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].

[1] B.M. Friedrich *et al.*: Chemotaxis of sperm cells, *PNAS* **33**, 2007. [2] L. Alvarez *et al.*: The computational sperm cell, *Trends in Cell Biology* **24**, 2014.

BP 20.11 Tue 12:15 BH-N 128

Complex lane formation in asystem of dipolar mircroswimmers — •Florian Kogler and Sabine H. L. Klapp — Institute of Theoretical Physics, Secr. EW 7-1, Technical University Berlin, Hardenbergstrasse 36, D-10623 Berlin, Germany

We investigate the non-equilibrium structure formation of an experimentally motivated [1] two-dimensional (2D) binary system of dipolar colloids propelling in opposite directions. Using Brownian Dynamics simulations we find a transition towards a laned state, reminiscent of the laning transition in colloidal systems with isotropic repulsive inter actions. However, the strongly anisotropic dipolar interactions induce two novel features: First, lanes are characterized by a complex internal structure. Second, the laning transition displays reentrance with respect to the interaction strength. We interprete our findings by simple theoretical arguments relating the observed behaviour to general equilibrium properties of phase-separating fluids [2].

[1] S. Gangwal and O. J. Cayre and M. Z. Bazant and O. D. Velev, PRL 100 (2008) 058302.

[2] F. Kogler and S. H. L. Klapp, preprint

BP 21: Complex Contagion Phenmomena (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 networks 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[1], Li Chen[2], Weiran Cai[3], and Peter Grassberger[4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Robert Koch- Institute, 13353 Berlin, Germany — [3]TU Dresden, Germany — [4]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.
[1] F. Ghanbarnejad, M. Gerlach, J. M. Miotto, and E. G. Altmann, "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 chen[1,2] and •dirk brockmann[1,2] — [1]Robert-Koch Institute, Berlin, Germany — [2]Humboldt 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 as 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 diseases — •Olga Baranov[1] and Dirk Brockmann[1,2] — [1]Robert Koch Institut, Berlin — [2]HU 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 'egocentric' 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 modelled 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 where the interaction of economic constraints with disease spread transforms 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 into "explosive" spread if the cost of recovery is above a critical cost. The transition to this explosive regime is discontinuous – once there are signs of a transition it can no longer be prevented. In the second case I will show you how the information resolution available to individuals determines the effectiveness of voluntary vaccination decisions. Although an epidemic cannot be contained when individuals use global information, the successful eradication of a disease can occur in an intermediate region of information resolution between the local and the global.

BP 21.7 Tue 12:15 MA 001

Virus transmission on a network of injecting drug users — •Cornelia Metzig 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 highy clustered, assortive 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 is. These phenomena can be captured in a network model where each connection describes only one sharing event. Simultaneous rewiring of the network and transmission are 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 21.8 Tue 12:30 MA 001

Spatio-temporal dynamics of the cholera epidemic of 1831/1832 in Austria — •Michael Leitner[1] and Gero Vogl[2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — [2]Fakultät 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 Weinviertel in Lower Austria (approx. 5000 km^2), 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 analyzes 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 Belik[1,2], Florian Fiebig[1], and Philipp Hövel[1] — [1]Institut für Theoretische Physik, TU Berlin — [2]Helmholtz-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 epidemics 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 Koher, Lucian Willareth, Hartmut Lenz, 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 thereby. We present an intuitive algebraic formalism by contrast, which is explicitly based on temporal networks and which allows to calculate potential paths of an infection. By applying the idea to a SIR (susceptible-infected-recovered) type of disease, we will present an elegant way to find all possibly affected nodes of an outbreak. The method can be efficiently implemented and will be demonstrated on a recorded data set.

BP 22: Posters: Cytoskeletal filaments

Time: Tuesday 14:00–16:00 Location: Poster A

BP 22.1 Tue 14:00 Poster A

Novel class of microtubules regulates the forces present in the mitotic spindle — •Maja Novak[1], Janko Kajtez[2], Anastasia Solomatina[2], Matko Glunčić[1], Iva M. Tolić[2,3], and Nenad Pavin[1] — [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 connect chromosomes with the spindle poles, exert forces on the chromosomes via protein complexes termed kinetochores. However, the forces acting on k-fibers and kinetochores are not known. We introduce a simple model in which pairwise k-fibers are described as elastic slender rods, with their tips being connected in a freely joint manner. Model includes a novel class of microtubules, termed bridging 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 of 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.

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 — •Clément Hémonnot[1], Oliva Saldanha[1], Rita Graceffa[1], Harald Herrmann[2], Britta Weinhausen[3], Manfred Burghammer[3], and Sarah Köster[1] — [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 windows, 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 core 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.

BP 22.3 Tue 14:00 Poster A

Object-adapted trapping and shape-tracking to probe a bacterial protein chain motor — •Julian Roth, Matthias Koch, and Alexander Rohrbach — Albert-Ludwigs-Universität Freiburg

The helical bacterium Spiroplasma is a motile plant and anthropod pathogen which swims by propagating pairs of kinks along its cell body. As a well suited model system for bacterial locomotion, understanding the cell's molecular motor is of vital interest also regarding the combat 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 ribbon's protein subunits.

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 Saldanha, Martha Brennich, Clément Hémonnot, Rita Graceffa, and Sarah Köster — Institute for X-ray Physics, Uni Göttingen

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 bundle 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.

BP 22.5 Tue 14:00 Poster A

Molecular assembly studied in microfluidic channels using fluorescence cross correlation spectroscopy — •Viktor Schroeder[1], Bernd Nöding[1], Harald Herrmann[2], and Sarah Köster[1] — [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 diffusive 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 data are collected at different 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.

BP 22.6 Tue 14:00 Poster A

Microrheological Properties of Keratin 8/18 Networks — •Tobias Neckernuss[1], Ines Martin[1], Katinka Mertens[1], Tobias Paust[1], Harald Herrmann[2], Michael Beil[3], and Othmar Marti[1] — [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 $MgCl_2$. With an optical tweezers we are able to determine mechanical properties of the network by trapping and exciting an embedded polystyrene bead to oszillations. The moving bead exerts a force which is transferred via the network to 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

microrheology.

BP 22.7 Tue 14:00 Poster A

Elastic Properties and Morphological Instability of Semiflexible Filament Networks: Application to Dendritic Actin Networks — •Thomas Stöter[1,3], Karin John[2,3], Denis Caillerie[4,5], and Chaouqi Misbah[2,3] — [1]Otto-von-Guericke Universität Magdeburg, FNW/ITP, D-39106 Magdeburg — [2]Univ. Grenoble Alpes, LIPHY, F-38000 Grenoble, France — [3]CNRS, LIPHY, F-38000 Grenoble, France — [4]Univ. Grenoble Alpes, 3SR, F-38000 Grenoble, France — [5]CNRS, 3SR, F-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 a 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.

BP 22.8 Tue 14:00 Poster A

Drebrin-like protein (DBN-1) is a novel sarcomere component which stabilizes actin filaments during muscle contraction — Eugenia Butkevich[1], Kai Bodensiek[1], Nikta Fakhri[1], Kerstin von Roden[1], Iwan T. Schaap[1,2], Irina Majoul[3], Christoph F. Schmidt[1], and •Dieter R. Klopfenstein[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Center for Nanoscale Microscopy and Molecular Physiology of the Brain (CNMPB), Göttingen — [3]Institute of Biology, University of Lübeck, Ratzeburger Allee 160, 23538 Lübeck - Germany

Actin filament organization and stability in the sarcomeres of muscle cells are critical for force generation. Here, we have identified and functionally characterized a C. elegans drebrin-like protein DBN-1 as a crucial constituent of the muscle-contraction machinery in the nematode. In vitro, DBN-1 exhibited actin filament binding and bundling activity. High-resolution AFM showed single DBN-1 molecules decorating the sides of actin filaments. In vivo, DBN-1 is expressed in body wall muscles constituting an essential sarcomere component. Surprisingly, during muscle contraction, DBN-1 alternated location between myosin- and actin-rich regions of the myofilament lattice likely regulating proper spacing of alpha-actinin and tropomyosin. A loss-of-function mutation in dbn-1 resulted in the partial depolymerization of F-actin upon muscle contraction. Taken together, DBN-1 organizes the muscle contractile apparatus maintaining the spatial relationship between actin-binding proteins and strengthening actin filaments by bundling.

BP 22.9 Tue 14:00 Poster A

Mechanical properties of single Vimentin Filaments — •Johanna Block[1], Andrea Candelli[2], Bernd Nöding[1], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]Physics of Living Systems, VU Amsterdam, Netherlands

Intermediate Filaments (IFs) are one of the three major components of the cytoskeleton of eukaryotic cells. Research during the last decade gave evidence that the IFs play a fundamental role for the morphology and the mechanical properties of cells, especially in cells that are subjected to mechanical stress. By analyzing single vimentin IFs with optical tweezers in solution - and thus avoiding influences by substrates (AFM) or a dense network (rheology) - we expect to gain deeper insights into the mechanical properties of this important cellular building block. Simultaneously imaging the filaments ensures that we measure single filaments and provides the opportunity to relate the mechanical behavior to the structural build-up of the filaments. Our results show major differences in stability and stiffness between homogenous and polymorphous vimentin filaments. We are able to reproduce the high stretchability of vimentin filaments up to 2.5 times of their length but in contrast to what was expected from simulations with comparatively low forces (less than 1 nN). Experimental data and theoretical modeling enables us to describe the mechanical properties of single vimentin filaments.

BP 22.10 Tue 14:00 Poster A

active transport along cytoskeletal filaments in the presence of anisotropy — •zeinab sadjadi and m reza shaebani — Department of Theoretical Physics, Saarland University, Saarbrucken, 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 of anisotropy are investigated in the framework of a previously developed analytical approach, and the results are compared with Monte Carlo simulations.

BP 22.11 Tue 14:00 Poster A

Cooperative Microtubule Dynamics within a closed Elastic Membrane — •Jonas Hegemann and Jan Kierfeld — TU Dortmund, 44221 Dortmund, Germany

Microtubules as an essential part of the cytoskeleton are known to interact mechanically with the cell membrane. Since local pertubations 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 microtubule oscillations from catastrophe and rescue events synchronize. Furthermore, we show that the centrosome performs a random walk.

BP 22.12 Tue 14:00 Poster A

Active Microrheology: Mechanical Properties of Keratin 8/18 Networks — •Katinka Mertens[1], Tobias Neckernuss[1], Tobias Paust[1], Ines Martin[1], Harald Herrmann[2], Michael Beil[3], and Othmar Marti[1] — [1]Institute for Experimental Physics, Ulm University, D-89081 Ulm, Germany — [2]Division of Molecular Genetics, German Cancer Research Center, D-69120 Heidelberg, Germany — [3]Department of Internal Medicine I, Ulm University, D-89081 Ulm, Germany

Intermediate filaments are part of the cytoskeleton and increase the mechanical stability of cells. Keratin 8 and 18 are common intermediate filaments in epithelial cells. We investigate mechanical properties of keratin 8/18 networks using active multi-point microrheology. Polystyrene beads, embedded in the keratin networks, are dynamically deflected with an optical trap. Surrounding beads are excited due to the transmission of stress by the network. Correlating the motion of the beads, we determine the isotropy of networks and their force transmission. Thus, we explore the locally complex tensorial elastic response of heterogeneous networks.

BP 22.13 Tue 14:00 Poster A

Stochastic mechanochemical simulation of microtubule dynamics — •Matthias Schmidt and Jan Kierfeld — Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund

Microtubules are filaments in eukaryotic cells made of alpha-beta-tubulin heterodimers which display a complex polymerization dynamics involving catastrophe and rescue events. This dynamics is a result of the interplay of polymerization, hydrolysis, and mechanical forces within the microtubule, which arise from dimer-bending due to hydrol-

ysis.

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, dimer-dependent depolymerization and hydrolysis 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 Jourdain[1], Anne Bernheim[2], and Karsten Kruse[1] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Ben 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 Golde[1], Martin Glaser[1], Carsten Schuldt[1], Jörg Schnauss[1], Harald Herrmann[2], and Josef Käs[1] — [1]University of Leipzig, Faculty of Physics, Soft Matter Physics Division, Leipzig, Germany — [2]German 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 — •Franziska Decker[1,2], Joachim Rosenberger[1,2], and Jan Brugués[1,2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Max 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 proteins turn over within 20s 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 do 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 Rieckhoff[1,2], Franziska Decker[1,2], Joachim Rosenberger[1,2], and Jan Brugues[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max 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 cryogenic and living *Dictyostelium discoideum* — •Marius Priebe[1], Marten Bernhardt[1], Christoph Blum[2], Marco Tarantola[2], Eberhard Bodenschatz[2], and Tim Salditt[1] — [1]Georg-August-Universität Göttingen, Institut für Röntgenphysik — [2]Max-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 differential phase contrast is evaluated in terms of the projected electron density and additional x-ray fluorescence aquisitions 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 — •Mohammadhosein Razbin[1], Martin Falcke[2], Panayotis Benetatos[3], and Annette Zippelius[1] — [1]Max Planck Institute for Dynamics and Selforganization, Am Fassberg 17 and Institute for Theoretical Physics, Georg August University, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany; — [2]Max Delbrück Center for Molecular Medicine, Robert Rössle Str. 10, 13092 Berlin, and Dept. of Physics, Humboldt University, Newtonstr. 15, 12489 Berlin, Germany — [3]Department 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 forces on the membrane. The forces 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 Faivre, and Stefan 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.

BP 22.21 Tue 14:00 Poster A

Lateral Filopodial Movement in Fibroblasts on Microcontact Printed Substrates — •Julia Strübig, Erik Bernitt, and Hans-Günther Döbereiner — Institut for Biophysics, University of Bremen, 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 (Oldenbourg 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, Saarbrucken, 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 molecular 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* — •Marius Priebe[1], Marten Bernhardt[1], Christoph Blum[2], Marco Tarantola[2], Eberhard Bodenschatz[2], and Tim Salditt[1] — [1]Georg-August-Universität Göttingen, Institut für Röntgenphysik — [2]Max-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

Time: Tuesday 14:00–16:00 Location: Poster A

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 Equation 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.

[1] I. Goychuk, arXiv:1410.2416 [physics.bio-ph] (2014).
[2] I. Goychuk, Adv. Chem. Phys. **150**, 187 (2012).
[3] I. Goychuk, V. Kharchenko, R. Metzler, PLoS ONE **9**, e91700 (2014); Phys. Chem. Chem. Phys. **16**, 16524 (2014).

BP 23.2 Tue 14:00 Poster A

A mechanism to generate stable microtubule overlaps — Dennis Johann, Debajit Goswami, •Christopher Zapp, and Karsten Kruse — Saarland University, Saarbrücken, Germany

The mitotic spindle is a structure generated during cell division that serves to segregate the chromosomes onto the two daughter cells. It consists of microtubules spreading from each of the cell poles towards the division plane. In the spindle, the minus-ends of the tubules are pointing towards the poles, thus generating overlaps of antiparallel filaments near the centre of the cell that are stabilized by proteins, so-called crosslinkers. Controlling these overlaps is vital to the cell as it influences the physical properties of the spindle. In this work, we study a mechanism to generate and control stable overlaps of antiparallel microtubules using the interplay between different crosslinking proteins.

BP 23.3 Tue 14:00 Poster A

Towards synthetic molecular motors: a model study — •Amartya Sarkar and Alexander Mikhailov — Fritz Haber Institute, Berlin 14195, Germany

We study the model of a synthetic molecular motor, whose operation closely emulates that of real molecular motors. The motor is described in terms of an elastic network and is able to perform cyclic conformational motions which in turn is capable of uni-directionally transporting a filament. The mechano-chemical motions are due to energy supplied by the binding of a ligand, its conversion to a product, and the subsequent release of the product. Stochastic simulations of this model motor system under the conditions of both weak and strong coupling with the filament, under varying temperatures, has been performed. A continuous transition between two regimes of operation, from that a deterministic ratchet mechanism to a Brownian ratchet mechanism, has been demonstrated. Further it is shown that the mo-

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 Location: Poster A

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

Modelling the Red Blood Cell membrane — •Daniel Schmidt[1,2], Udo Seifert[2], and Ana-Sunčana Smith[1] — [1]Inst. f. Theor. Physik and Excellence Cluster "Engineering of Advanced Materials", Universität Erlangen-Nürnberg — [2]II. Inst. f. Theor. Physik, Universität Stuttgart

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 accordingly 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, •Yohsuke Imai, Takami Yamaguchi, and Takuji Ishikawa — 6-6-01, Aramaki Aza Aoba, Aoba ku, Sendai, 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 that 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 Brüning[1,2], Martin Kreuzer[1,3], and Roland Steitz[1] — [1]Helmholtz-Zentrum Berlin, Berlin, Germany — [2]Delft University of Technology, Delft, Netherlands — [3]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 mimick 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].

[1] B. Brüning and B. Farago; Perfluorooctanoic acid rigidifies a model lipid membrane; Physical Review E 89, 040702(R) (2014).

BP 24.5 Tue 14:00 Poster A

UV induced Polymerization of Phospholipids at Langmuir Blodgett Through — •Roland Hillmann, Marius Dotter, Sören Grannemann, Lukas Galla, Andy 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 analyzation by AFM or HIM.

BP 24.6 Tue 14:00 Poster A

Exocytotic activity of living cells imaged with surface plasmon resonance microscopy — Stephan Michael, •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 equilibrate their osmolarity by releasing 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 — •Susann Spindler, Jens Ehrig, and Vahid 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].

[1] C.-L. Hsieh, S. Spindler, J. Ehrig, and V. Sandoghdar, J. Phys. Chem. B 118 (2014)

BP 24.8 Tue 14:00 Poster A

Direct Measurement of Mechanical Properties of Unsupported Lipid Bilayer under Hydrodynamic Deformation — •Cornelia Walter[1], Michael Hein[1], Ralf Seemann[1,2], and Jean-Baptiste Fleury[1] — [1]Saarland University, Experimental Physics, Saarbruecken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen, 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 — •Anna Lippert[1,2], Navid Bonakdar[1], and Vahid Sandoghdar[1] — [1]Max Planck Institute for the Science of Light , Günther-Scharowsky-Str. 1 D-91058 Erlangen — [2]Friedrich- Alexander Universität Erlangen-Nürnberg, Schloßplatz 4, 91054 Erlangen

The goal of our project is the establishment of a biological microreactor, enabling the production of complex metabolites. As a first simple system we report on our efforts to incorporate the necessary enzymes and transporter proteins to import and convert sucrose into glucose-6-phosphat in a giant unilamellar vesicle (GUV). We aim to use this platform to study confined kinetics, diffusion and transporter activity under controlled conditions.

BP 24.10 Tue 14:00 Poster A

Fabrication of Giant Unilamellar Vesicles — •Hannah Stein[1,2], Susann Spindler[1], and Vahid Sandoghdar[1] — [1]Max Planck Institute for the Science of Light Günther-Scharowsky-Str. 1 D-91058 Erlangen — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg D-91058 Erlangen

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 50-100um 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. — •Bartosz Kowalik[1], Emanuel Schneck[2], Matej Kanduč[1], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Biomaterials Department, Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, 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 — Marcelo Cisternas[1,2], Alvaro Henrriquez[1,2], Heman Bhuyan[1,2], Maria Retamal[1,2], Mario Favre[1,2], •Ulrich Volkmann[1,2], Darina Manova[3], Stephan Mandl[3], and Fernando Guzman[4] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]CIEN-UC, Santiago, Chile. — [3]Leibniz-Institut für Oberflächenmodifizierung, Leipzig, Germany — [4]4Depto. De Fisica FCFM, Universidad de Chile, 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 phospholipids 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.

BP 24.13 Tue 14:00 Poster A

Receptor-mediated wrapping of nanoparticles — •Karandeep Singh, Sabyasachi Dasgupta, Thorsten Auth, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

Cargo is internalized by biological cells using different internalization processes, e. g. endocytosis, phagocytosis, and pinocytosis. In all cases, the cargo is inside 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 System — •Davit Hakobyan and Andreas 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 3-particle lattice model the phase separation of saturated and unsaturated lipids and choles-

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 their characteristic properties 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 unsataurated 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 Schlaich[1], Matej Kanduc[1], Emanuel Schneck[2], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, D-14195 Berlin, Germany — [2]Max 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 Aland[1], John Lowengrub[2], and Jun Allard[2] — [1]Institut für wissenschaftliches Rechnen, TU Dresden, Germany — [2]Department 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 Location: Poster A

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 a prebiotic evolution. Theory shows that non-equilibrium conditions in form of a temperature gradient should allow the enhanced polymerization from cyclic nucleotides in a thermophoretic molecule trap. The local accumulation of monomers shift the polymerization towards ever longer RNA. It appears possible that RNA polymerization can be triggered using purely physical means without using any catalysts or highly tuned activation chemistry of the monomer.

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 Elsaesser — Max-Born-Institut für Nichtlinear Opitk 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 linkage and the furanose ring structure display subpico- to picosecond 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, Tihomir 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 protecion 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 hydrogene bonds with compatible solute concentration which leads to higher scattering probablities 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 — •Marc Benjamin Hahn, Susann Meyer, Tihomir Solomun, Heinz Sturm, and Hans-Jörg Kunte — BAM - Federal Inst. Mater. Res., Berlin, Germany

Radiation protecion 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 Oprzeska-Zingrebe and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

The formation of specific DNA secondary and tertiary structures have 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 Si_2N_3 membranes both uncoated and lipid-coated [2]. Additionally, measurements of controlled dsDNA translocation through carbon nanomembranes (CNM) and through MoS_2 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.

[1] S. Knust et. al., Rev. Sci. Instrum. **83**, 103704 (2012)
[2] L. Galla et. al., Nano Lett. **14**, 4176 (2014)

BP 25.7 Tue 14:00 Poster A

Modelling the mechanisms of backtrack and recovery in RNA polymerases I and II — Ana Lisica[1,2], Marcus Jahnel[1,2], Christoph Engel[3], •Edgar Roldan[4,5], Patrick Cramer[3], and Stephan Grill[1,2,4] — [1]BIOTEC, Technische Universität Dresden, Tatzberg 47/49, 01307 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstrassüe 108, 01307 Dresden, Germany — [3]Max Planck Institute for Biophysical Chemistry, Am Fassberg 11, 37077 Göttingen, Germany — [4]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 81, 01187 Dresden, Germany — [5]GISC - 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 micromehanical 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 Cruz[1], Claudia Danilowicz[2], Chantal Prevost[3], Mara Prentiss[2], and Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Physics Department, Harvard University, Cambride, MA, USA — [3]LBT - CNRS and Univ Paris Diderot, Sorbonne Paris Cite, 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.

BP 26: Posters: Statistical Physics of Biological Systems

Time: Tuesday 14:00–16:00 Location: Poster A

BP 26.1 Tue 14:00 Poster A

Broken detailed balance in active fluctuations of semiflexible filaments — •Jannes Gladrow[1], Nikta Fakhri[2], Chase P. Broedersz[3], Fred C. MacKintosh[4], and Christoph F. Schmidt[1] — [1]Georg-August Universität Göttingen, Germany — [2]Massachusetts Institute of Technology, USA — [3]Princeton University, USA — [4]Vrije Universiteit, Netherlands

Non-equilibrium microscopic force generation in cells often results in stochastic steady-state fluctuations. In the cell cytoskeleton, for example, cytoplasmic myosins can drive vigorous conformational fluctuations of actin filaments and microtubules. We here present an analytical and numerical analysis of randomly driven shape fluctuations 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.

BP 26.2 Tue 14:00 Poster A

Thermodynamic uncertainty relation for biomolecular processes — •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 ϵ requires at least a cost of $2k_BT/\epsilon^2$ independent of the time required to generate the output.

BP 26.3 Tue 14:00 Poster A

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.

BP 26.4 Tue 14:00 Poster A

How molecular knots can pass through each other — •Jonathan Siebert[1], Benjamin Trefz[1,2], and Peter Virnau[1] — [1]Department of Physics, Johannes Gutenberg University of Mainz, D-55128 Mainz, Germany — [2]Graduate 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_BT. Therefore, it is not only of aesthetic interest, but may also play a role in technological applications, e.g. nanopore sequencing.

BP 26.5 Tue 14:00 Poster A

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

BP 26.6 Tue 14:00 Poster A

Specialization and bet hedging in heterogeneous populations — •Steffen Rulands[1,2], Benjamin D. Simons[1], and Erwin Frey[1] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, UK — [2]Department of Physics, Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München, Germany

How can cells specialize to a niche and at the same time be able to survive in a variety of different environments? In recent years it has become increasingly clear that bacterial, stem cell and even tumor cell populations exhibit a surprisingly high degree of heterogeneity. Genetic diversity and phenotypic heterogeneity are commonly used as a strategy to rapidly adapt to changing conditions. For example, some bacteria switch between phenotypic states in order to survive antibiotic attacks and embryonic stem cell populations exhibit heterogeneous capacities for pluripotency.

We investigate how and under which conditions genetic diversity and phenotypic heterogeneity develop and sustain. Studying paradigmatic ecological scenarios we show that the degree of genetic diversity and the persistence of phenotypic heterogeneity qualitatively change with type of competition between cells and the degree of diffusive motion in the population. While direct competition generally promotes persistence of phenotypic heterogeneity, specialization dominates in models with indirect competition irrespective of the degree of mobility.

BP 26.7 Tue 14:00 Poster A

Knotted protein folding as an ordered sequence of events — •Saeed Najafi and Raffaello Potestio — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

A small but relevant number of proteins whose native structure is known features nontrivial topology, i.e. they are knotted. Understanding the process of folding from a swollen conformation to the biologically-relevant conformation is, for these proteins, particularly difficult, due to the complex pathways leading to entangled state.To shed some light into this problem we introduced a native structure-based coarse-grained model of the protein, in which the information about the folded conformation is encoded in local, short-ranged interactions. Making use of a stochastic search scheme in the parameter space we can identify a set of interactions that maximize the folding probability to the native state.

BP 26.8 Tue 14:00 Poster A

Influence of genetic interactions schemes on adaptive walks — •Stefan Nowak and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln

The NK landscape is a model for a genotype to fitness mapping where epistatic interactions between loci can be explicitly defined. We study adaptive walks on this landscape to analyse the effects of different interaction schemes. For simple versions of the model, the length of the walk and the attained fitness can be computed exactly. For general NK landscapes, we show by Monte Carlo simulations that these quantities

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

BP 26.9 Tue 14:00 Poster A

Phase transition in random adaptive walks on correlated fitness landscapes — Su-Chan Park[1], Ivan Szendro[2], •Johannes Neidhart[2], and Joachim Krug[2] — [1]The Catholic University of Korea, Bucheon, Korea — [2]Institut für Theoretische Physik, Universität zu Köln, Deutschland

We study biological evolution on a random fitness landscape with linear fitness gradient. When selection is strong and mutations rare the dynamics is an uphill walk that terminates at a local fitness maximum. The mean walk length is a function of the genome size L. We show that if and only if the random contribution to the fitness is exponentially distributed, the mean walk length displays a phase transition as a function of the strength of the fitness gradient. For all other distributions only a single phase exists. The considered process is equivalent to a zero temperature Metropolis dynamics for the random energy model in an external magnetic field which leads to a connection to the aging dynamics of spin glasses. See also arXiv:1408.4856.

BP 26.10 Tue 14:00 Poster A

Statistical properties of Fisher's geometric model — •Sungmin Hwang, Ivan Szendro, and Joachim Krug — Insitute for Theoretical Physics, University of Cologne, Germany

Fisher's geometric model has played an important role for providing a connection between the phenotypic space and the fitness landscape while it remains simple enough to be analytically tractable. As complete or partial structures of fitness landscapes in many microbial organisms have been experimentally explored, the extensive effort has been made to understand the epistasis of the fitness landscape, i.e., the genetic interaction among mutations. In this work, we calculated the properties of epistasis distribution under various conditions in the frameworks of Fisher's geometric model. Especially, we focus on the case where the two single mutants have the same selection coefficient in order to analyze how epistasis varies in terms of the selection coefficient of the single mutants. Finally, we compare this result with experimental data to check the validity of our result.

BP 26.11 Tue 14:00 Poster A

Theory of rapid force spectroscopy — •Jakob Tómas Bullerjahn, Sebastian Sturm, and Klaus Kroy — Universität Leipzig, Faculty of Physics & Earth Sciences, Institute for Theoretical Physics, Brüderstr. 16, 04103 Leipzig, Germany

Dynamic force spectroscopy allows the experimentalist to gauge the underlying free energy landscape of single molecular bonds by enforcing their rupture with external loading. At low loading rates, the experimentally measured distributions of rupture forces can be analysed using Kramers' theory of spontaneous unbinding, whereas the extreme forces observed in full-scale molecular simulations can be treated with deterministic methods. Starting from a rigorous probabilistic model of bond dynamics, we develop a unified systematic theory [1] that provides exact closed-form expressions for the rupture force distributions and mean unbinding forces, valid for all loading rates save for a narrow region close to a critical loading rate. Our results, in combination with Bayesian methods of data analysis, yield an accurate tool for analysing and comparing force spectroscopy data from a wide range of experiments and simulations.

[1] J. T. Bullerjahn, S. Sturm & K. Kroy, Nat. Comm. 5, 4463 (2014).

BP 26.12 Tue 14:00 Poster A

Increasing complexity of linear, prevailing, autocatalytical molecules — •Philipp Zimmer[1], Emanuel Gregor Worst[2], Eva Wollrab[2], Albrecht Ott[2], and Karsten Kruse[1] — [1]Universität des Saarlandes, Theoretische Physik, Postfach 151150, 66041 Saarbrücken — [2]Universität des Saarlandes, Biologische Experimentalphysik, Postfach 151150, 66041 Saarbrücken

Two common concepts of Darwinian evolution are mutation and selection. In natural evolution, these processes have permanently generated increasingly complex species. Nevertheless evolution has maintained to avoid dead ends such that a further development is proceeding. This process is not well understood. Performing stochastic simulations as well as experiments with DNA, we find that our system evolves reproducibly towards consecutive states of increasing complexity, if the autocatalytic activity exceeds a critical value.

BP 26.13 Tue 14:00 Poster A

Modeling chromosomes during meiosis in fission yeast — •Wenwen Huang[1], Yen Ting Lin[1], Daniela Frömberg[1], Petrina Delivani[2], Mariola Chacón[2], Iva Tolic[2], Frank Jülicher[1], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, 01307, Dresden, Germany

During the 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 the function of time and amplitude of oscillations and compare it to the experimental data. Our results provide a quantitative characterization of of chromosome movements and help to understand the role of nuclear oscillations on the alignment of chromosomes during meiosis.

BP 26.14 Tue 14:00 Poster A

Evolutionary accessibility in the NK Model for fitness landscapes — •Benjamin Schmiegelt — Institute for Theoretical Physics, Cologne, Germany

Fitness landscapes are biological evolution's equivalent to energy landscapes, on which populations move as genotype distribution clouds [1]. In the limit of weak mutation and strong selection, the population's dynamic can be described by an uphill climb. Accessibility refers here to the probability that the landscape's global maximum is reachable from the antipodal genotype [2]. The NK model for such a landscape with L binary loci resembles a spin glass where each spin/locus interacts with k other spins/loci. A key determinant of evolutionary accessibility is the degree of sign epistasis, the fraction of loci having both positive and negative fitness effects depending on the state of other loci. Using that the NK model at fixed k for $L \to \infty$ almost surely exhibits global reciprocal epistasis, i.e. reciprocal sign epistasis between two loci on all generic background, it is shown that the accessibility tends to zero, and does so faster than in the House-of-Cards model (random energy model), generalizing results obtained previously for a special case of the NK-model where the groups of interacting loci are disjoint [3].

[1] J.A.G.M. de Visser and J. Krug, Nature Reviews Genetics 15, 480-490 (2014)

[2] J. Franke, A. Klözer, J.A.G.M. de Visser and J. Krug, PLoS Computational Biology 7, e1002134 (2011).

[3] B. Schmiegelt and J. Krug, Journal of Statistical Physics 154, 334-355 (2014).

BP 26.15 Tue 14:00 Poster A

Stochastic Terminal Dynamics in Epithelial Cell Intercalation — •Matthias Häring[1], Stephan Eule[1], Jakob Metzger[1], Lars Reichl[1], Deqing Kong[2], Yujun Zhang[2], Jörg Grosshans[2], and Fred Wolf[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg, 37077 Göttingen, Germany — [2]Institute for Developmental Biochemistry, Medical School, University of*Göttingen, Justus-von-Liebig Weg 11, 37077 Göttingen, Germany

We found that the constriction of epithelial cell contacts during intercalation in germ band extension in Drosophila embryos follows intriguingly simple quantitative laws. The mean contact length $\langle L \rangle$ follows $\langle L \rangle(t) \sim (T-t)^{\alpha}$, where T is the finite collapse time; the time dependent variance of contact length is proportional to the square of the mean; finally the time dependent probability density of the contact lengths remains close to Gaussian during the entire process. These observations suggest that the dynamics of contact collapse can be captured by a single stochastic differential equation in a small noise regime. Here, we present such a model, providing an effective description of the non-equilibrium statistical mechanics of contact collapse. All model parameters are fixed by measurements of time dependent mean and variance of contact lengths. Our model predicts the existence of a quasi-stationary distribution of contact lengths. We investigate this quasi-stationary distribution numerically and present an analytical solution for model parameters that are close to the measured values.

BP 27: Posters: Complex Fluids and Soft Matter

Time: Tuesday 14:00–16:00 Location: Poster A

BP 27.1 Tue 14:00 Poster A

Flux simulations of anisotropic particles in different geometries using lattice Boltzmann method — •Lukas Schrack and Stephan Gekle — 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 of such 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.

[1] M. Trebbin et al., *PNAS* **110**, 17 (2013)

[2] A. Arnold et al., *Meshfree Methods for Partial Differential Equations VI, Lecture Notes in Computational Science and Engineering* **89**, 1 23 (2013), Springer

BP 27.2 Tue 14:00 Poster A

Nonlinear Dynamics Model Of Epithelial Tissue — •Wei-Lung Lo and Hsuan-Yi Chen — Department of Physics, Nation Central University, Jhongli, 32001, Taiwan.

In spite of recent experimental and theoretical advances in the study of the homeostasis of biological tissues, not much is known about the relaxation dynamics of a tissue toward its homeostasis state. In this work we propose a theoretical model to study this problem. The tissue is composed of stem cells and terminal differentiated cells (TDs). The stem cells divide at a rate r*s and TD cells undergo apoptosis at a rate rd. The self-renewal probability of a stem cell after cell division is assumed to be P*(N*_D) , a function of the total number of TD cells. Our model shows that a biological tissue could allow the existence of multiple steady states. The relation between the steady state properties of the tissue and the corresponding biomolecular processes is addressed. Furthermore, the stability of the homeostasis for a stratified epithelium is studied. We show that the relaxation rate of a tissue towards its homeostasis state is controlled by (i) viscous flow induced by tissue surface tension (ii) adjusted cell proliferation rate (iii) coupling between cell proliferation and flow field in the tissue. The question of how tissue competition affects the relaxation of tissue around a homeostasis state is addressed.

BP 27.3 Tue 14:00 Poster A

Extended X-ray absorption fine structure investigation of aqueous salt solutions under high pressure — •Karin Julius[1], Christian Sternemann[1], Michael Paulus[1], Thomas Büning[1], Karin Esch[1], Julian Schulze[1], Patrick Degen[2], Ralph Wagner[3], and Metin Tolan[1] — [1]Fakultät Physik / Delta, TU Dortmund, 44221 Dortmund, Germany — [2]Ruhr-Universität Bochum, Lehrstuhl für Physikalische Chemie, 44780 Bochum, Germany — [3]Fachbereich C Physik, Bergische Universität Wuppertal, Gaußstr. 20, 42097 Wuppertal, Germany

The study of the structural impact that water (de)stabilizing agents have upon the bulk solvent medium under high hydrostatic pressure can give comprehensive insight to the stabilization or destabilization of proteins in solution. We use extended X-ray absorption fine structure (EXAFS) analysis in order to investigate the influence of pressures up to 5 kbar on the local water network around Rb^+ and Y^{3+} in 0.1 M salt solutions of RbCl and YCl_3. The EXAFS measurements have been performed at beamline BL8 of DELTA (Dortmund) with a high pressure cell in vicinity of the Rb and the Y K-edge. Within the limits of the experiment, the spectra show evidence that the first hydration shells around Rb^+ and Y^{3+} are not influenced by the pressure increase while the surrounding bulk water gets compressed. MD-simulations of the salt solutions in a pressure range from 50 to 5000 bar were performed to discuss the experimental results.

BP 27.4 Tue 14:00 Poster A

Micropipette force sensors for biomechanics and soft matter adhesion studies — •Marcin M. Makowski and Oliver Baeumchen — 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 e.g. 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. (EPJE 30, 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.

BP 27.5 Tue 14:00 Poster A

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 interprete 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.

BP 27.6 Tue 14:00 Poster A

Microscopic structure of supercooled water studied by x-ray Compton scattering and x-ray Raman scattering — •Juri Nyrow[1], Felix Lehmkühler[2], Mikko Hakala[3], Thomas Büning[1], Ingo Steinke[2], Christoph J. Sahle[4], Karin Julius[1], Agnieszka Poulain[4], Ali Al-Zein[4], Thomas Buslaps[4], Metin Tolan[1] und Christian Sternemann[1] — [1]Fakultät Physik/DELTA, TU Dortmund, GE-44221 Dortmund — [2]Deutsches Elektronen-Synchrotron DESY, GE-22607 Hamburg — [3]Department of Physics, University of Helsinki, FI-00014 Helsinki — [4]ESRF, FR-38043 Grenoble Cedex 9

The microscopic structure of water at ambient and in supercooled conditions is controversially discussed, e.g. with respect to a mixture of low and high density water phases [1]. Recently, x-ray absorption and diffraction studies reported an increasing contribution of tetrahedrally coordinated low density water on cost of a highly disturbed hydrogen bonding network at supercooled conditions [2,3]. We investigated changes of the molecular structure in supercooled water for temperatures down to 255 K by x-ray Compton scattering and x-ray Raman scattering. The results indicate a strengthening of the tetrahedral hydrogen bond network, accompanied by a shortening of the intramolecular OH bond length upon supercooling. These findings will be discussed using structural models with different local bonding configurations [4].

[1] C. Huang et al. PNAS 106, 15214 (2009).
[2] J. A. Sellberg et al. J. Chem. Phys. 141, 034507 (2014).
[3] J. A. Sellberg et al. Nature 510 (7505), 381-384 (2014).

[4] M. Hakala et al. Phys. Rev. B 73, 035432 (2006).

BP 27.7 Tue 14:00 Poster A

The role of detailed balance in chemically active droplets — •Rabea Seyboldt[1], David Zwicker[1,2], and Frank Jülicher[1] — [1]Max-Planck Institut für Physik komplexer Systeme, Dresden — [2]School 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.

BP 27.8 Tue 14:00 Poster A

The mechanical properties of early Drosophila embryos measured by high-speed video microrheology — •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 microrheology. 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 anphase where we observe directed motion.

BP 28: Posters: Biomaterials and Biopolymers

Time: Tuesday 14:00–16:00 Location: Poster A

BP 28.1 Tue 14:00 Poster A

Raman spectroscopic analysis of drug-target interactions in malaria disease — •Torsten Frosch[1,2] and Juergen Popp[1,2] — [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 be 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.

References: [1] Frosch, T.; Yan, D.; Popp, J. Anal Chem 2013, 85, 6264-6271. [2] Frosch, T.; Schmitt, M.; Noll, T.; Bringmann, G.; Schenzel, K.; Popp, J. Anal. Chem. 2007, 79, 986-993. [3] Frosch, T.; Meyer, T.; Schmitt, M.; Popp, J. Anal. Chem. 2007, 79, 6159-6166.

BP 28.2 Tue 14:00 Poster A

The effect of urea on the swelling and collapse behavior of poly-N-isoproylacrylamide: a computational study — •Julian Michalowsky[1], Samantha Micciulla[2], Regine von Klitzing[2], and Jens Smiatek[1] — [1]Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Stranski-Laboratorium, Institut für Chemie, Technische Universität Berlin, 10623 Berlin, Germany

The effect of urea on the swelling and collapse properties of poly(N-isopropylacrylamide) (PNIPAM) molecules is presented. The results of all-atom Molecular Dynamics simulations imply that the macroscopic changes induced in the system by the increase of temperature and urea concentration can be related to microscopic details. The numerical simulations elucidate the main mechanism leading to the observed effects, which are the result of a subtle interplay between hydration properties and a concentration-dependent urea binding behavior. In particular, at low osmolyte concentration a small amount of direct bonded urea molecules to PNIPAM in addition to the hydrating water molecules leads to the stabilization of a more extended conformation. In contrast, at high osmolyte concentrations the binding between PNIPAM and urea becomes more favorable such that the number of hydrating water molecules is significantly decreased. Our numerical results therefore imply that a concentration-dependent binding behavior of urea governs the experimentally observed collapse and swelling properties of PNIPAM brushes in aqueous solution.

BP 28.3 Tue 14:00 Poster A

Swelling behaviour of individual corneocytes — •Hannes Heinel, Diana Voigt, and Robert Magerle — Chemische Physik, Fakultät für Naturwissenschaften, TU Chemnitz, 09107 Chemnitz, Germany

Corneocytes are dead, cornified cells that compose the outmost layer of the skin, known as stratum corneum. They contain a network of keratin intermediate filaments encased by a protein envelope, and display an extreme and reversible swelling upon hydration. M. E. Evans et al. have shown, that the expansion is due to the particular three-dimensional packing of keratin intermediate filaments [1,2]. With atomic force microscopy (AFM) we study the changes of morphology and nanomechanical properties of individual corneocytes upon hydration in humid air. Isolated corneocytes from a human donor are deposited on different substrates and imaged with AFM. The relative humidity of air is changed in-situ. [1] M. E. Evans, R. Roth, PRL **112**, 038102 (2014); [2] M. E. Evans, S. T. Hyde, J. R. Soc. Interface **8**, 1274 (2011)

BP 28.4 Tue 14:00 Poster A

Microrheological characterization of DNA nanotube networks — •Tina Händler[1], Carsten Schuldt[1,2], Martin Glaser[1], Jörg Schnauss[1], Josef A. Käs[1], and David M. Smith[2] — [1]University of Leipzig, Soft Matter Physics Division, Leipzig — [2]Fraunhofer Institute for Cell Therapy and Immunology, Leipzig

Studying the mechanics and dynamics of biopolymers has inspired many ideas and theories in polymer physics. One prominent example is actin, being the best-studied semiflexible polymer. Unfortunately, naturally occurring protein-based biopolymers are limited in their properties such as length, stiffness and interaction strengths. This highlights the advantage of having "programmable" model polymers at hand, which give the opportunity to experimentally test parameters otherwise unavailable in natural systems, and therefore expand theoretical approaches. Nanotubes formed from synthetic DNA strands are an ideal match to this need: they are semiflexible over their typical length scale and can be hybridized to have characteristics such as persistence length which are similar actin filaments or can be varied in a

controllable way. We use this model system to measure the mechanical properties and dynamics of entangled networks with microrheological methods. The results can be employed to re-examine theories of semiflexible polymers and provide an insight into the internal structural dynamics of DNA helix tubes.

BP 28.5 Tue 14:00 Poster A

A unified theoretical approach to the inelastic mechanics of biopolymer gels, cells and cell aggregates — •Andrea Kramer[1], Matti Gralka[2], and Klaus Kroy[1] — [1]Institute for Theoretical Physics, Universität Leipzig, Germany — [2]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].

[1] L. Wolff et al., New J. Phys. 12, 053024 (2010)
[2] S. Münster et al., PNAS 110, 12197 (2013)
[3] T.V. Stirbat et al., Eur. Phys. J. E 36, 84 (2013)

BP 28.6 Tue 14:00 Poster A

Higher ordered assembly of rigid biopolymers induced by depletion forces — •Martin Glaser[1], Teresa Tschirner[1,2], Maximilian Moebius-Winkler[2], Carsten Schuldt[1,2], Tina Händler[1], Tom Golde[1], Josef Käs[1], David Smith[2], and Jörg Schnauss[1] — [1]University of Leipzig, Faculty of Physics and Earth Sciences: Soft Matter Division, Leipzig, Germany — [2]Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany

The influence of depletion forces on processes like cellular organization has long been underestimated. An attractive potential induced within a system of rigid biopolymers can lead to the formation of higher ordered structures. The biopolymer actin can assemble, to loose networks, bundles and also clusters in a higher-level assembly like asters and nematic phases. In particular, the formation of asters was usually attributed to active processes driven by the molecular motor myosin. We present experimental evidence of bundle arrangements in star-like structures independent of other associated proteins. For the formation, we use established actin-bundling mechanisms such as counter-ion clouds and depletion forces. These structures can be formed solely by altering the concentration of actin and the according bundling agent in the system. Since no other proteins are involved, this effect demonstrates that higher ordered structure formations can be controlled only by self-assembly and accordingly energy minimization of the system. To demonstrate generality of this ordering effect beyond cellular biopolymers, we additionally present first experimental results on the formation of higher ordered structures by artificially designed DNA tubes.

BP 29: Posters: Systems biology

Time: Tuesday 14:00–16:00 Location: Poster A

BP 29.1 Tue 14:00 Poster A

Control of ventricular tachycardia under myocardial ischemic conditions and infarction — •Edda Boccia and Stefan 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 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 rotating waves to and from infarction zones using pulsed electric fields. We will discuss the implications of our findings for the development and optimization of low energy control of cardiac arrhythmias including Low-Energy Anti-Fibrillation Pacing (LEAP, Luther & Fenton et al., Nature 2011).

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[1], gaetano campi[2], inna bukreeva[1], michela fratini[1], giuliana tromba[3], maddalena mastrogiacomo[4], ranieri cancedda[4], and manfred burghammer[5] — [1]ipcf-cnrc/o Physics Departement- Sapienza University- Rome-Italy. — [2]Istituto di Cristallografia- CNR, Monterotondo Rome, Italy. — [3]Sincrotrone Trieste SCpA, 34149 Basovizza (Trieste), Italy. — [4]Dipartimento di Medicina Sperimentale-Università di Genova — [5]esrf-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 (XRPCT) the most effective tool to investigate the structural features of this tissue at different length scales.In particular we use XRPCT 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 image by XRPCT the 3D microvascular networks in different bone-engineered constructs.

BP 29.3 Tue 14:00 Poster A

Modeling of gene silencing in RNA interference — •Simon Dornseifer[1], Georg Sczakiel[1], Tobias Restle[1], and Jens Christian Claussen[2] — [1]IMM, Universität zu Lübeck, Germany — [2]Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

RNA interference (RNAi) is a mechanism of post-transcriptional gene silencing that, since its discovery, gained high attention, and gave rise to the development of new nucleic acid-based tools. Here we propose and investigate a computational systems biology model of siRNA-mediated RNAi in human cells in order to link precise quantitative kinetic data and new molecular findings with a quantitative and time-resolved understanding of RNAi in the human system. Cell culture experiments suggest 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 (here, cleaved RNA fragments) leaves the complex in a slow step. Here, we investigate an alternatice, 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 mRNA 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 29.4 Tue 14:00 Poster A

Modeling of gene silencing in RNA interference — •Simon Dornseifer[1], Georg Sczakiel[1], Tobias Restle[1], and Jens Christian Claussen[2] — [1]IMM, Universität zu Lübeck, Germany — [2]Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

RNA interference (RNAi) is a mechanism of post-transcriptional gene silencing that, since its discovery, gained high attention, and gave rise to the development of new nucleic acid-based tools. Here we propose and investigate a computational systems biology model of siRNAmediated RNAi in human cells in order to link precise quantitative kinetic data and new molecular findings with a quantitative and timeresolved understanding of RNAi in the human system. Cell culture experiments suggest 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 mRNA 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

Time: Tuesday 14:00–16:00 Location: Poster A

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

Der durchschlagende Erfolg der Mikrofluidik ist unter anderem der Laminarität der Strömung (Reynoldszahl << 1) sowie dem preiswerten Einsatz von sehr effizienten Mikrofabrikationsmethoden zu verdanken. Leider sind Mikrokanäle nicht immer geeignet, insbesondere, wenn man größere Zellkulturen, Co-Kulturen oder sogar Organkulturen untersuchen 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 Antwort präsentieren wir ein Perfusionssystem, welches laufende Strömungen im Bereich mehrerer Milliliter/Sekunde präzise schalten und steuern kann. Bis zu 8 verschiedene Lösungen können völlig unterbrechungsfrei geschaltet werden. Als Anwendung werden Messungen an Chlorid-Kanälen präsentiert - eine Verbindung also von Meso- und Nanofluidik. Dieses System eignet sich hervorragend für die Messung von Kinetiken und Dynamiken von der molekularen bis zur multizellulären Skala.

BP 30.2 Tue 14:00 Poster A

Effect of Sr on the microstructure and properties of Mg-6Al alloy — •Tayebeh Nayeri and Sina Sadreddini — Department of Materials Science and Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran.

In this study, microstructures and properties of the Mg*Al alloy with strontium addition are studied. After the addition of strontium, structure analysis was performed to investigate phase evaluation. The potentiostate were also carried out in 3.5% Nacl solution with the results showing that the effect of adding strontium element to magnesium-aluminum alloys on corrosion behavior of this metal was strongly dependent on microstructure of the final alloy (e.g. grain size, type, intermetallic compounds, etc.).The major second phase included Al4Sr and Al2Sr, but the amount and morphology of these compounds was different in the alloys. The results indicated a reduction in the amount of Mg17 Al12 phase and corrosion rate as well as a rise in the resistance to cavitations.

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

Time: Tuesday 14:00–16:00 Location: Poster A

BP 31.1 Tue 14:00 Poster A

Intrinsic muscle design: influence on human motor control — •Alexandra Bayer[1,2], Syn Schmitt[1,2], Michael Guenther[1], and Daniel Fabian Benjamin Haeufle[1] — [1]Universität Stuttgart, Institut für Sport- und Bewegungswissenschaft, Allmandring 28, D-70569 Stuttgart, Germany — [2]Universität 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 investigated, 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 nonlinear musculoskeletal model and four lumped muscle-tendon complexes. 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 mathematical representation of the biochemical and biomechanical model parts on movement speed in fast goal-directed arm movements. Already exchanging the description of activation dynamics revealed significant 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.

BP 32: Evolutionary Game Theory II (joint SOE/BP/DY)

Time: Tuesday 14:00–16:15 Location: MA 001

BP 32.1 Tue 14:00 MA 001

Frequency-Dependent Selection at Rough Expanding Fronts — •Jan-Timm Kuhr and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin

Microbial colonies are a formidable model system to study longstanding 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 mutation and selection 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.

[1] J.-T. Kuhr, M. Leisner, and E. Frey, New J. Phys. **13**, 113013 (2011).

BP 32.2 Tue 14:15 MA 001

Evolutionary Fitness in Variable Environments — •Anna Melbinger 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 often are much smaller than expected.

BP 32.3 Tue 14:30 MA 001

Non-selective evolution of growing populations — •Karl Wienand[1], Matthias Lechner[1], Felix Becker[2], Heinrich Jung[2], and Erwin Frey[1] — [1]Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians Universität, Munich, Germany — [2]Biozentrum, Ludwig-Maximilians Universität, Munich, Germany

Evolution results from the interplay between directed selection and non-selective effects. Most theoretical analyses of non-selective evolution rely on constant population sizes and result in some trait taking over the entire population. However, bacterial populations both in nature and in the laboratory are often observed during their exponential growth. In this work we show that, during growth, populations "freeze" to a random steady state composition. To show this, we employed theoretical models based on Pólya urns and performed experiments on two *Pseudomonas putida* strains in non-selective conditions. We found excellent agreement between experiments and theory. We were 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.

BP 32.4 Tue 14:45 MA 001

Counterintuitive findings for evolution on networks — •Laura Hindersin and Arne Traulsen — Max Planck Institute for Evolutionary Biology, Plön, 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 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 populations.

[1] Hindersin L, Traulsen A. 2014 Counterintuitive properties of the fixation time in network-structured populations. J. R. Soc. Interface 11: 20140606. http://dx.doi.org/10.1098/rsif.2014.0606

BP 32.5 Tue 15:00 MA 001

The Cost and Dynamics of Competence in *Bacillus subtilis* — •Jeffrey Power, Melih Yüksel, and Berenike Maier — 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. Competence presents the opportunity for the acquisition and implementation of new genes, but at the cost of a reduced growth rate.

To better understand the advantage of stochastic switching, stationary phase competition assays were carried out competing strains with various fractions of competent cells against the wild type. Flow cytometry was used to monitor changes in the mixed populations over time, and fitness advantages were quantified by means of selection coefficients. We found selection coefficients of s = 0.04(1) for the non-competent *comK* strain and s = -0.07(1) for the hypercompetent *rok* strain, indicating that competence development has a large cost.

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.

BP 32.6 Tue 15:15 MA 001

A Two-Player Game with Linear State-Dependent Payoff Function — •Tim Herrmann[1], Mark Kirstein[2], and Katharina Fischer[3] — [1]TU Dresden — [2]TU Dresden, Chair of Managerial Economics — [3]TU 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.

BP 32.7 Tue 15:30 MA 001

Evolutionary Coalitional Games — •Tadeusz Płatkowski — Faculty of Mathematics, Informatics, and Mechanics \\ University of Warsaw, Warsaw, Poland

We introduce the concept of evolutionary coalitional 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

Evolutionary games of condensates in coupled birth-death processes — •Johannes Knebel, Markus F. Weber, Torben Krüger, and Erwin Frey — Ludwig-Maximilians-Universität, München, Deutschland

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 driven-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 32.9 Tue 16:00 MA 001

Length selection and replication in a thermal flow chamber — •Simon A. Lanzmich[1], Lorenz M. R. Keil[1], Moritz Kreysing[2], and Dieter Braun[1] — [1]Systems Biophysics, LMU Munich, Germany — [2]MPI of Molecular Cell Biology and Genetics, Dresden, Germany

The replication of long nucleic acids is central to life. On the early Earth, suitable non-equilibrium boundary conditions were required to surmount the effects of thermodynamic equilibrium such as dilution and degradation of oligonucleotides. One particularly intractable experimental finding is that short genetic polymers replicate faster and outcompete longer ones, leading to ever shorter sequences and the loss of genetic information. We show in theory and experiment that heat flux across an open chamber in submerged rock concentrates replicating oligonucleotides from a constant feeding flow and selects for longer strands. The thermal gradient triggers a complex interplay of molecular thermophoresis, external flow and laminar convection, where the latter drives strand separation and exponential replication. The measurements are understood quantitatively based on the calculation of stochastic trajectories inside the chamber using a two-dimensional random walk model. This allowed to derive lifetimes and thermal oscillation frequencies of the nucleic acids. In an intermediate range of external velocities, the superposition of flow fields retains strands of 75 bases, while strands half as long die out, inverting above dilemma of the survival of the shortest. The combined feeding, thermal cycling and positive length selection opens the door for stable molecular evolution in the long-term micro-habitat of asymmetrically heated porous rock.

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

Time: Wednesday 9:30–13:15 Location: H 1058

Invited Talk BP 33.1 Wed 9:30 H 1058

Feeling for cell function: Mechanical phenotyping at 100 cells/sec — •Jochen 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 diverse applications in biology, biotechnology and medicine.

BP 33.2 Wed 10:00 H 1058

Characterizing viscoelastic properties of the cortex in mitotic cells — •Elisabeth Fischer-Friedrich[1,2], Jonne Helenius[3], Anthony Hyman[2], Daniel Müller[3], and Frank Jülicher[1] — [1]MPI PKS, Nöthnitzerstr. 38, 01187 Dresden, Germany — [2]MPI CBG, Pfotenhauerstr. 108, 01307 Dresden, Germany — [3]D-BSSE, 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 Hemmerle[1], Jörn Hartung[1], Oskar Hallatschek[1,2], Lucas Goehring[1], and Stephan Herminghaus[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Department 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 ($\simeq$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 cohesiveness, 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-

vestigation — •Viktor Heinrichs[1,2], Sabine Dieluweit[1], Jörg Stellbrink[2], Rudolf Merkel[1], and Dieter Richter[2] — [1]ICS-7 Forschungszentrum Jülich GmbH, Jülich, Germany — [2]ICS-1 Forschungszentrum Jülich GmbH, Jülich, Germany

Most animal cells are strongly influenced by the elasticity and topography of their environment. For clear-cut investigation of cellular mechanobiology elastic model substrates are required. These materials should be biocompatible, transparent, suitable for micro structure fabrication and their elasticity should be tuneable in a wide range. However, a Young's modulus of 1 kPa (ultra-soft, necessary to model, e.g., brain or glial tissues) is difficult to achieve [1, 2]. These challenges can be tackled with cross-linked polydimethylsiloxane (PDMS) with the additional benefit of long shelf-life. We created a new PDMS material that meets all requirements in cell mechanics and examined it explicitly on viscoelastic properties with a strain controlled rheometer. The elasticity of the PDMS network was tuned via selection of the precursor polymers and their mixing ratio. Values as low as 1.5 kPa have been reliably achieved. First cell mechanical experiments on this novel material basis are underway. [1] C. M. Cesa, N. Kirchgeßner, D. Mayer, U. S. Schwarz, B. Hoffmann, R. Merkel. Rev. Sci. Instrum. 2007, 78, 034301. [2] D. T. Butcher, T. Alliston, V. M. Weaver, Nature Rev. Cancer 2009, 9, 108-122.

BP 33.5 Wed 10:45 H 1058

Molecular stress sensors constructed from DNA — •Meenakshi Prabhune[1], Jonathan Bath[2], Andrew Turberfield[2], Florian Rehfeldt[1], and Christoph F Schmidt[1] — [1]Third Institute of Physics-Biophysics, Georg August University, Göttingen, Germany — [2]University of Oxford, Department of Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK

Molecular stress generation in cells is spatially and temporarily organized in complex patterns to drive meso-scale active processes such as intracellular transport, cell migration, or cell division. To quantitatively understand how these processes are driven, it is necessary to map local stresses inside cells, which is hard due to the lack of appropriate probes. We have designed a molecular-scale probe consisting of a self-assembled DNA hairpin with a fluorophore - quencher pair that responds to small forces applied to its ends. We demonstrate the working of this force sensor in vitro and explore possibilities for in vivo application to map local stress fields in cells.

BP 33.6 Wed 11:00 H 1058

Shape 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 impedance long-term trend. 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

BP 33.7 Wed 11:45 H 1058

Probing the role of cytoplasmic flows in embryogenesis — •Matthäus Mittasch[1], Peter Gross[1,2], Stephan Grill[1,2], and Moritz Kreysing[1] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany — [2]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 downregulation. 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 micron-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 multipoles 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.

BP 33.8 Wed 12:00 H 1058

Force fluctuations in three-dimensional suspended fibroblasts — •Florian Schlosser, Christoph F. Schmidt, 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 attached 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.

Schlosser, Rehfeldt, Schmidt, *Phil. Trans. R. Soc. B* 20140028, **2014**

BP 33.9 Wed 12:15 H 1058

Buckling dynamics of freely diffusing single erythrocytes — •Michael Göllner, 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 diffusing inside microchambers without adhesive interactions to the glass coverslip or the use of optical tweezers. By increasing the surrounding osmotic pressure, erythrocytes are exhibiting a buckling transition which is described by means of radial Fourier analysis. Temporal evolution of the modal decomposition of cell edge movement leads to characterization of osmolarity-dependent fluctuations of freely diffusing single RBCs.

BP 33.10 Wed 12:30 H 1058

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

In cell physiology and pathology mechanical signaling plays an important role. Many cell types, including central nervous system cells, respond 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.

BP 33.11 Wed 12:45 H 1058

Properties of Single Squamous Cell Carcinoma Cells — •Susanne Steeger[1], Tanja Schreyer[1], Stefan Hansen[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Heinrich-Heine-Universität Düsseldorf, Deutschland — [2]Univ.-HNO-Klinik Düsseldorf, Deutschland

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 oft 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 cytosekelton which is reflected in the different elasticities of both cancer and comparable benign cells.

BP 33.12 Wed 13:00 H 1058

PAR polarity pattern in C. elegans zygotes establishes via a mechanochemical feedback module — •Peter Gross[1,2], K.Vijay Kumar[2,3], Nathan W. Goehring[4], Justin S. Bois[5], Frank Jülicher[3], and Stephan W. Grill[1,2,3] — [1]MPI-CBG, Dresden — [2]BIOTEC, TU Dresden — [3]MPI-PKS, Dresden — [4]London Research Institute, UK — [5]UCLA, Los Angeles, CA

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 spatiotemporal 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.

BP 34: Statistical Physics of Biological Systems II (joint BP/DY/CPP)

Time: Wednesday 9:30–13:15 Location: H 1028

BP 34.1 Wed 9:30 H 1028

Pinned polymer loops in external field: how to align chromosomes for recombination? — Yen Ting Lin[1], Daniela Frömberg[1], Wenwen Huang[1], Petrina Delivani[2], Mariola Chacón[2], Iva Tolic[2], Frank Jülicher[1], and •Vasily Zaburdaev[1] — [1]MPI for the Physics of Complex Systems, Dresden, Germany — [2]MPI of Molecular Cell Biology and Genetics

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.

BP 34.2 Wed 9:45 H 1028

Statistical Inference of E.Coli's tumbling behavior and chemotaxis strategy using Kramers-Moyal coefficients — •Oliver Pohl[1], Marius Hintsche[2], Carsten Beta[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin — [2]Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam

The bacterium Escherichia coli moves with alternating runs and tumbles that occur with a mean tumble rate. In the presence of gradients of a chemoattractant, E. coli performs chemotaxis. We set up a time-continuous model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed. The swimming direction updates according to rotational Brownian motion and additional shot noise, which initiates tumbling events. The speed is not constant as in previous models but decreases during the tumbling events.

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 predetermined. Furthermore, we can identify the bacteria's chemotaxis strategy by exploiting the Kramers-Moyal coefficients.

BP 34.3 Wed 10:00 H 1028

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 proteins 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.

BP 34.4 Wed 10:15 H 1028

Stochastic Dynamics of IFN Type I Signaling — •Nikolas Schnellbächer[1,2], Nils Becker[3], Thomas Höfer[3], and Ulrich Schwarz[1,2] — [1]Institute for Theoretical Physics, University of Heidelberg, Heidelberg, Germany — [2]BioQuant, University of Heidelberg, Heidelberg, Germany — [3]German Cancer Research Center, Heidel-

berg, Germany

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 active ternary signaling 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 notoriously 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[1] and Dave Thirumalai[2] — [1]IMT Lucca Institute for Advanced Studies, Lucca Italy 55100 — [2]University 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 reduced simple equations that can be solved asymptotically. We are able to accurately recover the well known Odijk scaling of $F \sim L/l_d$, 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 $F \sim L/l_t$ for a tensile length scale $l_t \sim (l_p/\beta f)^{1/2}$. Our results may be relevant in the mechanical unbinding of histone-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 Dieterich[1], Joan Camunas-Soler[2,3], Marco Ribezzi-Crivellari[2,3], Udo Seifert[1], and Felix Ritort[2,3] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Germany — [2]Departament de Física Fonamental, Universitat de Barcelona, Spain — [3]CIBER-BBN de Bioingeniería, Biomateriales y Nanomedicina, Instituto de Salud Carlos III, Madrid, Spain

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 Noe — FU Berlin, Arnimallee 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 — •Andreas Mader[1], Benedikt von Bronk[1], Benedikt Ewald[1], Sara Kesel[1], Karin Schnetz[2], Erwin Frey[1], and Madeleine Opitz[1] — [1]Faculty of Physics, LMU München, Germany — [2]Institute 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 induction via stress. A 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 *cel* (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[2], •Daniel Midtvedt[1], Elisabeth Nüske[2], Shovamayee Maharana[2], Sonja Kroschwald[2], Doris Richter[2], Vasily Zaburdaev[1], and Simon Alberti[2] — [1]Max Planck Institut für Physik komplexer Systeme — [2]Max 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.

BP 34.11 Wed 12:45 H 1028

Detailed balance violations in mesoscopic biological systems — •Christopher Battle[1], Chase P. Broedersz[2], Nikta Fakhri[1], Fred C. MacKintosh[3], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August Universitaet, Goettingen, Germany — [2]Lewis-Sigler Institute for Integrative Genomics and Department of Physics, Princeton University, Princeton, NJ, USA — [3]Dept. 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 violate fundamental tenets of equilibrium, such as the principle of detailed balance. While some cellular processes show unmistakable non-equilibrium characteristics, e.g. persistent 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 34.12 Wed 13:00 H 1028

Genetic networks specifying the functional architecture of orientation domains in V1 — •Joscha Liedtke and Fred Wolf — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Goettingen (Germany)

Although genetic information is critically important for brain development and structure, it is widely believed that neocortical functional architecture is largely shaped by activity dependent mechanisms.

Here we show theoretically that mathematical models of genetic networks of principal neurons interacting by long range axonal morphogen transport can generate morphogen patterns that exactly prescribe the functional architecture of the primary visual cortex (V1) as experimentally observed. We analyze in detail an example genetic network that encodes the functional architecture of V1 by a dynamically generated morphogen pattern. We use analytical methods from weakly non-linear analysis [Cross & Hohenberg 1993] complemented by numerical simulations to obtain solutions of the model. In particular we find that the pinwheel statistics are in quantitative agreement with high precision experimental measurements [Kaschube et al. 2010].

This theory opens a novel perspective on the experimentally observed robustness of V1's architecture against radically abnormal developmental conditions such a dark rearing [White et al. 2001]. Furthermore, it provides for the first time a scheme how the pattern of a complex cortical architecture can be specified using only a small genetic bandwidth.

BP 35: Membranes and vesicles II (joint BP/CPP)

Time: Wednesday 15:00–18:30 Location: H 1028

Invited Talk BP 35.1 Wed 15:00 H 1028

Caged Hyperpolarized Xenon in Phospholipid Membranes for NMR Sensing Applications — •Leif Schröder — Leibniz-Institut für Molekulare Pharmakologie (FMP), Berlin, Germany

Spin-hyperpolarized xenon comes with high sensitivity and specificity for NMR spectroscopy due to the large chemical shift range of the dissolved gas. Recent developments in indirect detection of temporarily caged atoms through chemical exchange saturation transfer with hyperpolarized nuclei (Hyper-CEST) allows to sense for the molecular environment of the NMR-active isotope Xe-129 despite being a noble gas. In fact, its tendency to participate in labile van der Waals interactions facilitates very sensitive NMR detection. The hydrophobicity of xenon causes easy partitioning into phospholipid membranes where it can be combined with hydrophobic molecular cages as their hosts that confer a specific chemical shift to the guest nuclei for easy Hyper-CEST detection. The CEST effect is sensitive to exchange dynamics and can therefore be used to characterize the conditions for the specific host-guest system in various environments. This talk will give an overview about applications such as sensing for membrane fluidity and integrity or NMR imaging studies of liposome tracking for targeted drug delivery.

BP 35.2 Wed 15:30 H 1028

Lipid composition in fusion of model membrane systems studied by x-ray diffraction — •Sebastian Köhler[1], Yihui Xu[1], Ziad Khattari[2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Georg-August-Universität Göttingen — [2]Department of Physics, Hashemite University, Zarqa, Jordan

We have investigated the structure and interaction of solid-supported multilamellar phopholipid 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.

BP 35.3 Wed 15:45 H 1028

VSG dynamics on the Trypanosome and on model membranes — Marius Glogger[1], Marie Spindler[1], Andreas Hartel[1,2], Nicola Jones[1], Markus Engstler[1], and •Susanne Fenz[1] — [1]Biocenter: Cell and Developmental Biology, University of Würzburg, Würzburg, Germany — [2]Department of Electrical Engineering, Columbia University, New York, New York 10027, United States

Trypanosomes are the pathogens of sleeping sickness in humans and Nagana in cattle. They exhibit a uniform surface coat of multiple copies of variable surface glycoproteins (VSGs). Trypanosomes use this extremely dense, albeit highly dynamic surface coat for protection against the host's innate immune response. The entire VSG surface coat can be exchanged by endocytosis of the old VSG and parallel exocytosis of a new VSG variant within 10 minutes. However, both processes are restricted to a small membrane invagination of the cell surface, the so-called flagellar pocket. The mobility of VSG is essential for the parasite's survival and the focus of our research interest. Trypanosomes are excellent model organisms because 95% of their surface coat consists of VSGs. Thus, comparable measurements in live cells and model membranes will allow us to separate active motion from passive diffusion. As VSGs are abundant they can be easily purified and subsequently integrated into supported lipid bilayers via their membrane anchor. We apply single-molecule fluorescence microscopy to study VSG dynamics in immobilized trypanosomes and model membranes with special emphasis on the modulating character of protein glycosylation.

BP 35.4 Wed 16:00 H 1028

Al3+ binding effects on lipid membrane structure — Hannah Wayment-Steele[1], Sofia Svedhem[2], Lewis E. Johnson[3], Malkiat S. Johal[1], Björn Agnarsson[2], and •Angelika Kunze[4] — [1]Dept. of Chemistry, Pomona College, CA, USA — [2]Dept. of Applied Physics, Chalmers Univ. of Technology, Göteborg, Sweden — [3]Dept. of Chemistry, Univ. of Washington, Seattle, WA, USA — [4]Inst. of Physical Chemistry, Univ. of Göttingen, Göttingen, Germany

Aluminum is found in daily life as a contaminant in food-contact articles as well as in medical and cosmetic products. However, the aluminum ion has been identified as a neurotoxin; several studies have suggested that increased Al3+ concentrations are correlated with increased risks for Alzheimer's disease. The toxicity of the Al3+ derives

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 — Maria J. Retamal[1,2], Marcelo A. Cisternas[1,2], Sebastian E. Gutierrez-Maldonado[3], Tomas Perez-Acle[3], Birger Seifert[1,2], Mark Busch[4], Patrick Huber[4], and •Ulrich G. Volkmann[1,2] — [1]SurfLab UC, Instituto de Fisica, Pontificia Universidad Catolica de Chile (UC), Santiago, Chile — [2]CIEN-UC, Santiago, Chile — [3]DLab, Fundación Ciencia y Vida, Santiago, Chile — [4]Institute of Materials Physics and Technology, Hamburg Univ. 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/publishing/journal-highlights/artificial-membranes-silicon

BP 35.6 Wed 16:30 H 1028

Attraction between hydrated hydrophilic surfaces — •Matej Kanduc[1], Emanuel Schneck[2], and Roland Netz[1] — [1]Department of Physics, Free University Berlin — [2]Max 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 all-atom 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 contact angles of 135°) to hydrophilic surfaces exhibiting complete wetting. Indeed, for a finite range of contact angles between 65° and 90°, we find a regime where hydrophilic surfaces attract at subnanometer separation and stably adhere without intervening water, in good agreement with experiments. Analysis of the total number of hydrogen bonds (HBs) formed by water and surface groups rationalizes this crossover between hydration repulsion and hydrophilic attraction in terms of a subtle balance [2]. Such solvent reorganization forces presumably underlie also other important phenomena, such as selective ion adsorption to interfaces as well as ion pair formation.

[1] M. Kanduc, A. Schlaich, E. Schneck, and R. Netz; Adv. Colloid Interface Sci. 208, 142 (2014).

[2] M. Kanduc, E. Schneck, and R. Netz; Chem. Phys. Lett. 610, 375-380 (2014)

15 min break

BP 35.7 Wed 17:00 H 1028

Vesicles-on-a-chip: versatile fabrication of liposomes and polymersomes in microfluidic environment — •Julien Petit, Ingmar Polenz, Stephan Herminghaus, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Synthetic biology recently appeared as an emerging field of research for mimicking and understanding natural systems from a fundamental point of view. This "bottom-up" approach involves the investigation of the biological and physical properties and mechanisms of functional biological systems (from basic modules/parts of living cells to more complicated systems). One key challenge relies on the fabrication of compartments such as vesicles, that can be viewed as model membranes, as demonstrated by numerous studies during the past decades. Despite this fact, reliable methods for high-throughput production of vesicles (liposomes as well as polymersomes) in an easy and well-controlled manner are still in progress. In this scope, we propose a versatile method for producing monodisperse vesicles in a microfluidic environment from double-emulsions templates. The combination of the microfluidic chip design and the original channel treatment as well as the new fluid systems employed in the present study allows the production and manipulation of liposomes and polymersomes on demand. This new technique opens a playground for fundamental studies, e.g. on the collective behavior of vesicle clusters and their self-organization, as well as applications such as protein or drug encapsulation and mechanisms of targeted delivery.

BP 35.8 Wed 17:15 H 1028

High resoultion mapping of the surface charge density of lipid bilayers under physiological conditions — •Thomas Fuhs, Lasse Hyldgaard Klausen, Flemming Besenbacher, and Mingdong Dong — Interdisciplinary Nanoscience Center (iNANO), Aarhus University, Aarhus, Denmark

The surface charge density of lipid bilayers governs the cellular uptake of charged particles and guides cell-cell and cell-surface interactions. Direct probing of the potential requires sub nanometer distances as the electrostatic potential is screened by high physiological salt concentrations. This prevented direct measurement of the SCD under physiological conditions. In this study we investigate supported bilayers of lipid mixtures that form domains of distinct surface charges, submerged in 150mM NaCl. We use a scanning ion-conductance microscope (SICM) setup to measure the ionic current through a nanopipette as the pipette is scanned several nm above the sample. The charged headgroups of the lipids attract counter ions leading to a charge dependent enhancement of the ion concentration near the surface. This creates a measurable change of conductivity in the vicinity of the surface. As the dependency of the current on the SCD and pipette potential is nontrivial we characterized it using numerical solutions to Poisson and Nernst-Planck equations. Based on the simulation results we propose an imaging method. We confirm feasibility of the proposed method by experimentally mapping the local surface charge density of phase separated lipid bilayers.

BP 35.9 Wed 17:30 H 1028

From destruction to protection - following peptide interactions with membrane interfaces — •Johannes Franz[1], Denise Schach[1], Joe E. Baio[2], Dan Graham[3], David G. Castner[3], Mischa Bonn[1], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Oregon State University, Corvallis, OR, USA — [3]University 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.

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 mono- and bilayers.

BP 35.10 Wed 17:45 H 1028

Addressing Multivalent Interactions Using Single Particle Tracking — •Stephan Block, Srdjan Acimovic, Mikael Käll,

and Fredrik Höök — Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden

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 particles 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 Sandoghdar — 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 endocytotic 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 Backus — 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 are not surface-active at the bare water-air interface, they do interact strongly with the lipid monolayer. The presence of dendrimers in the solution 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: Cell adhesion, mechanics and migration II

Time: Wednesday 15:00–18:30 Location: H 1058

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 CT26. 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 Erzberger[1], Martin Bergert[2,3], Ewa Paluch[3], and Guillaume Salbreux[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]currently at: Laboratory of Thermodynamics in Emerging Technologies, ETH Zuerich, Switzerland — [3]MRC 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 — •Erik Bernitt, Malte Ohmstede, and Hans-Günther Döbereiner — 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 experiments in which we shift the cell's position of the chemical equilibrium between f- and g-actin using latrunculin A.

BP 36.4 Wed 15:45 H 1058

Catching a target with directed run and tumble motion — •Pawel Romanczuk[1] and Guillaume Salbreux[2] — [1]Dept. of Ecology and Evolutionary Biology, Princeton University, NJ 08544 — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden

During Zebrafish development progenitor cells are required to arrive with high temporal and spatial precision at specific targets sites. On the one hand this directed migration is associated with the presence of chemical cues, and on the other hand it was reported to consist of phases of persistent motion ("runs") interrupted by reorientation events associated with cell repolarization ("tumbles") [1]. Here we consider a minimal model of chaser particles undergoing directed migration towards a target with noisy information on the target position, e.g. due to chemotactic sensing. The chaser moves by switching between two phases of motion (run and tumble), reorienting itself towards the target during tumble phases, and performing a persistent random walk during run phases. We show that the chaser average run time can be adjusted to minimize the catching time or the spatial dispersion of the chasers. We obtain analytical results for the catching time and for the spatial dispersion in the limits of small and large ratios of run time to tumble time, and scaling laws for the optimal run times. Finally, we discuss the possibility of an optimal chemotactic strategy in animal cell migration by analyzing in-vivo experiments together with simulation of a more detailed stochastic model fitted to experimental data.

[1] M. Reichman-Fried et al., Developmental Cell 6, 589 (2004)

BP 36.5 Wed 16:00 H 1058

Bistable forespore engulfment in *B. subtilis* by a zipper mechanism in absence of the cell wall — •Nikola Ojkic[1], Javier López Garrido[2], Kit Pogliano[2], and Robert G. Endres[1] — [1]Department of Life Sciences, Imperial College, London, United Kingdom — [2]Division of Biological Sciences, University of California, San Diego, La Jolla, California, USA

To survive starvation, the bacterium *Bacillus subtilis* forms durable spores. The initial step of sporulation is asymmetric cell division, leading to a large mother-cell and a small forespore compartment. After division is completed, the mother cell engulfs the forespore in a slow process based on cell-wall degradation and synthesis. However, recently a new cell-wall independent mechanism was shown to significantly contribute, which can even lead to fast engulfment in ~ 60 % of the cases when the cell wall is removed. In this backup mechanism, strong ligand-receptor binding between mother-cell protein SpoIIIAH and forespore-protein SpoIIQ leads to zipper-like engulfment, but quantitative understanding is missing. We combined florescence image analysis and stochastic Langevin simulations of the fluctuating membrane to investigate the origin of fast bistable engulfment in absence of the cell wall. We predict regions of osmotic pressure and membrane-surface tension that produce successful engulfment. Our cell morphologies compare favorably with experimental time-lapse microscopy, with engulfment sensitive to the number of SpoIIQ-SpoIIIAH bonds in a threshold-like manner. Indeed, decreasing the medium osmolarity in experiments prevents engulfment in line with predictions.

BP 36.6 Wed 16:15 H 1058

Modeling crawling cell motility — •Jakob Löber[1], Falko Ziebert[2], and Igor Aranson[3] — [1]Institut für Theoretische Physik, TU Berlin — [2]Albert-Ludwigs-Universität, Freiburg, Germany — [3]Argonne National Laboratory, Argonne, USA

Self-propelled motion, emerging spontaneously or in response to external cues, is a hallmark of living organisms. Self-propulsion relies on the force transfer to the surrounding. While self-propelled swimming in the bulk of liquids is fairly well characterized, many open questions remain in our understanding of self-propelled motion of cells along substrates. Here we present a phenomenological model for crawling cells based on an advected phase field model and other reaction-diffusion equations. The force transfer from the cell to the substrate is explicitly taken into account, giving rise to complex modes of cell movement such as bipedal motion and stick-slip motion. The model captures the generic structure of the traction force distribution and faithfully reproduces experimental observations, like the response of a cell on a gradient in substrate elasticity (durotaxis). Collective states of motion such as concerted rotation arises for multiple interacting cells on patterned substrates.

30 min break

BP 36.7 Wed 17:00 H 1058

Spontaneous actin dynamics in contractile rings — Viktoria Wollrab[1,2], Raghavan Thiagarajan[1,2], Daniel Riveline[1,2], and •Karsten Kruse[3] — [1]Laboratory of Cell Physics, Institut de Science et d'Ingénierie Supramoléculaires, 67083 Strasbourg, France — [2]Laboratory of Cell Physics, Institut de Génétique et de Biologie Moléculaire et Cellulaire, 67404 Illkirch, France — [3]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany

Networks of polymerizing actin filaments are known to be capable to self-organize into a variety of structures. For example spontaneous actin polymerization waves have been observed in living cells in a number of circumstances, notably, in crawling neutrophils and slime molds. During later stages of cell division, they can also spontaneously form a contractile ring that will eventually cleave the cell into two daughter cells. We present a framework for describing networks of polymerizing actin filaments, where assembly is regulated by various proteins. It can also include the effects of molecular motors. We show that the molecular processes driven by these proteins can generate various structures that have been observed in contractile rings of fission yeast and mammalian cells. We discuss a possible functional role of each of these patterns.

BP 36.8 Wed 17:15 H 1058

Characterizing Cell Motility and Transmigration on Ring Shaped Micro Patterns — •Christoph Schreiber, Felix Jakob Segerer, and Joachim Oskar Rädler — Fakultät für Physik, Ludwig-Maximilians-Universität München, Germany

Cell migration is important in many biological processes such as embryogenesis, wound healing, or cancer metastasis. To understand the formation of tumors and the effect of drugs, a detailed characterization of the migration behavior is important. Furthermore the ability to overcome barriers like the basement membrane is a key indicator for the aggressiveness of different cancer cells. Therefore a systematic approach for studying transmigration behavior is necessary to characterize the invasiveness of cancer cells.
Here, we study single cell migration constrained to a micro-patterned ring-shaped lane. On such tracks cells perform a 1D persistent random walk like movement that can be divided in a directional and a reorientation phase. Analyzing large arrays in parallel, we are able to evaluate characteristic velocities and persistence times of a cell line with high accuracy. By introducing a gap of defined size and chemical composition in the ring shaped lane we study how cell migration is affected by the encounter with a chemical barrier. At the chemical border cells either turn around or transmigrate over the barrier. Studying the transmigration probability systematically, we find a steady decrease of transition probability with increasing barrier width.

BP 36.9 Wed 17:30 H 1058

Is the wound healing mechanism an accelerating one? — •Damir Vurnek, Sara Kaliman, and Ana-Sunčana Smith — Theoretical Physics I, FAU Erlangen

Morphogenesis and wound healing both require migration of large number of constituent cells. We address these problems by using MDCK II model epithelium grown on collagen I coated glass substrates. Usually, to study such a system, a part of an expanding monolayer is carefully analyzed. Here we take the complementary approach and look at the global development of an, initially droplet seeded, system of cells which is allowed to expand freely over time. In contrast to most studies majority of our experiments performed have very long time windows of at least 10 days. On the basis of experimental findings the known model of exponential growth of small ($< 0.1\text{mm}^2$) cell clusters is expanded with an additional parameter which accounts for the slowing down of area growth. Thus, with the use of a simple differential equation, and easily interpreted parameters - initial colony area (A_0), colony doubling time (τ) and effective slowing down of growth (b) - one can successfully predict the area expansion of clusters in the range of four orders of magnitude. Further data analysis shows a stunning picture of a perpetually accelerating monolayer edge, in stark opposition to the concept of constant speed limits supposedly reached by macroscopic ($> 10\text{mm}^2$) monolayers. These findings raise the questions of accumulating stress levels such epithelial tissues endure before breaking or buckling, or even just slowing down.

BP 36.10 Wed 17:45 H 1058

Migration patterns of dendritic cells in response to chemokines — •Veronika Bierbaum, Jan Schwarz, Eva Kiermaier, Michael Sixt, and Tobias Bollenbach — IST AUSTRIA,

Am Campus 1, 3400 Klosterneuburg

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 cell motion. In these assays, cells 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 motion. In soluble gradients of CCL19 and CCL21, dendritic cells maintain their directionality towards the chemokine source over a large range of concentrations. However, in linear and exponential gradients of immobilized CCL21 the cells' directionality depends on chemokine concentration and is maximal at low concentrations. To rationalize these observations we develop a theoretical model of chemokine signal detection and interpretation. This experimental-theoretical approach can reveal general principles of cell migration in response to chemokines.

BP 36.11 Wed 18:00 H 1058

Stress induced collective cell migration in epithelial sheets — •Michael Köpf — Departement de Physique, Ecole Normale Superieure Paris, France

Stress normal to the boundary of an epithelial sheet can arise in constrained and unconstrained cell layers through pushing and pulling of surrounding tissue and wettability of the substrate, respectively. A continuum model describes the epithelium as a polarizable and chemomechanically interacting layer under the influence of such stresses. This model links the experimentally observed formation of finger-like protrusions at the edge of unconstrained spreading cell monolayers to substrate wettability [1]. Statistics of the velocity orientation shows a strong alignment in the fingers opposed to an isotropic distribution in the bulk, in agreement with measurements by Reffay et al [2]. The model further exhibits a stress accumulation within the tissue that proceeds in form of a mechanical wave, starting at the wound edge [3].

Additionally, four types of spreading and motility can 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 [4].

[1] Köpf, Pismen, *Soft Matter* **9** (2013) 3727-3734
[2] Reffay et al., *Biophysical Journal* **100** (2011) 2566-2575
[3] Serra-Picamal et al., *Nature Physics* **8** (2012) 628-634
[4] Köpf (2014) in preparation

BP 36.12 Wed 18:15 H 1058

Polarization of motile amoeboid cells under confinement — •Oliver Nagel[1], Can Guven[2], Matthias Theves[1], Megan Driscoll[2], Wolfgang Losert[2], and Carsten Beta[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Germany — [2]Department of Physics, University of Maryland, 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 Location: EW 202

Invited Talk BP 37.1 Wed 15:00 EW 202

The cost of moving optimally — •Dinant Kistemaker — 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 inconsistent 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 input 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 effort with information entropy: a new method applied to complex biological movement — •Daniel Häufle[1], Michael Günther[1], Günter Wunner[2], and Syn Schmitt[1,3] — [1]Human Movement Simulation Lab, Universität Stuttgart — [2]Institut für Theoretische Physik 1, Universität Stuttgart — [3]Stuttgart Research Centre for Simulation Technology, Universität Stuttgart

Recently, a new measure has been proposed to quantify control effort of biological and technical movement. This measure was developed to enable a quantitative evaluation of a long standing hypothesis stating that the physical structure of humans and animals allow movement generation with less control effort. In particular, it has been hypothesized that muscles with their nonlinear contraction properties reduce control effort. This new measure is based on Information Entropy and reveals that the control effort for the simple movement task of periodic hopping is only I=32bit when generated with a muscle vs. I=660bit with a DC-motor. To further investigate this hypothesis, this approach has now been applied to human walking in comparison to robotic walking. Additionally, we will show that this measure can also be applied to microscopic active brownian motion swimmers of different shape to emphasize the wide application of our approach.

BP 37.3 Wed 15:45 EW 202

Predicted stop positions used to push pointing movements into the goal — •Karl Kalveram — Tu Darmstadt and Uni Duesseldorf

Recently we performed experiments with human forearm-movements used in pointing to a remote goal. The movements were perturbed by artificial changes of the geometry of the arm-pointer arrangement. Under discontinuous visual feedback (the pointer's location being visible only at beginning and ending of the movement), the error (difference between the goal and the pointer's location at movement end) was relatively high and varied with the perturbations. Under continuous visual feedback of the pointer's momentary location, however, the error remained low and was un-correlated with the perturbations. Inspection of the kinematics revealed that ordinary negative feedback control could not explain this effect.

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 principally enables predicting the stop position from any interim 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

Reafference Principle 2.0 — •Kim Joris Boström and Heiko Wagner — Motion Science, University of Münster, Germany

The reafference 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 it learns 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 reafference principle by computer simulations.

BP 37.5 Wed 16:15 EW 202

Wobbling masses: definite costs and potential benefits — •Michael Günther[1,3] and Syn Schmitt[1,2] — [1]Universität Stuttgart, Human Movement Simulation Lab — [2]Stuttgart Research Centre for Simulation Technology — [3]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 Location: C 130

Invited Talk BP 38.1 Wed 15:00 C 130

Ultraslow dynamics of hydrated metal ions at the water-solid interface observed by atomic force microscopy — •Kislon Voitchovsky — 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.

[1] M. Ricci, P. Spijker, F. Stellacci, J.-F. Molinari, K. Voitchovsky, Langmuir, 29, 2207 (2013) [2] M. Ricci, P. Spijker, K. Voitchovsky, Nature Commun., 5, 4400 (2014)

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 interfaces 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 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, unlikely 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 the AFM measured force curves 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 heterogeneous 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 unprecedentedly high resolution.

BP 38.4 Wed 16:00 C 130

Ion adsorption-induced wetting transition in oil-water-

mineral systems — •Frieder Mugele, Bijoy Bera, Andrea Cavalli, Igor Siretanu, Armando Maestro, Dirk van den Ende, Michel Duits, and Martien Cohen-Stuart — University of Twente, MESA+ 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 10° 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 Kensbock, Heiko Ahrens, Andreas Gröning, Thomas Ortmann, and Chrisitane 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 — •Mischa 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 — •Eva Brandes[1], Peter Karageorgiev[1], Padmanabhan Viswanath[2], and Hubert Motschmann[1] — [1]Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany — [2]Centre 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 investigated 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 nonmonotonous concentration profile.

BP 38.8 Wed 17:30 C 130

Macro- and Microrheology of Heterogeneous Microgel Packings — Fany Di Lorenzo[1,2] and •Sebastian Seiffert[1,2] — [1]Freie Universität Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Germany

Microgels are soft deformable colloids that can be packed by external compression. Such packing transforms a suspension of loose microgel particles into an arrested state with properties similar to that of a macroscopic gel. We follow this idea and prepare microgel packings that consist of both soft, loosely crosslinked particles and stiff, densely crosslinked particles, considering packing fractions that cover the range from the onset of particle contact to particles that are strongly packed, deformed, and deswollen. With this strategy, we investigate the transition from a particulate suspension to a macrogel-type system with defined, purposely imparted sub-micrometer scale spatial heterogeneity. We study these inhomogeneous composites from macro- and microscopic perspectives by oscillatory shear rheology and by fluorescence recovery after photobleaching to probe their macroscopic mechanics and the microscopic mobility of flexible linear tracer polymers that diffuse through them.

References: F. Di Lorenzo, S. Seiffert, Macromolecules 2013, 46, 1962. F. Di Lorenzo, S. Seiffert, Colloid Polym. Sci. 2013, 291, 2927.

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.

BP 39: Physics of Sustainability and Human-Nature Interactions I (joint SOE/DY/jDPG/BP/AKE)

Time: Wednesday 16:45–18:30 Location: MA 001

Topical Talk BP 39.1 Wed 16:45 MA 001

The Industrial Society's natural Sustainability — •Hans G. Danielmeyer 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 Word War II and 1980; increase retirement age; continue innovation; and defend the G7 position globally. Believing in the Neoclassical Paradigm of exponential growth is already Chinas problem because it wastes resources with unsustainable investments.

[1] H. G. Danielmeyer and T. Martinetz, An exact theory of the industrial evolution and national recovery, www.inb.uni-luebeck.de, 2009 pdf. [2] C. Teuling and R.Baldwin, Secular Stagnation: Facts, Causes and Cures, CEPR London 2014, www.voxeu.org/sites/default/files/Vox_secular_stagnation.pdf

BP 39.2 Wed 17:15 MA 001

The decoupling of CO2 emissions and human development — Kai Kornhuber[1], Dominik Reusser[1], •Luis Costa[1], Jürgen Kropp[1,2], Rybski Diego[1], and Schellnhuber Joachim[1,3] — [1]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [2]University of Potsdam, Potsdam, Germany — [3]Santa Fé Institute

Evidence of a decoupling between greenhouse gas emission and socioeconomic development would benefit international climate negotiations 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 Fluschnik, Steffen Kriewald, Anselmo García Cantú Ros, Bin Zhou, Dominik Reusser, Jürgen Peter Kropp, and Diego Rybski — 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-exponents as 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 Sterzel, Prajal 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 — •Prajal Pradhan[1], Dominik Reusser[1], Matthias Lüdeke[1], and Juergen Kropp[1,2] — [1]Potsdam Institute for Climate Impact Research, Potsdam — [2]University 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 environmental 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 $CO_{2eq.}$/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

Sustainabilty for a Warming Planet — •Humberto Llavador[1,2], John Roemer[3], and Joaquim Silvestre[4] — [1]Universitat Pompeu Fabra (Barcelona) — [2]Barcelona GSE — [3]Yale University — [4]University 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 bargaining problem between developing and developed nations requires recognizing the relationship between economic growth and the climate problem. We propose that the dates at which developing countries converge in living standards to those of developed countries should

not be altered by the agreement. This principle, along with sustainability, 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 Location: H 1058

Discussion

BP 41: Protein structure and dynamics I

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

Invited Talk BP 41.1 Thu 9:30 H 1058

Probing the downhill folding kinetics of Lambda repressor variants with optical tweezers — Ann Mukhortava, Andreas Hartmann, and •Michael Schlierf — B CUBE - Center for Molecular 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 folding using optical tweezers that provide the possibility to measure structural 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/Q33Y/G46,48A) and LambdaHA (Y22W/Q33H/G46,48A). We show that force perturbation of the energy 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 dependence. 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 Mauri[1,2], Tobias Weidner[2], and Heike Arnolds[1] — [1]Surface Science Research Centre, University of Liverpool, UK — [2]Max Planck institute for polymer research, Mainz, Germany

The adsorption of insulin at surfaces is a ubiquitous problem of interest in various fields of biotechnology and pharmaceutical applications. Studying protein structure at surfaces is generally though a challenging 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 calculations 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. Insulin is present in Nature mainly as hexamers, dimers and monomers. While the first two are stable, monomers do denaurate 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 versatility 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 Schmüser[1], Nadja Hellmann[2], Mischa Bonn[1], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Institute for Molecular Biophysics, Jakob Welder Weg 26, 55128 Mainz, Germany

Information about the 3D structure of proteins at interfaces is essential 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 structure are insufficient to understand many protein functions, which arise from protein dynamics: Protein folding, reorientation and motion. A well-established tool to study static protein structures is X-ray crystallography. But with this method it is still challenging to follow protein conformational change, folding or refolding in real time. We use vibrational sum frequency generation spectroscopy (SFG) to follow conformational changes of proteins at interfaces. The aim is to combine time resolved SFG with molecular dynamics simulations to glean information 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 Köhler[1,2] and Giovanni Settanni[1,3] — [1]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, D-55128 Mainz — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, D-55128 Mainz — [3]Max 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 protein 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 electrostatic interactions between the protein and the silicate surface as well as the counter ion layer. Preferred adsorption orientations for the globular 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 Lorenzo[1], Hadi RAmezani-Dakhel[2], Hendrik Heinz[2], and Marialore Sulpizi[1] — [1]Johannes Gutenberg University Mainz, Staudinger Weg 7 55099 Mainz — [2]epartament 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 biointerfaces for medical and bio-technological applications. In this contribution we aim to provide a characterization of different peptides / gold interactions at a molecular level in order to explain and interpret 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 theory (DFT) calculations are also discussed. Results for aminoacids and

nucleic acids nano assembly different gold surfaces are presented.

[1] V. Humblot, A. Tejeda, J. Landousi, A. Vallee, A. Naitabdi, A. Taleb, C.-M. Pradier. Surface Science 2014, 628, 24-29.

[2] Heinz H, Vaia RA, Farmer BL, Naik RR J. Phys. Chem. C 2008, 112, 17281 17290; Heinz H, Farmer BL, Pandey RB, Slocik JM, Patnaik SS, Pachter R, Naik RR. J. Am. Chem. Soc. 2009, 131, 9704-9714

30 min break

BP 41.6 Thu 11:30 H 1058

Self-assembled protein nanofibers as basis for novel biomaterials — •Christian Helbing[1], Gang Wei[2], Tanja Deckert-Gaudig[3], and Klaus D. Jandt[1] — [1]Chair of Materials Science (CMS), Otto-Schott-Institute of Materials Research (OSIM), Friedrich Schiller University Jena, Jena, Germany — [2]Hybrid Materials Interfaces Group, University of Bremen, Bremen, Germany — [3]Institute for Photonic Technology, Jena, Germany

Protein nanofibers (PNFs) are promising materials for numerous applications in the field of biomedical 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 Adamczyk[1], Niall Simpson[1], Gregory M. Greetham[2], Andrea Gumiero[3], Martin A. Walsh[3], Michael Towrie[2], Anthony W. Parker[2], and Neil T. Hunt[1] — [1]University of Strathclyde, Glasgow, UK — [2]Central Laser Facility, Rutherford Appleton Laboratory, Didcot, UK — [3]Diamond 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 dependence of the vibrational relaxation parameters of the NO stretching vibration is observed indicating that water molecules interact directly with the haem ligand. Furthermore, IR pump-probe data feature quantum beats originating from the preparation of a coherent superposition of low-frequency vibrational modes in the active site of catalase that are coupled to the haem ligand stretching vibration. Together, the data establishes a strong interaction between the haem ligand and a water-mediated H-bond network in catalase that is likely to be pivotal to proton transfer events during the enzymatic cycle.

BP 41.8 Thu 12:00 H 1058

Structural mechanics of 2D and 3D lattices from clathrin proteins — •Mitja Platen[1], Philip N. Dannhauser[2], Heike Böning[2], Huberta Ungewickell[2], Ernst Ungewickell[2], and Iwan A.T. Schaap[1] — [1]IIIrd Institute of Physics, Georg August University Göttingen, Germany — [2]Institute of Cell Biology, Centre of Anatomy, Hannover Medical School, Hannover, Germany

In the cell clathrin proteins can form polyhedral scaffolds that facilitate the formation of highly curved vesicles (~100 nm) from lipid bilayers. These vesicles are involved in intracellular transport but also in the transport of compounds in and out the cell. We recently developed the methodology to reconstitute clathrin lattices in a minimal system, with and without lipid bilayers. With AFM imaging we are able to reconstruct the orientation of the clathrin triskelia in a planar lattice and to quantify the mechanical role of the clathrin light chains in the lattice. Our current efforts are aimed to measure the forces that are exerted by clathrin lattice to bend the lipid bilayer into vesicles.

BP 41.9 Thu 12:15 H 1058

Effects of molecular noise on bistable protein distributions in rod-shaped bacteria — •Lukas Wettmann, Mike Bonny, and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

The distributions of many proteins in rod-shaped bacteria are far from homogeneous. Often they accumulate at the cell poles or in the cell centre. At the same time, the copy number of proteins in a single cell is relatively small making the patterns noisy. To explore limits to protein patterns due to molecular noise, we studied a generic mechanism for spontaneous polar protein assemblies in rod-shaped bacteria, which are based on cooperative binding of proteins to the cytoplasmic membrane. For mono-polar assemblies, we find that the switching time between the two poles increases exponentially with the cell length and 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 yet it 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, it has been noted that phase contrast 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 Grimaldo[1,2], Felix Roosen-Runge[1], Fajun Zhang[2], Frank Schreiber[2], and Tilo Seydel[1] — [1]Institut Laue-Langevin, Grenoble, France — [2]Institut 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 IN16B, 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].

[1] M. Grimaldo, F. Roosen-Runge, F. Zhang, T. Seydel, F. Schreiber, J. Phys. Chem. B **118**, 7203 (2014) [2] M. Grimaldo, F. Roosen-Runge, N. Jalarvo, M. Zamponi, F. Zanini, M. Hennig, F. Zhang, F. Schreiber, T. Seydel, submitted

BP 42: Cytoskeletal filaments (joint BP/CPP)

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

Invited Talk BP 42.1 Thu 9:30 H 1028

Microtubules adapt to mechanical stress through spontaneous intra-lattice repair — Laura Schaedel[1], Karin John[1], Jeremie Gaillard[1], Maxence Nachury[2], Laurent Blanchoin[1], and •Manuel Thery[1,3] — [1]UMR5168, CEA/CNRS/INRA/Université Grenoble-Alpes, Grenoble, France — [2]Stanford University School of Medicine, CA 94305, USA. — [3]Hôpital Saint Louis, UMRS1160, INSERM/AP-HP/Université Paris Diderot, Paris, France

Microtubule arrays define the shape of axons, cilia and 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[1], Catherine Do[2], and •Henry Hess[1] — [1]Department of Biomedical Engineering, Columbia University, New York, New York 10027, USA — [2]Institute for Cancer Genetics, Columbia University Medical Center, New York, New York 10032, USA

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 Lansky[1,2,5], •Marcus Braun[1,2,5], Annemarie Lüdecke[1,2], Michael Schlierf[1], Pieter Rein ten Wode[3], Marcel Janson[4], and Stefan Diez[1,2] — [1]B CUBE, TU Dresden, Germany — [2]MPI-DBG, Dresden, Germany — [3]AMOLF, Amsterdam, The Netherlands — [4]Laboratory of Cell Biology, Wageningen University, The Netherlands — [5]equal contribution

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 crosslinkers 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 Jakobs — 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[1], Lora Winters[2], Iva Tolić[2], and Nenad Pavin[1] — [1]Faculty of science , University of Zagreb, Croatia — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

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 as 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 — •Emanuel Reithmann, Louis Reese, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, München

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/cytoplasm. 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-

locity ensuing from diffusion and capture can effectively be computed within a Michaelis-Menten framework. We predict that diffusion and capture would significantly beat the (three-dimensional) Smoluchowski diffusion limit for the rate of direct protein association to filament ends for practically all proteins that are known to diffuse on microtubules and actin-filaments.

15 min break

Invited Talk BP 42.7 Thu 11:30 H 1028

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.

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 John[1], Denis Caillerie[2], Thomas Stoeter[1,3], and Chaouqi Misbah[1] — [1]Université Grenoble Alpes/ CNRS, LIPHY, F-38000 Grenoble, France — [2]Université Grenoble Alpes/CNRS, 3SR, F-38000 Grenoble, France — [3]Otto-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 a 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 Schnauss[1], Tom Golde[1], Carsten Schuldt[1], Sebastian Schmidt[1], Martin Glaser[1], Dan Strehle[1], Josef Käs[1], and Claus Heussinger[2] — [1]Institute for Experimental Physics I, University of Leipzig , Linnéstraße 5, 04103 Leipzig , Germany — [2]Institute 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 crowding regime is well below the macromolecular 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

Organisation dynamics of stress fibers in adult stem cells — •Carina Wollnik[1], Benjamin Eltzner[2], Stephan Huckemann[2], and Florian Rehfeldt[1] — [1]Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — [2]Institute for Mathematical Stochastics, Georg-August-University, Göttingen, Germany

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].

[1] A. Engler et al., Cell (2006); [2] A. Zemel et al., Nature Physics (2010); [3] B. Eltzner et al., arXiv:1408.4002, 2014; [4] S. Huckemann et al., arXiv:1404.3300, 2014;

BP 42.11 Thu 12:45 H 1028

Elasticity of 3D networks with rigid filaments and compliant crosslinks — •Knut M. Heidemann[1], Abhinav Sharma[2], Florian Rehfeldt[2], Christoph F. Schmidt[2], and Max Wardetzky[1] — [1]Institut für Numerische und Angewandte Mathematik, Georg-August-Universität, Göttingen — [2]Drittes Physikalisches Institut – Biophysik, Georg-August-Universität, Göttingen

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 suggested in prior work, the model system studied here cannot provide an explanation for the experimentally observed linear scaling of the modulus with the stress in filamentous networks.

BP 43: Networks: From Topology to Dynamics II (joint SOE/DY/BP)

Time: Thursday 12:00–13:15 Location: MA 001

BP 43.1 Thu 12:00 MA 001

Sensitivity against author name disambiguation of a motif-based success score in coauthorship networks — •David F. Klosik[1], Stefan Bornholdt[1], and Marc-Thorsten Hütt[2] — [1]Institut für Theoretische Physik, Universität Bremen — [2]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. Weihe, 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)].

BP 43.2 Thu 12:15 MA 001

Random Walks on Citation Networks — •Vimal Kishore and Eduardo G. Altmann — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Scientific papers are the main source of communication of scientific ideas and are connected to each other through citations. The digitalization of articles allows scientists to easily trace not only the citations contained in a paper but also the citations a paper received. This motivates us to consider random walks on citation networks as models of the search of scientific information scientists perform. The spreading of the random walkers in the network provides information on the flow of scientific ideas across different publications and fields. We discuss different mechanisms leading to a sub-linear growth of the number of discovered papers as a function of random-walk steps.

BP 43.3 Thu 12:30 MA 001

Restricting the h-index to a citation time window: A case study of a timed Hirsch index — •Michael Schreiber — Institut 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.

BP 43.4 Thu 12:45 MA 001

An Interacting Network Perspective on Global Trade — •Julian Maluck 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.

BP 43.5 Thu 13:00 MA 001

From diffussion to evolutionary game theory on the multilayer — •Rubén J. Requejo, Nikos E. Kouvaris, and Albert Díaz-Guilera — Foundamental Physics Department, Universitat de Barcelona

I will present some results obtained within the LASAGNE project (multi-LAyer SpAtio-temporal Generalized NEtworks), starting with the effect of the multiplex structure on the diffusion of particles, following with the extension of agent-based dynamics to the multiplex by means of an evolutionary game theoretical model of interacting metapopulations, which shows the effect of the multilayer structure on the replicator dynamics, and finishing with the observation of chimera states in the multiplex for a public goods game with cooperators, defectors and jokers.

BP 44: DNA/RNA and related enzymes

Time: Thursday 15:00–17:00 Location: H 1058

Invited Talk BP 44.1 Thu 15:00 H 1058

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.

BP 44.2 Thu 15:30 H 1058

Mechanisms of backtrack recovery by RNA polymerases I and II — •Ana Lisica[1,2], Marcus Jahnel[1,2], Christoph Engel[3], Edgar Roldan[4,5], Patrick Cramer[3], and Stephan Grill[1,2,4] — [1]BIOTEC, Dresden, Germany — [2]MPI CBG, Dresden, Germany — [3]MPI PBC, Göttingen, Germany — [4]MPI PKS, Dresden, Germany — [5]GISC, Madrid, Spain

RNA polymerases (Pol) backtrack frequently during transcription elongation. To recover from the backtracked state, Pol I uses a strong transcript 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 44.3 Thu 15:45 H 1058

Fast Chromatin Assembly facilitated by Nucleosome Breathing and Replication-Guided Packing — •Johannes Nuebler[1], Brendan Osberg[1], Philipp Korber[2], and Ulrich Gerland[1] — [1]Theory of Complex Biosystems, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]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 biologically 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.

[1] R. Padinhateeri, J.F. Marko, PNAS 108, 7799 (2011).

[2] B. Osberg, J. Nuebler, P. Korber, U. Gerland, Nucleic Acids Res. doi: 10.1093/nar/gku1190 (2014)

BP 44.4 Thu 16:00 H 1058

Gene regulation on the RNA level. The B12 dependent btuB riboswitch studied with single molecule FRET. — •Richard Börner, Michelle Schaffer, Sofia 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 the 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.

1. Perdrizet, G. A., et al. 2012. Proc. Natl. Acad. Sci. U. S. A. 109:3323-3328. 2. Choudhary, P. K. and R. K. Sigel. 2014. RNA 20:36-45. 3. Sindbert, S., et al. 2011. J. Am. Chem. Soc. 133:2463-2480.

BP 44.5 Thu 16:15 H 1058

Random association of neighbouring replicons creates DNA replication factories. — •Jens Karschau[1,2], Nazan Saner[3], Toyaki Natsume[3], Renata Retkute[4], Conrad A. Nieduszynski[5], J. Julian Blow[3], Alessandro P.S. de Moura[2], and Tomozuki U. Tanaka[3] — [1]MPI PKS, Dresden, Germany — [2]University of Aberdeen, U.K. — [3]University of Dundee, U.K. — [4]University of Nottingham, U.K. — [5]University of Oxford, U.K.

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.

BP 44.6 Thu 16:30 H 1058

Vibrational dynamics and hydration of the DNA backbone — •Biswajit Guchhait, Yingliang Liu, Rene Costard, Torsten Siebert, and Thomas Elsaesser — Max-Born-Institut für Nichtlinear Opitk 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 H_2O. This behavior is attributed to steric hindrance and the action of strong electric fields at the interface.

BP 44.7 Thu 16:45 H 1058

Continuous, sequence dependent gelation of nucleic acids driven by a thermal gradient. — •Christof 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.

BP 45: Systems biology

Time: Thursday 15:00–16:15 Location: H 1028

BP 45.1 Thu 15:00 H 1028

Centriole Centering in Centrosomes: Behavior of Catalytic Particles in Active Droplets — •David Zwicker[1,2], Anthony A. Hyman[3], and Frank Jülicher[2] — [1]Harvard University, Cambridge MA, USA — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Max Planck Institute of Cell Biology and Genetics, Dresden, Germany

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 centrioles 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.

BP 45.2 Thu 15:15 H 1028

Reaction-diffusion processes and molecular crowding — •David Gomez and Stefan Klumpp — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The interior of a living cell is a highly crowded environment, with macromolecules occupying up to 20-40% of the total cell volume. Molecular crowding affects both the thermodynamics and the kinetics of molecular binding, via their equilibrium constant and the diffusion coefficients, respectively. Using random walk on a lattice as well as off-lattice simulations with the simulation software ReaDDy, we consider reactions that uncouple the effects of molecular crowding on binding equilibria and the effects on molecular diffusion. As an application of our method, we combine the two uncoupled reactions into a Michaelis-Menten-like reaction and study the effects of molecular crowding on the overall product synthesis rate. The conditions to obtain the maximal product synthesis rate depend on crowding levels and other parameters intrinsic to the reaction.

BP 45.3 Thu 15:30 H 1028

Spatio-temporal dynamics of segregation in gonococcal populations — •Enno R. Oldewurtel, Nadzeya Kouzel, and Berenike Maier — Department of Physics, University of Cologne

Various bacterial pathogens evolved to escape the host immune system by reversibly switching off the generation of surface molecules via mutations. This can generate heterogeneity within a population. However, new mutant cells are likely to get lost again due to stochastic fluctuations before increasing in number. Hence, it is unclear how heterogeneity can evolve and be maintained.

The human pathogen *Neisseria gonorrhoeae* can undergo frequent changes in its major virulence factor, a long polymeric cell appendage, called type IV pilus. It can switch on and off modifications or production of this structure. Type IV pili mediate aggregation among bacteria. Thus changes in the pilus, can lead to changes in the physicochemical interaction between cells. Here, we address the spatio-temporal dynamics of emergence and spreading of bacteria with modified or lacking type IV pili, within a growing colony of *N. gonorrhoeae*.

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.

BP 45.4 Thu 15:45 H 1028

Scaling and regeneration of self-organized patterns — •Steffen Werner[1], Tom Stückemann[2], Manuel Beirán Amigo[1,3], Jochen C. Rink[2], Frank Jülicher[1], and Benjamin M. Friedrich[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Universidad 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 chemical pattern formation, yet the resulting Turing patterns usually do not scale with system size, but are governed by characteristic length scales. Here, we introduce a generalization of 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**

BP 45.5 Thu 16:00 H 1028

Competition between nucleosomes and transcriptional machinery determines the timing of genome activation in the zebrafish embryo — •Stefanie Belohlavy[1], Jens Karschau[1], Shai R. Joseph[2], Mukesh Kumar[2], Andrej Shevchenko[2], Nadine L. Vastenhouw[2], and Vasily Zaburdaev[1] — [1]MPI PKS, Dresden, Germany — [2]MPI CBG, Dresden, Germany

In a developing embryo, many identical cells are formed by rapid cell divisions from one single egg cell. Initially, DNA is not readable for protein synthesis, and cells only rely on egg-provided resources. Then, once a certain number cells have been produced, DNA transcription starts. Why DNA is initially transcriptionally silent is a topic of strong debate. Previously, biological models of a repressor silencing DNA were proposed. In analogy to this idea, we experimentally show nucleosomes to act as a highly abundant repressor in zebrafish. To fully explain transcriptional activation, we propose a theoretical competition model. It consists of an activator (which only binds to specific sites) and a repressor (which has uniform probability to bind anywhere on the DNA). The exponential increase of DNA lowers the free repressor pool. Whenever a repressor leaves an activator site, activators rebind to it instead of a repressor triggering DNA transcription. Our model is consistent with our experimental advances: variations in the ratio of DNA to repressor shift the time of transcriptional onset. Future modifications to the strength of binding sites will help us to identify particular activators as theory and experiment continue to advance side by side.

BP 46: Biomaterials and Biopolymers II (joint CPP/BP)

Time: Thursday 15:00–18:00 Location: C 264

BP 46.1 Thu 15:00 C 264

Dynamic and static force measurements on (PLL/HA)n multilayer films by atomic force microscopy — •Johannes Hellwig and Regine von Klitzing — Stranksi-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.

(1) Volodkin, D. V.; Larionova, N. I.; Sukhorukov, G. B. Biomacromolecules 2004, 5, 1962.

(2) Decher, G. Science 1997, 277, 1232.

(3) Üzüm, C.; Hellwig, J.; Madaboosi, N.; Volodkin, D.; v. Klitzing, R. Beilstein J. Nanotechnol. 2012, 3, 778.

BP 46.2 Thu 15:15 C 264

Mechanical characterization of recombinant spider silk: yarn tensile testing and single fiber deformation via AFM — •Benedikt Neugirg[1], Gregor Lang[2], Thomas Scheibel[2], and Andreas Fery[1] — [1]Physical Chemistry II, University of Bayreuth — [2]Biomaterials, 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.

We found 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.

BP 46.3 Thu 15:30 C 264

Wang-Landau simulation of protein-like Gō model molecules — •Arne Böker and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg

The Wang-Landau method is a recent addition to the Monte Carlo family, able to provide complete thermodynamic information about a system. Contrary to Markovian Monte Carlo, it works in a generalized statistical ensemble, giving the opportunity to access quantities of microcanonical and canonical ensembles in one simulation.

Gō-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 Gō 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 Gō model on these properties.

BP 46.4 Thu 15:45 C 264

The effect of specific interactions on the state diagram of a hard-sphere chain model — •Benno Werlich[1], Timur Shakirov[1], Mark Taylor[2], and Wolfgang Paul[1] — [1]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Halle(Saale), Germany — [2]Department of Physics, Hiram College, Ohio, USA

Secondary structure formation in proteins is generated by an interplay of unspecific and specific interactions. We employ a coarse-grained, one-bead protein-like model to qualitatively understand the importance of the specific interactions. Based on a hard-sphere chain model with unspecific square well attractions we introduce specific interactions as additional square well potentials. These interactions are selective and correspond to a simple donor acceptor representation in the context of hydrogen bonds. The donor acceptor interaction strength can be changed via variation of the well depth of the square well potential. A comparison between hard-sphere chains with and without specific interactions shows a strong deviation in certain ranges of the density of states (DOS). The DOS is the basic function which encodes the whole thermodynamics and thus the microcanonical and canonical analysis give a more detailed insight. To generate the DOS we applied the Stochastic Approximation Monte Carlo method.

BP 46.5 Thu 16:00 C 264

Characterization of a liposomal drug carrier with continuous contrast variation in SAXS — •Raul Garcia-Diez[1], Christian Gollwitzer[1], Michael Krumrey[1], and Zoltan Varga[2] — [1]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [2]Biological Nanochemistry Research Group, Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Magyar Tudosok korutja 2, H-1117, Budapest, Hungary

Doxorubicin is an anticancer drug known for its high cardiotoxicity, though a liposomal formulation of it can reduce this side-effect significantly and improve the pharmacokinetics of the drug. In this work, the mean size and average density of pegylated liposomal doxorubicin (Caelyx®) was determined by continuous contrast variation in SAXS with iodixanol, an iso-osmolar suspending medium. The study is focused on the isoscattering point position and the analysis of the Guinier region of the scattering curves recorded at different solvent densities at the four-crystal monochromator beamline of PTB at the synchrotron radiation facility BESSY II. The response of the liposome to increasing solvent osmolality and the structure of the liposome-encapsulated doxorubicin fiber after the osmotic shrinkage of the liposome are evaluated with sucrose contrast variation in SAXS/WAXS.

BP 46.6 Thu 16:15 C 264

Binding of amino acids to bioactive calcite surface — •Robert Stepić[1], Zlatko Brkljača[1], David M. Smith[2,3], and Ana-Sunčana Smith[1] — [1]Institute for Theoretical Physics and Excellence Cluster: Engineering of Advanced Materials, FAU Erlangen-Nürnberg, Nägelsbachstraße 49b, Erlangen, 91052, Germany — [2]Division of Organic Chemistry and Biochemistry, Rudjer Bošković Institute, Bijenička 54, 10000, Zagreb, Croatia — [3]Center for Computational Chemistry, FAU Erlangen-Nürnberg, Nägelsbachstraße 25, Erlangen, 91052, Germany

Biomineralization is a process by which living organisms form minerals. This process is controled mainly by proteins and the resulting end products have distinctively different properties than minerals produced by abiotic mineralization. Better understanding of underlying mechanisms of biomineralization could help us make use of them in wide range of applications. Our goal is to gain further insight into the role of proteins in biomineralization by taking their elementary building blocks, amino acids, and investigating their interactions with a calcite surface in water. To achieve this we use a well established theoretical framework of molecular dynamics implemented in free GROMACS package. Efficient sampling of the phase space is done using the harmonic bias potential along the suitable reaction coordinate. This allows us to construct the potential of mean force and determine the free energies of binding to the surface of various amino acids. Results of this research will give us clues as to what amino acids play a key role in proteins that control the process of biomineralization.

15 min. break

BP 46.7 Thu 16:45 C 264

Investigation of the lateral arrangement of phospholipid monolayers with respect to the adsorption of hyaluronan* — •Florian Wieland[1], Thomas Zander[1], Sören Gayer[1], Andra Dedinaite[2], Per Claesson[2], Vasyl Haramus[1], and Regine Willumeit-Römer[1] — [1]Helmholtz Zentrum Geesthacht, Max Planck Str. 1, 21502 Geesthacht — [2]KTH 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.

BP 46.8 Thu 17:00 C 264

Interaction of Hyaluron and Phospholipids at high hydrostatic pressure — •Thomas Zander[1], Florian Wieland[1], Min Wang[2], Akanksha Raj[2], Per Claesson[2,3], Andra Dedinaite[2,3], Vasyl Haramus[1], Regine Willumeit-Römer[1], and Andreas Schreyer[1] — [1]Helmholtz Zentrum Geesthacht, Institute for Materials Research, DE-21502 Geesthacht — [2]KTH Royal Institute of Technology, School of Chemical Sciences and Engineering, SE-10044 Stockholm — [3]SP 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.

BP 46.9 Thu 17:15 C 264

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.

BP 46.10 Thu 17:30 C 264

Characterising the water vapour sorption behaviour of wood — •Alexander Murr and Roman Lackner — Institut for Structural Engineering and Material Science, University of Innsbruck

Wood is a cellular material with a hierarchical structure based on polymers (cellulose, hemicelluose and lignin). As variations of humidity causes a change of its physical properties, a detailed knowledge of the interaction between water and wood is of importance. A common method for such investigations are water vapour sorption (wvs) experiments where relative humidity is varied and the related change of sample mass is measured. As this change of mass deviates from classical diffusion, various macroscopic models appeared in literature, ranging from relaxation limited to transport limited approaches. To identify which of these descriptions could be used for further investigations, a precise identification of the macroscopic behaviour is necessary.

In the given presentation the sorption kinetics of Norway spruce wood (Picea abies) will be discussed. Based on a series of wvs experiments on grained wood the influence of grain size and temperature on the sorption behaviour will be shown. A comparison of similar sample masses with different grain sizes illustrates diffusion along the cell wall not being the limiting factor in the observed sorption experiments. Additionally, an outlook on further theoretical and experimental investigations shall be given.

BP 46.11 Thu 17:45 C 264

Kinetics of mutarotation in fucose-saccharides as monitored by dielectric and infrared spectroscopy — •Wilhelm Kossack[1], Wycliffe Kiprop Kipnusu[1], Mateusz Dulski[2], Karolina Adrjanowicz[2], Olga Madejczyk[2], Emanuel Urandu Mapesa[1], Martin Tress[1], Kamil Kaminski[2], and Friedrich Kremer[1] — [1]University of Leipzig, Linnestr. 5, Leipzig, Germany — [2]University 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 anomeric 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 (α-) 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 α-relaxation. This reflects the fact that the α-relaxation monitors the equilibration at a mesoscopic length scale, resulting from fluctuations in the anomeric composition.

BP 47: Microswimmers, Active Liquids I (joint CPP/BP/DY)

Time: Thursday 15:45–18:00 Location: PC 203

Invited Talk BP 47.1 Thu 15:45 PC 203

Flagellar synchronisation through direct hydrodynamic interactions — •Marco Polin[1], Douglas Brumley[2], Kirsty Wan[3], and Raymond Goldstein[3] — [1]University of Warwick, Coventry. UK — [2]MIT, Boston, MA. US — [3]University 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 behind 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 dynamic flagellar 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 emerging collective behavior. Hydrodynamic interactions lead to a clustering transition dependent on swimmer type [3] or to the formation of fluid pumps in 3D harmonic traps [4]. Self-phoretic active colloids show biomimetic autochemotactic behavior, which can induce dynamic clustering, oscillating clusters, or a chemotactic collaps [5].

[1] R. Vogel and H. Stark, Phys. Rev. Lett. **110**, 158104 (2013).
[2] D. Alizadehrad et al., to be published in PLoS Comp. Biol.
[3] A. Zöttl and H. Stark, Phys. Rev. Lett. **112**, 118101 (2014).
[4] M. Hennes et al., Phys. Rev. Lett. **112**, 238104 (2014).
[5] O. Pohl and H. Stark, Phys. Rev. Lett. **112**, 238303 (2014).

BP 47.3 Thu 16:45 PC 203

Collective behavior and clustering of self-propelled rod shaped catalytic motors: A theoretical study — •Davoud Pouladsaz[1] and Zahra Eskandari[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max 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 — •Lorenz Huber, Jonas Denk, Emanuel Reithmann, and Erwin Frey — Ludwig-Maximilians-Universität, München, Deutschland

During bacterial cytokinesis FtsZ filaments assemble into a ring-like structure. Recent experiments with reconstituted FtsA-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 effective propulsion. The FtsZ filaments are assumed to sterically repel each other. Employing Brownian dynamics simulations and a kinetic Boltzmann ansatz to study these systems on microscopic and mesoscopic length scales, respectively, we identify activity, intrinsic curvature, and steric repulsion as sufficient to control the stability of vortex patterns. In our microscopic approach we modeled the FtsZ membrane dynamics as a two-dimensional system of propelled elastic polymers and find a parameter regime of dense and stable vortices. Furthermore, we employed a mesoscale description in terms of a kinetic Boltzmann approach to investigate general effects of intrinsic curvature on collective behavior in active systems. We obtain a phase diagram featuring a confined parameter region of steady dense swirls. Our results provide a generic and robust mechanism for pattern formation in actual biological systems of curved filaments.

BP 47.5 Thu 17:15 PC 203

The many faces of drag in micro-swimming — •Jayant Pande[1], Laura Merchant[1,2], Jens Harting[3], and Ana-S. Smith[1,4] — [1]Inst. for Theo. Phys., Friedrich-Alexander Univ., Erlangen, Germany — [2]School of Phys. and Astronomy, Univ. of St. Andrews, Scotland — [3]Dept. of Appl. Phys., Eindhoven Univ. of Technology, Eindhoven, the Netherlands — [4]Ruđer 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 Kümmel[1], Parmida Shabestari[1], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universität Stuttgart, D-70569 Stuttgart, Germany — [2]Max-Planck-Institut für Intelligente Systeme, D-70569 Stuttgart, Germany

Artificial active swimmers, i.e. Janus particles, suspended in a critical binary mixture, are capable of a self-diffusiophoretic 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 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.

[1] VOLPE G, BUTTINONI I, VOGT D, KÜMMERER H J AND BECHINGER C 2011 MICROSWIMMERS IN PATTERNED ENVIRONMENTS SOFT MATTER 7, 8810 (2011) [2] B. TEN HAGEN, F. KÜMMEL, R. WITTKOWSKI, D. TAKAGI, H. LÖWEN, AND C. BECHINGER, NATURE COMMUNICATIONS 5 (2014)

BP 47.7 Thu 17:45 PC 203

Detention times of microswimmers close to surfaces — •Andreas Zöttl[1], Konstantin Schaar[1,2,3], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin — [2]Robert Koch-Institut, D-13353 Berlin — [3]Institut für Theoretische Biologie, Humoldt 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 interaction with the surface for the dynamics of microswimmers at a surface has been discussed controversially.

In our work we study theoretically the collision of microswimmers with surfaces by including both hydrodynamic interactions and noise. 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 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.

BP 48: Physics of Sustainability and Human-Nature Interactions II (joint SOE/DY/jDPG/BP/AKE)

Time: Thursday 17:00–18:30 Location: MA 001

Topical Talk BP 48.1 Thu 17:00 MA 001

Critical Transitions in Socio-econo-ecological Systems—A Global Adaptive Model of the Regional Transitions to Agriculture 8000 BC to AD 500 — •Carsten Lemmen and Kai W. Wirtz — Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

Critical transitions in societies emerge as boundaries between cultural "ages", e.g. the transition from the Industrial to the Information Age, or from the Holocene to the Anthropocene. Societal transitions are believed to emerge from nonlinear feedbacks between environment, economy, and society, but hypotheses have been difficult to test so far.

We propose to employ "numerical experiments in history" and consider one of the major critical transitions in world history—the abandonment of a foraging lifestyle in favor of agriculture and pastoralism. We investigate this transition with a deterministic and dynamic model of society. The global model resolves regional-scale human-environment interactions in space and time, based on only few prognostic adaptive societal traits and their co-evolutionary dynamics with population size.

We successfully reproduced the agropastoral transition as seen in archaeological data; we tested demic and cultural hypotheses about its expansion, finding both equally consistent with the data; we explored the stability of the expansion pattern facing large-scale palaeoenvironmental excursions and found strong resilience of populations and their key traits. Our model enabled us to quantify global and regional emissions of CO_2 and the sustainable population size for the past 10000 years.

BP 48.2 Thu 17:30 MA 001

Evaluating a Socio-environmental Complex Adaptive System: The Case of Self-Organized Socio-environmental Development in State Chiapas. — •Felipe Lara-Rosano[1] and Adriana Quiroga-Carapia[2] — [1]Universidad Nacional Autonoma de Mexico (UNAM), Mexico City, Mexico — [2]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.

BP 48.3 Thu 17:45 MA 001

Macroscopic description of complex adaptive networks coevolving with dynamic node states — •Marc Wiedermann[1,2], Jonathan F. Donges[1,3], Jobst Heitzig[1], Wolfgang Lucht[1,2], and Jürgen Kurths[1,2] — [1]Potsdam Insitute for Climate Impact Research, Germany — [2]Humboldt University, Berlin, Germany — [3]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.

BP 48.4 Thu 18:00 MA 001

Exploring the safe and just operating space in an inhomogeneous world — •Wolfram Barfuss[1,2], Boyan Beronov[1,3], Marc Wiedermann[1,4], and Jonathan Donges[1,5] — [1]Potsdam Institute for Climate Impact Research, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]Ludwig-Maximilians-Universität München, Germany — [4]Humboldt-Universität zu Berlin, Germany — [5]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 an existing conceptual coevolutionary 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 Heitzig[1] and Tim Kittel[1,2] — [1]Potsdam Institute for Climate Impact Research — [2]Humboldt 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 of 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

Time: Thursday 16:45–18:45 Location: H 1028

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 Urbanska[1], Karl Duderstadt[2], Annemarie Lüdecke[1], Wim Walter[3], Antoine van Oijen[2], and Stefan Diez[1] — [1]B CUBE, TU Dresden, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [3]Biozentrum Klein Flottbek, Uni Hamburg, Germany

Cytoskeletal motor proteins are essential for long-range, directed transport within 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-um beads were attached to the SNAP-tag-labelled tails of kinesin-1 motors via λ-DNA linker. Such motor-DNA-bead complexes were applied to surface-immobilized microtubules 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 processivity by its C-terminal domain — Matthew Nicholas[1], Peter Höök[2], Sibylle Brenner[1], Caitlin Lazar[3], Richard Vallee[3], and •Arne Gennerich[1] — [1]Albert Einstein College of Medicine, Bronx, NY 10128 — [2]University of Notre Dame, Notre Dame, IN 46556 — [3]Columbia Uuniversity, New York, NY 10032

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 of rat 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.

BP 49.4 Thu 17:45 H 1028

Segregation of diffusible and directionally moving particles on a polar filament — •Denis Johann, Debajit Goswami, and Karsten Kruse — Saarland University, Saarbrücken, Germany

Directed transport in living cells relies on the action of motor proteins. These enzymes can transform chemical energy into mechanical work and move directionally along filamentous tracks. At the same time, these filaments serve as a substrate for the binding of proteins performing other functions, but that also obstruct the motors' motion. Motivated by the mobile cross-linker Ase1, we theoretically study a system of molecular motors in the presence of diffusible particles. Both the motors and the obstacles shuttle between the filament and its surrounding. Numerical simulations of this system show a segregation between motors and obstacles if the filament ends act as diffusion barriers for the obstacles. A phenomenological mean-field theory captures the essential effects observed in the simulations [1].

[1] Johann, Goswami, and Kruse, Phys. Rev. E **89**, 042713 (2014)

BP 49.5 Thu 18:00 H 1028

Time scales explain different transport behavior of elastically coupled molecular motors — •Florian Berger[1], Corina Keller[2], Stefan Klumpp[2], and Reinhard Lipowsky[2] — [1]Howard Hughes Medical Institute and Laboratory of Sensory Neuroscience, The Rockefeller University, 10065 New York, USA — [2]Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

Cellular transport is achieved by the cooperative action of molecular motors which are elastically linked to a common cargo. When the motors pull on the cargo at the same time, they experience fluctuating elastic strain forces induced by the stepping of the other motors. These elastic coupling forces can influence the motors' stepping and unbinding behavior. To develop an intuitive understanding of cargo transport by two elastically coupled motors exposed to an external load force, we introduced four different time scales for four different processes: (i) spontaneous unbinding, (ii) force induced unbinding, (iii) force induced stalling and (iv) load sharing. In particular the time scale for load sharing allows us to predict how the regulation of single motor

parameters influence the cooperativity.

BP 49.6 Thu 18:15 H 1028

Filamin Inhibition of Myosin Groups Potentiates with Group Size — Zsombor Balassy[1], •Lennart Hilbert[1,2], Nedjma B Zitouni[1], and Anne-Marie Lauzon[1] — [1]McGill University, Montréal, Canada — [2]Center for Systems Biology, Dresden, Germany

Filamin is an actin-actin crosslinker found in smooth muscle and non-muscle cells and inhibitis actin filament sliding in *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 ($L = 1.0\,\mu$m). 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 $L = 1.7\,\mu$m). 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 locally 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

BP 49.7 Thu 18:30 H 1028

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 F_1-ATPase and the kinesin motor.

BP 50: Biotechnology and bioengineering

Time: Thursday 17:30–18:45 Location: H 1058

BP 50.1 Thu 17:30 H 1058

Real-time deformability cytometry: On-the-fly mechanical phenotyping for label-free cell functional assays — •Oliver Otto[1], Philipp Rosendahl[1], Alexander Mietke[1,2], Stefan Golfier[1], Angela Jacobi[1], Christoph Herold[1], Daniel Klaue[1], Nicole Töpfner[1], Salvatore Girardo[1], Elisabeth Fischer-Friedrich[2], and Jochen Guck[1,3] — [1]Biotechnology Center, Technische Universität Dresden, Dresden, Germany — [2]Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Cavendish 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 analysis rates in excess of 100 cells/s. Cells are driven through a microfluidic channel leading to deformations due to hydrodynamic stresses only, 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.

BP 50.2 Thu 17:45 H 1058

Interaction between Polyelectrolytes and Proteins in aqueous solution. — •Shun Yu, Xiao Xu, Joachim Dzubiella, and Matthias Ballauff — Helmholtz-Zentrum Berlin, Intitute 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/-physics and medicine [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 pI", 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, 2553 (2013)
[2] Dubin et al., Separation & Purification Reviews 23, 1 (1994)
[3] Welsch et al., Polymer 12, 2835 (2013)

BP 50.3 Thu 18:00 H 1058

Diamondoid-functionalized Au(111) nanoelectrodes as probes for detecting DNA and mutations — •Ganesh Sivaraman[1], Rodrigo Garcia Amorim[2], Ralph Scheicher[2], and Maria Fyta[1] — [1]Institute For Computational Physics , University of Stuttgart, Germany — [2]Division of Material Theory, Department of Physics and Astronomy, Uppsala University, Sweden

Solid state nanopores 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 nanopores by which the specific interaction of a "functionalizing 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-functionalization 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 functionalized 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.

BP 50.4 Thu 18:15 H 1058

Highly controllable synthetic neuronal circuits: Poly-L-lysine patterend semiconductor microtube substrates — •Jann Harberts[1], Aune Koitmäe[1], Gabriele Loers[2], Cornelius Bausch[1], Daniel Diedrich[1], David Sonnenberg[1], Christian Heyn[1], Wolfgang Hansen[1], and Robert H. Blick[1] — [1]CHYN & INF, University of Hamburg, Germany — [2]ZMNH, 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 25μm. The advantage of this method is the flexibilty of pattering. It serves a fast way to adapt new patterns to different layouts, where the minimum definable drop spacing is 5μm. Printing droplets of PLL enhances the yield of the axonguiding through the tubes and creates a highly controlled neural network.

BP 50.5 Thu 18:30 H 1058

IR-Spectroscopy and Multivariate Data Analysis in Point of Care Testing — •Anja Niedermayr[1,2], Peter B. Luppa[3], Carsten Giebeler[4], and Alexander M. Gigler[1,2,5] — [1]Siemens AG, Corporate Technology, Otto-Hahn-Ring 6, 81739 München — [2]Sect. Crystallography, LMU München, Theresienstr. 41, 80333 München — [3]Klinikum rechts der Isar, TU München, Clinical Chemistry and Pathobiochemistry, Ismaninger Str. 22, 81675 München — [4]Pyreos Ltd., Scottish Micro Electronics Centre, West Mains Road, Edinburgh EH9 3JF, Scotland, UK — [5]Center for NanoScience (CeNS), LMU München, Schellingstr. 4, 80799 Munich

In medicine, an early decision on the right course of treatment can make the difference between life and death. Therefore, the rapid availability of test results is crucial. Devices that facilitate medical testing at or near the point of patient care (Point-of-care Testing, POCT) significantly reduce the turn around time. This will become increasingly relevant in modern day diagnosis and therapy. At this point, parallel POCT is available for only few parameters since every single analyte requires a highly specific indicator substance. Infrared spectroscopy enables a marker free, parallel analysis of various medical parameters in one unaltered sample. In combination with multivariate statistical modeling a precise quantitative prediction of the investigated substances can be achieved. The prediction's accuracy and reliability critically depends on the statistical method used to set up the model. Here, initial results of our study on the determination of selected high-content blood ingredients, i.e. alcohol and albumin, will be shown.

BP 51: Physics of Food (joint CPP/BP)

Time: Thursday 18:00–18:30 Location: C 264

BP 51.1 Thu 18:00 C 264

Small-angle scattering study on the structure of the lecithin stabilizer layer in tetracosane-water nanoemulsions and -suspensions — •Martin Schmiele and Tobias Unruh — Physik Department, Friedrich-Alexander-Universität Erlangen–Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany

Tetracosane (C_{24}, TCS) o/w nanoemulsions stabilized by the lecithin 1,2-dimyristoyl-sn-glycero-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 super-cooling (ΔT about 20 K) and crystallize in a for TCS unusual orthorhombic crystal structure (space group $Pca2_1$ as verified by wide-angle x-ray scattering).

Using small-angle x-ray and neutron scattering and nanodispersions with different neutron scattering contrasts for the TCS 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 interpenetration between TCS and the acyl chains of DMPC. For the nanosuspensions 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 51.2 Thu 18:15 C 264

Lipid migration in multicomponent food products such as chocolate — •Svenja Reinke[1], Stephan V. Roth[2], Gonzalo Santoro[2], Josélio Vieira[3], Stefan Palzer[4], and Stefan Heinrich[1] — [1]Hamburg University of Technology, Denickestr. 15, 21073 Hamburg, Germany — [2]DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]Nestlé Product Technology Centre York, P.O. Box 204, Haxby Road, York YO91 1XY, United Kingdom — [4]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 analysis of wetting 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.

BP 52: Protein structure and dynamics II

Time: Friday 9:30–11:45 Location: H 1028

Invited Talk BP 52.1 Fri 9:30 H 1028

Biophysics of light-activated ion transporters — Arend Vogt, Jonas Wietek, and •Peter Hegemann — Humboldt-Universität zu Berlin

The field of optogenetics utilizes light-activated ion transporters as channelrhodopsins (ChRs) and Arch3 for specific neuronal activation or inactivation. Recently we characterized a light-driven proton pump CsR of the arctic alga Coccomyxa subellipsoidea. Owing to the fact that the photocurrents are very large in Xenopus oocytes, we have taken this advantage to analyze the function of individual positions at the extracellular side of the retinal Schiff base chromophore respective relevance for proton transport. Modification of the highly conserved proton shuttling residue R83 or its interaction partner Y57 strongly reduced the power of the pumps and converted CsR at moderate electrochemical load into an operational proton channel with inward or outward rectification depending on the replacement. We compared these proton selective channels with various natural and artificial light-activated channels (channelrhodopsins) that are selective for protons, sodium and chloride and we derived principle for light-depending gating, ion conductance and selectivity of microbial rhodopsins.

BP 52.2 Fri 10:00 H 1028

Electrochromic shift calculations reveal the structural changes between red- and green-sensitive rhodopsins — •Florimond Collette, Marcel Schmidt am Busch, and Thomas Renger — Institut für Theoretische Physik, Johannes Kepler Univer-

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 absorbance in the red- and green-sensitive visual pigments.

[1] F. Collette *et al.*, *J. Phys. Chem. B* **118**, 11109 (2014).

BP 52.3 Fri 10:15 H 1028

Photo-dynamics of photo-activated adenylyl cyclase NgPAC3 from the amoeboflagellate *Naegleria gruberi* **NEG-M strain** — •Alfons Penzkofer[1], Meenakshi Tanwar[2], Sinddu Kandoth Veetil[2], Suneel Kateriya[2], Manuela Stierl[3], and Peter Hegemann[3] — [1]Fakultät für Physik, Universität Regensburg, Universitätsstraße 31, D-93053 Regensburg, Germany — [2]Department of Biochemistry, University of Delhi South Campus, Benito Juarez Road, New Delhi 110021, India — [3]Institut für Biologie/Experimentelle Biophysik, Humboldt Universität zu Berlin, Invalidenstraße 42, D-10115 Berlin, Germany

The absorption and emission spectroscopic behavior of the photo-activated adenylyl cyclase NgPAC3 from the amoeboflagellate *Naegleria gruberi* NEG-M strain was studied [1]. The flavin cofactor was found to be partly fully oxidized and partly fully reduced. The typical BLUF domain (BLUF = Blue Light sensor Using Flavin) fully oxidized flavin absorption photo-cycle dynamics with about 14 nm flavin absorption red-shift in the signaling state was observed. The quantum efficiency of signaling state formation was determined to be $\phi_s = 0.66 \pm 0.03$. A bi-exponential signaling state recovery to the dark-adapted receptor state was observed with the time constants $\tau_{rec,f} = 275s$ (fraction 0.29) and $\tau_{rec,sl} = 45min$ (fraction 0.71). The thermal irreversible protein unfolding was studied and a protein melting temperature of $\vartheta_m \approx 50°C$ was found. NgPAC3 showed light-gated adenylate cyclase activity upon illumination with blue light.

[1] A.Penzkofer et al., J.Photochem.Photobiol.A:Chem. 287(2014)19.

15 min break

BP 52.4 Fri 10:45 H 1028

Conformational Change of the Neuronal Calcium Sensor GCAP1 — •Jörg Robin, Jens Brauer, Stefan Sulmann, Christoph Lienau, and Karl-Wilhelm Koch — Carl von Ossietzky 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 intracellular 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 sequential step by step order mechanism [2] by conformational change due to binding of calcium. This conformational change has recently been investigated 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 local 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 simulations. In conclusion, GCAP1 undergoes conformational change, but distinctly different from GCAP2. [1] Pugh, E. N. Jr. & Lamb, T. D. Handb. Biol. Phys. 3, 183 (2000) [2] Koch, K-W. & Dell'Orco, D. ACS Chem. Neurosci. 4, 909 (2013) [3] Kollmann, H. et al. ACS Chem. Biol. 7, 1006 (2012)

BP 52.5 Fri 11:00 H 1028

Phase behavior of dense lysozyme solutions — •Julian Schulze[1], Johannes Möller[1], Michael Paulus[1], Julia Nase[1], Metin Tolan[1], and Roland Winter[2] — [1]Fakultät Physik/Delta, Technische Universität Dortmund, 44221 Dortmund , Germany — [2]Fakultät für Chemie und Chemische Biologie, Technische Universität Dortmund, 44221 Dortmund, Germany

In previous studies, small angle X-ray scattering (SAXS) in combination 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 conditions as protein concentration c, temperature T, pressure p or salt concentration I. While the repulsive Coulomb term of the DLVO potential 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 formation 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 l-l phase separation 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 Baeurle — Institut für Physikalische und Theoretische Chemie, Universität 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-dynamic information of protein solvent systems far from equilibrium over multiple 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 combination 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 (Cr-phot1). Our results demonstrate that in the signaling state the kinase is activated through the disruption of the Jalpha-helix from the light-oxygen-voltage-2-sensitive (LOV2) domain, which is followed by a stretching of the activation loop and broadening of the catalytic cleft of the kinase. Literature: [1] E. Peter, B. Dick, I. Stambolic, S.A. Baeurle, Prot. Struct. Funct. Bioinf. 82, 2018 (2014).

BP 52.7 Fri 11:30 H 1028

Dynamics of the Orange Carotenoid Protein (OCP) under Photoactivation — Evgeny Maksimov[2], •Franz-Josef Schmitt[1], Thomas Friedrich[1], and Vladimir Paschenko[2] — [1]Institute of Chemistry, Bioenergetics, TU Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany — [2]Department of Biophysics, Biology Faculty, Lomonosov Moscow State University, 119991 Moscow, Russia

The cyanobacterium Synechocystis sp. PCC6803 contains a photoswitchable protein, the orange carotenoid protein (OCP) which undergoes conformational changes under illumination in the blue spectral regime. After activation by light the OCP binds to the membrane extrinsic 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 mechanism. 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 photoactivation of OCP that leads to a significant red shift of the absorption spectrum. A distance change between Tyr-201, Trp-288 and the keto terminus of the pigment might break H-bonds between the protein and the chromophore which tilt the β-ring out of plane in the inactive form of OCP.

BP 53: Complex Fluids and Soft Matter (joint BP/DY/CPP)

Time: Friday 9:30–12:15 Location: H 1058

BP 53.1 Fri 9:30 H 1058

Anisotropic Diffusion of Macromolecules in the Contiguous Nucleocytoplasmic Fluid during Eukaryotic Cell Division — Nisha Pawar, Claudia Donth, 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.

[1] N. Pawar, C. Donth, and M. Weiss, Curr. Biol. 24, 1905 (2014).

BP 53.2 Fri 9:45 H 1058

Optical Shaking of Single Cells — •Carla Zensen[1,3], Isis E. Fernandez[2,3], Oliver Eickelberg[2,3], Theobald Lohmüller[1,3], and Jochen Feldmann[1,3] — [1]Chair for Photonics and Optoelectronics, Physics Department and CeNS, Ludwig-Maximilians-Universität, Munich, Germany — [2]Comprehensive Pneumology Center, Institute of Lung Biology and Disease, Ludwig-Maximilians-Universität and Helmholtz Zentrum, Munich, Germany — [3]Nanosystems 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.

[1] A. Ohlinger, A. Deak, A.A. Lutich, and J. Feldmann, Phys. Rev. Lett. 108, 018101 (2012)

BP 53.3 Fri 10:00 H 1058

***In vivo* mechanics measurements using ferrofluid droplets** — •Friedhelm Serwane, Alessandro Mongera, Payam Rowghanian, David Kealhofer, and Otger Campàs — Department of Mechanical Engineering, University of California, Santa Barbara, USA

The development of living tissues and organs depends on cell behavior strongly influenced by the mechanics of their microenvironment. A prime example is the ability of a tumor to spread which has been linked directly to the elasticity of the surrounding matrix.

This interplay between mechanical inputs and biological responses has remained poorly understood, mainly due to a lack of techniques to measure mechanical properties while characterizing the molecular signals *in vivo*.

Here 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.

BP 53.4 Fri 10:15 H 1058

Biomolecule dynamics in microfluidic pH gradients and prebiotic FeS membranes — •Friederike M. Möller[1], Dominic Berchtold[1], Franziska Kriegel[1], Laura Barge[2], Michael Russell[2], and Dieter Braun[1] — [1]Systems Biophysics, LMU München, Germany — [2]Jet 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. A rocky FeS membrane forms upon contact from the sulfuric S– and the Fe++ ions. 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.

BP 53.5 Fri 10:30 H 1058

Dynamics of biological membrane mimics - A combined QENS and MD simulation study — •Lisa Lautner[1], Martin Schmiele[1], Sebastian Busch[2], Michaela Zamponi[3], and Tobias Unruh[1] — [1]Chair for Crystallography and Structural Physics, FAU Erlangen-Nuremberg, Germany — [2]University of Oxford, United Kingdom — [3]Heinz 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. Quasielastic Neutron 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-glycero-3-phosphocholine) bilayers in the liquid crystalline ($L_{(}\alpha$)) 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

Bridging the scales: How is the large-scale deformation of a cellular network related to cell-scale processes? — •Matthias Merkel[1], Raphael Etournay[2], Suzanne Eaton[2], and Frank Jülicher[1] — [1]MPI for the Physics of Complex Systems, Dresden — [2]MPI of Molecular Cell Biology and Genetics, Dresden

We propose a method to study the deformation of two-dimensional cellular networks. To this end, we focus on biological tissues, which typically undergo large-scale deformations during the development of an organism. However, how these large-scale deformations correspond to the collective behaviour of individual cells is not fully understood yet. Today, experimentalists are able to image tissues with up to 10 000 cells at sub-cellular spatial resolution and at a time resolution of minutes. Nevertheless, there is still a lack of methods allowing us to exploit the full depth of this huge amount of information.

Here, we propose a geometrical framework that exactly decomposes large-scale deformations into contributions by different kinds of cellular processes, which comprise cell shape changes, cell rearrangements (T1 transitions), cell divisions, and cell extrusions (T2 transitions). As

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 demonstrate 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 — •Manuel Wolff, Michael Nash, and Dieter Braun — Center for Nanoscience, LMU, Munich, Germany

Thermal gradients drive molecules in solutions, an effect termed thermophoresis. Interest in aqueous thermophoresis was recently triggered by its widespread application in biomolecule affinity analysis using infrared-illuminated capillaries.

Theoretical models are debated, not least due to the fact that molecules in water seem to behave significantly different in non-aqueous fluids. By designing fluorescently labeled polymers that are either completely uncharged or whose charge can be tuned by a change in pH, we find that the temperature dependence of ionic and non-ionic polymers is very distinct. Building upon previous models, we find that increasing thermophoresis for rising temperature, often fitted 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 non-aqueous solutions.

BP 53.8 Fri 11:30 H 1058

How to regulate droplet position in a heterogeneous chemical environment? — •Samuel Krüger[1,2], Christoph Weber[1], Jens-Uwe Sommer[2,3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Leibniz Institute of Polymer Research Dresden e.V., Dresden — [3]Technische Universität Dresden, Institute of Theoretical Physics, Dresden, Germany

P granules are droplet-like structures consisting of RNA and proteins. They occur in Caenorhabditis elegans embryo and are known to determine its germ lineage. Interestingly, P granules are segregated to one side of the cell. There is evidence that the droplet position is regulated by a spatially inhomogeneous protein called Mex-5. Here we propose a model that simplifies the multicomponent nature of the cytoplasm as a ternary mixture: The P granule material, the background fluid, and a regulator mimicking Mex-5. Using our model we aim to understand the physical principles controlling the droplet position. To this end we consider lattice-based Monte Carlo simulations for a ternary mixture, where the microscopic interactions between the components are captured by three Flory-Huggins parameters. Considering a linear regulator gradient we observe two stationary states. Droplets localise in regions of lowest regulator concentration if the regulator exhibits a high affinity to the solvent, and vice versa. We present evidence that the transition between the localisation at highest and lowest regulator concentration can be regarded as a phase transition. Beyond biology, understanding how the droplet positions can be regulated offers the possibility to design switchable units for chemical computing.

BP 53.9 Fri 11:45 H 1058

Mechanical regulation of vein morphogenesis in plant leaves — •Jonathan E. Dawson[1], Franck A. Dintengou[2], Irina Kneuper[2], William Teale[2], Klaus Palme[2], and Eleni Katifori[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Insitute of Bioloy II, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany

Development of leaf veins is a highly dynamic and regulated process. 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 primordia. We investigate the formation of leaf primary vein by simulating tissue growth driven by inter-cellular diffusion of the plant hormone auxin, from auxin synthesizing cells. We show that dynamic modulation of the cell mechanical properties based on cell auxin concentration can reproduce realistic primary vein as observed in growing leaf primordia. We further tested our model by comparing with experiments in which auxin transport in affected.

BP 53.10 Fri 12:00 H 1058

Osmolyte effects: Impact on the aqueous solution around charged and neutral spheres — •Jens Smiatek — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

We have performed atomistic molecular dynamics simulations to study the solvation characteristics of model spheres for low concentrations of urea and hydroxyectoine in aqueous solution. The spheres are either positively or negatively charged with a valency of one or charge neutral. Our results illustrate that the presence of osmolytes influences the solvation properties of the spheres significantly. We have conducted a detailed investigation of water properties like the mean dipolar relaxation times, water orientation parameters around the spheres, dielectric constants, preferential binding behavior, water self-diffusion coefficients, and free energies of solvation by thermodynamic integration to study the influence of osmolytes in detail. Our findings indicate that several factors like the charge of the spheres as well as the characteristics of the osmolytes significantly influence the thermodynamic and dynamic properties of the local water shell and the solvation process with regard to varying enthalpic and entropic contributions.

BP 54: Microswimmers, Active Liquids III (joint DY/BP/CPP)

Time: Friday 9:30–11:30 Location: C 264

Invited Talk BP 54.1 Fri 9:30 C 264

From chemical nanomotors to biological microswimmers — •Peer Fischer — Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart — Institut für Physikalische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart

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 — •Felix Winterer[1,2], Christoph Maier[1,2], Theobald Lohmüller[1,2], and Jochen Feldmann[1,2] — [1]Photonics and Optoelectronics Group, Ludwig-Maximilians-Universität München, Munich, Germany — [2]Nanosystems Initiative Munich (NIM), Munich, Germany

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 focussed 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 — Andrey Pototsky[1], •Uwe Thiele[2], and Holger Stark[3] — [1]Department of Mathematics, Swinburne University of Technology, Hawthorn, Victoria, 3122, Australia — [2]Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [3]Institut 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. We study the intricate influence of these self-propelled insoluble surfactants on the stability of the film surface and show that depending on the strength of in-surface rotational diffusion and the absolute value of the in-surface 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 Adhyapak 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 bundling dynamics. In particular, we observe abrupt synchronization and bundling on time scales much shorter than those required when the cell movement is switched off to avoid entanglement. Although hydrodynamic interactions still play an important role, through a comparative investigation we conclude that flagellar entanglement generated by cell rotation predominantly affects the total time to synchronize and bundle. Cell movement modifies stationary bundling states too. Specifically, the length over which a bundle is closely pact varies over time, having an oscillatory behavior whose amplitude decreases with increasing number of flagella. At the end we discuss how strongly all these findings affect the overall propulsion of the bacterium.
[1] M. Reichert and H. Stark, Eur. Phys. J. E **17**, 493 (2005).
[2] S.Y. Reigh, R.G. Winkler, and G. Gompper, Soft Matter **8**, 4363 (2012).

BP 54.5 Fri 10:45 C 264

Reorientation of passive Janus type swimmer in an external temperature profile — •Andreas Bregulla and Frank Cichos — University of Leipzig, department for experimental physics, leipzig, germany

Swimming on the micrometer length 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 photon nudging algorithm to gather and collect a specific number of particles and study their interactions. The interactions themselves can be mediated through many different aspects like charges, 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 — •Marco Braun and Frank 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 relationship between an object's distance to the focal plane (z) and the observed intensity pattern, and assign z positions by maximizing image cross-correlations to a reference stack. We achieve micron-scale resolution in z, <0.5 μm resolution in x and y, a range of ~350x300x200 μm (x,y,z), a throughput of tens of bacteria, and a temporal resolution that is only limited by the detector readout rate. We demonstrate the application of this technique to a range of bacterial species, verify that we recover previously observed motility patterns, and reveal that bacterial individuality, rather than stochasticity, underlies the broad population distribution observed for a key motility parameter of V. alginolyticus.

[1] Berg & Brown, Nature 239:500, 1972. [2] Vater et al., PLoS ONE 9:e87765, 2014. [3] Molaei et al., PRL 113:068103, 2014.

BP 55: Networks: From Topology to Dynamics II (joint DY/BP/SOE)

Time: Friday 9:30–12:45 Location: BH-N 128

BP 55.1 Fri 9:30 BH-N 128

Networks: From Dynamics to Topology — •Jose Casadiego[1,3] and Marc Timme[1,2,3] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Institute for Nonlinear Dynamics, Faculty of Physics, University of Göttingen, 37077 Göttingen, Germany — [3]IMPRS Physics of Biological and Complex Systems, Göttingen Graduate School for Neurosciences, Biophysics and Molecular Biosciences, 37077 Göttingen, Germany

How single units interact in a complex network fundamentally underlies its collective dynamics. Yet, identifying the physical structure of interactions from recorded time series still poses a great challenge. Up-to-date methods either require (i) a detailed pre-knowledge of the units' dynamical features, (ii) to externally drive the network or (iii) the network dynamics to be at stable states, such as fixed points or limit cycles. Here we develop a theory to reveal physical interactions of networks that relies on recorded time series only. By decomposing the dynamics of single units in terms of network interactions of different orders (pairs, triplets, quadruplets,...), we pose network reconstruction as an error minimization problem. We propose a greedy algorithm to solve such minimization problems. Our approach is principally model independent, ensuring its generality and applicability in different fields and making it particularly suitable when structural connections are desired, dynamical features are unknown and perturbing the network is unfeasible. Thus, our approach may serve as a key stepping stone for the expanding field of model-independent network reconstruction.

BP 55.2 Fri 9:45 BH-N 128

Revealing the Topology of Circulatory Networks in Nature — •Mirko Lukovic[1] and Erik Martens[2,3] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [2]Department of Biomedical Sciences, University of Copenhagen, Denmark — [3]Department of Mathematical Sciences, University of Copenhagen, Denmark

Complex networks such as those used for communication, resource delivery and transportation are ubiquitous in nature and society. From the internet and urban traffic, to the intimate networks of the circulatory systems in our bodies, understanding how their topology and structure relate to their function and efficiency is an essential first step in their management. Given the wide variety of existing transport networks with structures that range from being tree-like to cases where there is an intricate arrangement of nested loops, our goal is to use circulation times of the flow in order to infer global properties of the underlying network structure. To this end we investigate circulatory transport networks by modeling the flow as a stochastic process whose first passage time properties we determine for a variety of different network topologies. We also set up a framework in which different branching rules of the flow can be tested and its effects on the first passage times analyzed. Our results will help develop an effective and non-invasive method for probing circulatory networks such as the human vascular system.

BP 55.3 Fri 10:00 BH-N 128

Symbolic Regression and Network Analysis for the prediction of El Nino — •Markus Abel[1], Markus Quade[1], Ruggero Vasile[1], Avi Goz[2], Shlomo Havlin[3], and Armin Bunde[4] — [1]Ambrosys GmbH, Albert-Einstein Str. 1-5 Potsdam, Germany — [2]Department of Solar Energy & Environmental Physics, Ben-Gurion University, Jerusalem, Israel — [3]Department of Physics Bar-Ilan University Ramat-Gan 52900 Israel — [4]Institute For Theoretical Physics, University of Giessen, Germany

In the context of the modeling of dynamical systems, statistical analysis and data-based modeling is a hihgly promising method. We use symbolic regression, in particular genetic programming and nonparamtric regression to find effective models for the prediction of el Nino events. The data used consist of a novel method to form a network from the correlations of grid points in the El Nino basin. We compare our results with existing methods. Depending on the method used a predictive power of up to 100% is achieved, i.e. all events are correctly predicted.

BP 55.4 Fri 10:15 BH-N 128

Model selection and hypothesis testing for large-scale network models with overlapping groups — •Tiago P. Peixoto — Institut für Theoretische Physik, Universität Bremen

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.

BP 55.5 Fri 10:30 BH-N 128

Breakdown of quantum transport in scale-free networks — •Nikolaj Kulvelis 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.

BP 55.6 Fri 10:45 BH-N 128

Two-dimensional unimodular Lattice Triangulations as small-world and scale-free networks — •Benedikt Krüger, Ella Schmidt, and Klaus Mecke — Institut für Theoretische Physik, Staudtstr. 7, 91058 Erlangen

Triangulations are an important tool in physics for describing curved geometries. Unimodular triangulations on 2d lattices can also be considered as connected, simple, and maximal planar graphs, which allows the appliance of methods from graph theory on triangulations. We calculate the scaling behaviour of the degree distribution, clustering coefficient and the average shortest path length for random triangulations. Introducing a simple measure for the order of a triangulation and interpreting it as the energy of the triangulation we measure canonical averages of these observables using Monte-Carlo-Simulations. We find a crossover behaviour of all considered observables at small negative temperatures and hints for small-world and scale-free behaviour in certain temperature ranges.

15 min. break

BP 55.7 Fri 11:15 BH-N 128

Nonlinear elasticity of athermal networks: a critical phenoemenon — •Abhinav Sharma[1], Albert Licup[1], Michael Sheinman[1], Karin Jansen[2], Gijse Koenderink[2], and Frederick Mackintosh[1] — [1]VU, Amsterdam, Netherlands — [2]AMOLF, 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 analogous 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 Koegel 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.

[1] P.G. De Gennes and A. Pincus, *Phys. Kondens. Mater.* **1**, 189 (1970).

[2] T. A. Prokopieva, V. A. Danilov, S. S. Kantorovich, Ch. Holm, *Phys. Rev. E* **80**, 031404 (2009).

[3] D. L. Blair, A. Kudrolli, *Phys. Rev. E* **67**, 021302 (2003).

[4] http://www.ep5.uni-bayreuth.de/de/research/Magnetic-Soft-Matter/video/ferronetwork.html

BP 55.9 Fri 11:45 BH-N 128

Exclusion processes on networks — •Izaak Neri[1,2], Norbert Kern[3], and Andrea Parmeggiani[3] — [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[1,2], Judith Lehnert[1], and Eckehard Schöll[1] — [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]

[1] C. Wille, J. Lehnert, and E. Schöll, Phys. Rev. E 90, 032908 (2014)

BP 55.11 Fri 12:15 BH-N 128

Efficient sampling of networks with high clustering — •Rico Fischer[1], Jorge Leitao[1], Tiago Peixoto[2], and Eduardo Altmann[1] — [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 — 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 disjunct fields of research.(Organizers J. Krug and H. Meyer-Ortmanns)

Time: Friday 9:30–12:00 Location: BH-N 334

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

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 — •Hildegard 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.

F. Ionita, H. Meyer-Ortmanns, Phys. Rev. Lett. 112, 094101 (2014).

BP 56.6 Fri 11:45 BH-N 334

Parametrization and interaction analysis of survival curves — Ivan G. Szendro[1], Rahul Marathe[2], Yidong Shen[3], Adam Antebi[3], and •Joachim Krug[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Department of Physics, IIT Delhi, India — [3]Max 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).