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Overview of Invited Talks and Sessions

(Lecture rooms ZEU 250, HÜL 386, and SCH A251; Poster P1A, P2-EG, P2-OG1 and P3)

Plenary Talk of BP

PV XIII	Wed	8:30– 9:15	HSZ 01	Characterization of Biological Photoreceptors in Space and Time — •PETER HEGEMANN
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Invited Talks

BP 1.1	Mon	9:30–10:00	ZEU 250	Conformational Transitions in the Presence of Solvent and Internal Memory Effects — •ROLAND NETZ, JULIAN KAPPLER, JAN DALDROP, BARTOSZ KOWALIK, FLORIAN BRÜNIC
BP 2.1	Mon	9:30–10:00	HÜL 386	Visualization and Manipulation of the Invisible — •HEINRICH LEONHARDT
BP 3.1	Mon	9:30–10:00	SCH A251	Cilia-based transport networks — •EBERHARD BODENSCHATZ
BP 4.1	Mon	15:00–15:30	ZEU 250	Antibiotic-induced gene expression noise and cross-protection at the single-cell level — •TOBIAS BOLLENBACH
BP 5.1	Mon	15:00–15:30	HÜL 386	Metal Induced Energy Transfer — •JÖRG ENDERLEIN
BP 6.1	Mon	15:00–15:30	SCH A251	Quantifying and modelling active motion in biological systems — •TIMO BETZ
BP 13.1	Tue	9:30–10:00	HÜL 386	X-ray imaging of Cells and Tissues — •TIM SALDITT
BP 14.1	Tue	9:30–10:00	SCH A251	Laminar mixing in tubular networks of plasmodial slime moulds — •MARCUS HAUSER
BP 16.1	Tue	11:30–12:00	HÜL 386	Control on the nanoscale with DNA origami — •TIM LIEDL
BP 38.1	Wed	9:30–10:00	HÜL 386	Simulations move toward the understanding of protein-mediated membrane fusion — •HERRE JELGER RISSELADA
BP 39.5	Wed	11:15–11:45	SCH A251	Navigating the cytoskeleton: new tools to dissect and direct intracellular transport — •LUKAS KAPITEIN
BP 42.1	Wed	15:00–15:30	ZEU 250	Linking AMPA receptor nanoscale organization and function at excitatory synapses — •DANIEL CHOQUET
BP 43.1	Wed	15:00–15:30	HÜL 386	Diffusive anchorage of molecular motors allows for adaptive force generation — •STEFAN DIEZ
BP 47.1	Thu	9:30–10:00	ZEU 250	Mechanotransduction in Collective Cell Migration — •JOACHIM SPATZ
BP 48.1	Thu	9:30–10:00	HÜL 386	Shaping membranes: ENTH activity as a function of membrane tension — •CLAUDIA STEINEM, MARTIN GLEISNER, BENJAMIN KROPPEN, NELLI TESKE, ANDREAS JANSHOFF, MICHAEL MEINECKE
BP 49.1	Thu	9:30–10:00	SCH A251	The Origin of Cellular Life — •JACK W SZOSTAK
BP 55.1	Thu	15:00–15:30	HÜL 386	Network heterogeneity regulates steering in actin-based motility — •LAURENT BLANCHON
BP 56.1	Thu	15:00–15:30	SCH A251	Biophysical Studies of Amyloid Formation and Its Inhibition — •SHEENA RADFORD

BP 59.1	Fri	9:30–10:00	HÜL 386	Spatially-resolved transcriptomics and single-cell lineage tracing — ●JAN PHILIPP JUNKER
BP 60.1	Fri	9:30–10:00	SCH A251	Spontaneous curvature and membrane curling for malaria-infected erythrocytes — ●MANOUK ABKARIAN, OCTAVIO ALBARRAN ARRIAGA, GLADYS MASSIERA, CYRIL CLAUDET, ANDREW CALLAN JONES, VLADIMIR LORMAN, CATHERINE BRAUN BRETON

Invited talks of the joint symposium Bioinspired Functional Materials: From Nature's Nanoarchitectures

See SYBM for the full program of the symposium.

SYBM 1.1	Tue	9:30–10:00	HSZ 02	New twists in biological photonics: circular polarisation and beyond. — ●PETE VUKUSIC, LUKE McDONALD, EWAN FINLAYSON
SYBM 1.2	Tue	10:00–10:30	HSZ 02	Bio-inspired materials and structures for technology and architecture — ●THOMAS SPECK
SYBM 1.3	Tue	10:30–11:00	HSZ 02	Cellulose bio-inspired hierarchical structures — ●SILVIA VIGNOLINI
SYBM 1.4	Tue	11:15–11:45	HSZ 02	Strong Flexible Bioenabled Nanocomposites for Sustainable Sensing — ●VLADIMIR TSUKURUK
SYBM 1.5	Tue	11:45–12:15	HSZ 02	3D laser nano-printing of rationally designed materials — ●MARTIN WEGENER

Invited talks of the joint symposium Physics of Collective Mobility (SYCM) organized by SOE

See SYCM for the full program of the symposium.

SYCM 1.1	Wed	9:30–10:00	HSZ 02	Mobility in shareability networks — ●MICHAEL SZELL
SYCM 1.2	Wed	10:00–10:30	HSZ 02	Trail-following bacteria: from single particle dynamics to collective behaviour — ANATOLIY GELIMSON, KUN ZHAO, CALVIN K. LEE, W. TILL KRANZ, GERARD C. L. WONG, ●RAMIN GOLESTANIAN
SYCM 1.3	Wed	10:30–11:00	HSZ 02	Mobility and Self-Organization in Multi-Layer Networks: A Meta-Foodweb example — ●THILO GROSS, ANDREAS BRECHTEL, PHILIPP GRAMLICH, DANIEL RITTERSKAMP, BARBARA DROSSEL
SYCM 1.4	Wed	11:15–11:45	HSZ 02	Temporal Percolation in Critical Collective Mobility Systems — ●ANDREAS SORGE, DEBSANKHA MANIK, JAN NAGLER, MARC TIMME
SYCM 1.5	Wed	11:45–12:15	HSZ 02	Modeling the evolution of cities — ●MARC BARTHELEMY

Sessions

BP 1.1–1.12	Mon	9:30–13:00	ZEU 250	Computational Biophysics (Joint Session BP/DY)
BP 2.1–2.10	Mon	9:30–12:45	HÜL 386	Bioimaging and Spectroscopy I
BP 3.1–3.10	Mon	9:30–13:00	SCH A251	Mechanics and Dynamics of 3D Tissues - Joint Focus Session (BP/CPP/DY) organized by Peter Loskill
BP 4.1–4.9	Mon	15:00–17:30	ZEU 250	Systems Biology & Gene Expression and Signalling
BP 5.1–5.9	Mon	15:00–17:30	HÜL 386	Single Molecule Biophysics
BP 6.1–6.6	Mon	15:00–16:45	SCH A251	Cell Mechanics (Joint Session BP/DY)
BP 7.1–7.7	Mon	17:30–19:30	P3	Posters - Mechanics and Dynamics of 3D Tissues (Focus Session)
BP 8.1–8.20	Mon	17:30–19:30	P3	Posters - Bioimaging and Spectroscopy
BP 9.1–9.16	Mon	17:30–19:30	P3	Posters - Cell Mechanics
BP 10.1–10.10	Mon	17:30–19:30	P3	Posters - Single Molecule Biophysics
BP 11.1–11.5	Tue	9:30–12:15	HSZ 02	Bioinspired Functional Materials: From Nature's Nanoarchitectures to Nanofabricated Designs (Joint Symposium CPP/BP/MM/DF/DY/MI)
BP 12.1–12.11	Tue	9:30–13:00	HÜL 186	Microswimmers I (Joint Session DY/BP)
BP 13.1–13.5	Tue	9:30–11:00	HÜL 386	Bioimaging and Spectroscopy II
BP 14.1–14.10	Tue	9:30–13:00	SCH A251	Physics of <i>Physarum polycephalum</i> and Other Slime Molds - Joint Focus Session (BP/DY) organized by Hans-Günther Döbereiner
BP 15.1–15.6	Tue	11:30–13:00	ZEU 255	Colloids and Complex Fluids I (Joint Session CPP/BP/DY)

BP 16.1–16.3	Tue	11:30–12:30	HÜL 386	Biotechnology and Bioengineering
BP 17.1–17.5	Tue	14:30–15:45	HÜL 186	Microswimmers II (Joint Session DY/BP)
BP 18.1–18.8	Tue	14:00–16:00	ZEU 118	Statistical Physics in Biological Systems II (Joint Session DY/BP)
BP 19.1–19.14	Tue	14:00–16:00	P1A	Posters - Computational Biophysics
BP 20.1–20.19	Tue	14:00–16:00	P1A	Posters - Physics of the Genesis of Life (Focus Session)
BP 21.1–21.14	Tue	14:00–16:00	P1A	Posters - Membranes and Vesicles
BP 22.1–22.9	Tue	14:00–16:00	P1A	Posters - Biomaterials and Biopolymers
BP 23.1–23.10	Tue	14:00–16:00	P1A	Posters - Statistical Physics of Biological Systems
BP 24.1–24.18	Tue	14:00–16:00	P1A	Posters - Protein Structure and Dynamics
BP 25.1–25.12	Tue	14:00–16:00	P2-EG	Posters - Cytoskeletal Filaments
BP 26.1–26.8	Tue	14:00–16:00	P2-EG	Posters - Cell Adhesion
BP 27.1–27.4	Tue	14:00–16:00	P2-EG	Posters - Microswimmers
BP 28.1–28.1	Tue	14:00–16:00	P2-EG	Posters - Cell Migration & Contraction
BP 29.1–29.12	Tue	14:00–16:00	P2-EG	Posters - Multi-Cellular Systems
BP 30.1–30.2	Tue	14:00–16:00	P2-OG1	Posters - Neurosciences
BP 31.1–31.4	Tue	14:00–16:00	P2-OG1	Posters - Biotechnology and Bioengineering
BP 32.1–32.2	Tue	14:00–16:00	P2-OG1	Posters - DNA/RNA
BP 33.1–33.8	Tue	14:00–16:00	P2-OG1	Posters - Systems Biology & Gene Expression and Signalling
BP 34.1–34.5	Tue	14:00–16:00	P2-OG1	Posters - Physics of <i>Physarum polycephalum</i> and Other Slime Molds (Focus Session)
BP 35.1–35.2	Tue	14:00–16:00	P2-OG1	Posters - Physics of Parasites (Focus Session)
BP 36.1–36.1	Wed	8:30– 9:15	HSZ 01	Plenary Talk
BP 37.1–37.5	Wed	9:30–12:15	HSZ 02	Physics of Collective Mobility (Joint Symposium SOE/DY/BP/jDPG)
BP 38.1–38.11	Wed	9:30–13:00	HÜL 386	Membranes and Vesicles I
BP 39.1–39.7	Wed	9:30–12:30	SCH A251	Optogenetics for the Cytoskeleton - Focus Session organized by Ulrich Schwarz
BP 40.1–40.9	Wed	10:15–13:00	ZEU 260	Colloids and Complex Fluids II (Joint Session CPP/BP/DY)
BP 41.1–41.15	Wed	15:00–19:00	HÜL 186	Active Matter I (Joint Session DY/BP/ CPP)
BP 42.1–42.8	Wed	15:00–17:30	ZEU 250	Neurosciences
BP 43.1–43.7	Wed	15:00–17:15	HÜL 386	Cytoskeletal Filaments
BP 44.1–44.8	Wed	15:00–17:15	SCH A251	Biomaterials and Biopolymers (Joint Session BP/ CPP)
BP 45	Wed	18:30–19:30	HÜL 386	Annual General Meeting of the BP Division (BP Mitgliederversammlung)
BP 46.1–46.12	Thu	9:30–13:00	HÜL 186	Active Matter II (Joint Session DY/BP/ CPP)
BP 47.1–47.4	Thu	9:30–10:45	ZEU 250	Cell Adhesion
BP 48.1–48.11	Thu	9:30–13:00	HÜL 386	Membranes and Vesicles II
BP 49.1–49.12	Thu	9:30–13:00	SCH A251	Physics of the Genesis of Life - Focus Session organized by Moritz Kreysing and Dieter Braun
BP 50.1–50.12	Thu	9:30–13:00	GÖR 226	Networks: From Topology to Dynamics I (Joint Session SOE/DY/BP)
BP 51.1–51.6	Thu	11:15–12:45	ZEU 250	Microswimmers III (Joint Session BP/DY)
BP 52.1–52.9	Thu	15:00–18:00	ZEU 260	Topological Problems in the Physics of Polymers, Biopolymers and Fibers I (Joint Focus Session CPP/BP)
BP 53.1–53.8	Thu	15:00–17:00	ZEU 118	Pattern Formation (Joint Session DY/BP)
BP 54.1–54.10	Thu	15:00–17:30	ZEU 250	Statistical Physics of Biological Systems I (Joint Session BP/DY)
BP 55.1–55.7	Thu	15:00–17:15	HÜL 386	Cell Migration and Contraction
BP 56.1–56.9	Thu	15:00–17:30	SCH A251	Protein Structure and Dynamics
BP 57.1–57.5	Thu	15:00–16:15	ZEU 147	Networks: From Topology to Dynamics II (Joint Session DY/BP/SOE)
BP 58.1–58.5	Fri	9:30–10:45	ZEU 250	DNA & RNA
BP 59.1–59.5	Fri	9:30–11:00	HÜL 386	Multi-Cellular-Systems
BP 60.1–60.6	Fri	9:30–12:15	SCH A251	Physics of Parasites - Joint Focus Session (BP/DY) organized by Holger Stark
BP 61.1–61.6	Fri	10:15–13:00	ZEU 222	Topological Problems in the Physics of Polymers, Biopolymers and Fibers II (Joint Focus Session CPP/BP)

Annual General Meeting of the Biological Physics Division (BP Mitgliederversammlung)

Wednesday, March 22, 2017 18:30–19:30 HÜL 386

- Report of the current speaker team
- Election of the new speaker team 2017-2019
- Award of the EPL poster prizes of the Biological Physics Division
- Miscellaneous

BP 1: Computational Biophysics (Joint Session BP/DY)

Time: Monday 9:30–13:00

Location: ZEU 250

Invited Talk

BP 1.1 Mon 9:30 ZEU 250

Conformational Transitions in the Presence of Solvent and Internal Memory Effects — ●ROLAND NETZ, JULIAN KAPPLER, JAN DALDROP, BARTOSZ KOWALIK, and FLORIAN BRÜNIG — Department of Physics, Free University Berlin, Arnimallee 14, 14195 Berlin, Germany

Conformational transitions of biological molecules are controlled by solvent friction. For fast transitions, such as dihedral-angle flips, the finite solvent memory time plays a role. General scaling laws for the transition time including inertial, friction and memory effects are presented. The interplay between fast molecular reconfigurations and long-time conformational relaxation and the coupling between solvent and internal friction effects is discussed.

BP 1.2 Mon 10:00 ZEU 250

Dynamics and energetics of elongation factor SelB in the ternary complex and the ribosome — ●LARS V. BOCK, NIELS FISCHER, HOLGER STARK, and HELMUT GRUBMÜLLER — Max Planck Institute for Biophysical Chemistry, Göttingen

SelB is an elongation factor specialized to deliver the selenocysteine (Sec) tRNA to the ribosome by recoding the UGA stop codon on the mRNA. Initially the tRNA is in complex with selB and GTP forming the ternary complex (TC). High-resolution cryo-EM structures of intermediates of the Sec incorporation pathway uncover large-scale conformational changes of the ribosome and the TC. To complement the structural information with energetics and rapid dynamics, we performed extensive all-atom molecular dynamics simulations of the ribosome with bound TC as well as of the free TC in solution. The simulations of the free TC were started after extracting the TC from the ribosome-bound cryo-EM structures. The TC was found to rapidly interconvert between the different conformations allowing us to construct the free-energy landscape of the involved motions. This free-energy landscape indicates that the intrinsic large-scale conformational changes of the tRNA and SelB during the delivery to the ribosome are not rate-limiting to the process. In simulations of the free TC started from the GTPase-activated ribosome-bound conformation, the TC rapidly transitions into an inactivated conformation, showing that the GTPase-activated state is strongly stabilized by the ribosome. The simulations of the full ribosome with bound TC in the intermediate states allow us to identify the motions that are rate-limiting to the process of tRNA delivery and to identify the molecular mechanism of the domain closure of small ribosomal subunit upon tRNA decoding.

BP 1.3 Mon 10:15 ZEU 250

Correction of Finite-Size Effects on Diffusion in Lipid Membrane Simulations — ●MARTIN VÖGELE and GERHARD HUMMER — Max-Planck-Institut für Biophysik, Frankfurt am Main

Calculating diffusion coefficients from the mean squared displacement is a common task in evaluating molecular dynamics simulations. However, periodic boundary conditions introduce artifacts caused by the self-interaction with the periodic image. In cubic simulation boxes, the diffusion coefficient converges for large sizes. However, this is not the case if the system size is increased asymmetrically. [1]

We specifically test the effect of box geometry on the diffusion in lipid membranes which are usually simulated in very flat periodic boxes. There we find a logarithmic (and therefore unbounded) increase with growing box width. We discuss consequences of the apparent inability to determine a well-defined lipid diffusion coefficient from simulation and present possible methods to rationalize difficulties in comparing simulation results to each other and to experiment.

[1] M. Vögele and G. Hummer, J. Phys. Chem. B, 2016, 120 (33)

BP 1.4 Mon 10:30 ZEU 250

A Monte Carlo Study of Knots in Long Double-Stranded DNA Chains — FLORIAN RIEGER and ●PETER VIRNAU — Johannes Gutenberg-Universität Mainz

We determine knotting probabilities and typical sizes of knots in double-stranded DNA for chains of up to half a million base pairs with computer simulations of a coarse-grained bead-stick model: Single trefoil knots and composite knots which include at least one trefoil as a prime factor are shown to be common in DNA chains exceeding 250,000 base pairs, assuming physiologically relevant salt conditions.

The analysis is motivated by the emergence of DNA nanopore sequencing technology, as knots are a potential cause of erroneous nucleotide reads in nanopore sequencing devices and may severely limit read lengths in the foreseeable future. Even though our coarse-grained model is only based on experimental knotting probabilities of short DNA strands, it reproduces the correct persistence length of DNA. This indicates that knots are not only a fine gauge for structural properties, but a promising tool for the design of polymer models.

F. Rieger, P. Virnau, PLoS Comp. Biol. 12(9), e1005029 (2016).

BP 1.5 Mon 10:45 ZEU 250

Interaction of hyperbranched polyglycerol sulfate with proteins: calorimetry versus computer simulations — ●XIAO XU^{1,2}, QIDI RAN³, RAINER HAAG³, MATTHIAS BALLAUFF^{1,2}, and JOACHIM DZUBIELLA^{1,2} — ¹Institut für Weiche Materie und funktionale Materialien, Helmholtz-Zentrum Berlin — ²Institut für Physik, Humboldt-Universität zu Berlin — ³Institut für Chemie und Biochemie, Freie Universität Berlin

Using Isothermal Titration Calorimetry (ITC) and coarse-grained (implicit solvent/explicit salt) Langevin computer simulations, we study the interaction of hyperbranched polyglycerol sulfate (hPGS) with two oppositely charged serum proteins, i.e. human serum albumin (HSA) (-) and lysozyme (+). The simulation reveals explicitly the structural properties of the complexation. We demonstrate that the driving force of the complexation in both cases originates mainly from the release of condensed counter-ions from the polymer upon binding. The binding constant fitted by single set of identical sites model shows very weak dependence on polymer size for both proteins. By applying an excluded-volume (EV) model to fit the ITC data the explicit profile of binding free energy for multi-site binding between lysozyme and hPGS can be obtained. The experimental data coincides with computer simulation quantitatively especially for high generation of hPGS, which makes the simulation a useful tool to predict hPGS binding to targeted proteins such as selectins.

15 min break

BP 1.6 Mon 11:15 ZEU 250

Adsorption, binding motifs and structural change of proteins on silica studied by Molecular Dynamics — ●NILS HILDEBRAND, MONIKA MICHAELIS, SUSAN KÖPPEN, and LUCIO COLOMBI CIACCHI — Bremen Center for Computational Materials Science, Bremen

The physisorption of chymotrypsin and lysozyme on amorphous silica is investigated by classical Molecular Dynamics (MD) methods in comparison to adsorption and circular dichroism (CD) experiments. The long-range protein-surface attraction field is calculated in an implicit solvent based on DLVO theory. These calculations reveal a preferred protein orientation, which could be confirmed in explicit solvent simulations. Driven by its large dipole moment, chymotrypsin adsorbs with its alpha-helical regions pointing towards the surface. Lysozyme adsorbs in a side-on orientation. Positively charged hydrophilic residues form dominant binding motifs by adsorbing in dense water layers around the deprotonated silanol surface groups. The amount of adsorbed proteins found in the experiment can be explained by a combination of the binding motifs stability and protein-protein interactions. No significant conformational changes are observed in MD simulations lasting 300 ns. In order to capture surface-induced conformational changes revealed by CD experiments, parallel tempering in combination with metadynamics is employed. In these simulations, the helical content of chymotrypsin is used as a reaction coordinate, as helical unfolding is believed to strengthen the adhesion to the surface.

BP 1.7 Mon 11:30 ZEU 250

Organic co-solutes in aqueous solution: The effect on local water dynamics — JOHANNES ZEMAN, FRANK UHLIG, and ●JENS SMIAŁEK — Institut für Computerphysik, Universität Stuttgart, D-70569 Stuttgart, Germany

We investigate the effect of the organic co-solutes ectoine, trimethylamine N-oxide (TMAO), urea, and guanidinium chloride by means of classical and ab-initio Molecular Dynamics simulations. Our results reveal distinct effects on the local water structure and the water dy-

namics for the different co-solutes. The analysis of the diffusion coefficients and the dielectric spectra demonstrate that ectoine and TMAO significantly slow down water dynamics by a strongly bound hydration shell whereas urea and guanidinium chloride have a weaker impact. In combination with a sodium chloride solution, our findings for ectoine imply compensatory effects in order to explain the high co-solute and salt concentration in halotolerant bacteriae [1].

[1] M. B. Hahn, F. Uhlig, T. Solomun, J. Smiatek, H. Sturm; Phys. Chem. Chem. Phys. 18, 28398 (2016)

BP 1.8 Mon 11:45 ZEU 250

Determinants of nanoparticle protein corona composition investigated with molecular dynamics simulations — ●GIOVANNI SETTANNI¹, JIAJIA ZHUO¹, TONGCHUAN SUO¹, SUSANNE SCHÖTTLER^{2,3}, KATHARINA LANDFESTER², FRIEDERIKE SCHMID¹, and VOLKER MAILÄNDER^{2,3} — ¹Department of Physics, Johannes Gutenberg University Mainz — ²Max-Planck Institute for Polymer Research — ³Department of Dermatology, University Medical Center Mainz

Therapeutic nanoparticles in contact with biological fluids (blood, lung surfactant, etc.) are quickly covered by a layer of proteins (corona), which determines the particle's fate in the host organism (circulation half-life, cellular uptake, tissue distribution, immune response, etc.). Nanoparticles' surfaces are often modified (adding polymer coatings, or functionalization groups etc.) to improve their therapeutic efficacy, which involve a modification of the nanoparticle protein corona composition. The molecular factors determining the corona composition of nanoparticles are not very well understood, yet. Here we use molecular dynamics simulations to investigate the non-covalent interactions taking place between several blood proteins and poly(ethylene glycol) (PEG), a hydrophilic polymer commonly used to coat nanoparticles for improved efficacies. The simulations reveal recurring patterns of interaction involving specific amino acids. The latter could be used for the development of coarse grained representations of protein-PEG interactions and may provide the basis for understanding the properties of protein coronas formed around PEGylated nanoparticles.

BP 1.9 Mon 12:00 ZEU 250

Monolayer-Protected Anionic Au Nanoparticles Walk into Lipid Membranes Step by Step — ●FEDERICA SIMONELLI¹, DAVIDE BOCHICCHIO¹, RICCARDO FERRANDO², and GIULIA ROSSI¹ — ¹Physics Department, University of Genoa, Via Dodecaneso 33, 16146 Genoa, Italy — ²Chemistry Department, University of Genoa, Via Dodecaneso 31, 16146 Genoa, Italy

The design of ligand-protected metal nano-particles (NPs) with biomedical applications relies on the understanding, at the molecular level, of their interactions with cell membranes. We study, via unbiased coarse grained molecular dynamics simulations, the kinetics and the thermodynamics of the interaction between anionic ligand-protected gold NPs and model lipid membranes. We find that the NP-membrane interaction is a three-step process: electrostatics-driven adhesion to the membrane surface, hydrophobic contact and final embedding in the membrane core via anchoring of the charged ligands to both membrane leaflets. Our free energy calculations show that anchoring is highly favorable and not reversible. Furthermore, the interaction pathway of NPs with random surface arrangement of anionic and hydrophobic ligands is characterized by two metastable configurations: adsorbed at the membrane surface, and membrane-embedded. Patched ligand arrangements, instead, lead to the stabilization of a third, intermediate metastable configuration, resulting in a much slower kinetics of interaction with the membrane.

BP 1.10 Mon 12:15 ZEU 250

Modeling epidemic patterns of multiple diseases with short-term non-specific immunity — ●GORM GRUNER JENSEN¹, FLORIAN UEKERMANN¹, KIM SNEPPEN¹, and LONE SIMONSEN² — ¹Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, Copenhagen 2100-DK, Denmark — ²Department of public health, University of Copenhagen, Øster Farimagsgade 5, Copenhagen 1014-DK, Denmark

A number of common respiratory viruses cause seasonal epidemics in

a particular sequential pattern. Seasonal drivers like reduced immune function in mid-winter have been proposed as a possible cause. While these drivers may be sufficient to explain mid-winter viruses such as influenza, it is not clear whether other viruses require different drivers to explain their occurrence in spring, summer or fall. Here we use a multi-disease model to explore the possibility that a short non-specific immunity explains their seasonal patterns as a consequence of interaction between the diseases rather than requiring multiple seasonal drivers or complex pairwise interaction.

In the presence of a single seasonal driver, working identically on all diseases, our model exhibits a variety of observed epidemic patterns, including ordered peaks of different diseases. As example for application to observed patterns, we show two disease simulations reproducing multiple features of the correlation between annual PIV-3 and biennial PIV-1 epidemic peaks.

BP 1.11 Mon 12:30 ZEU 250

Characterization of coarse-grained helix-coil transition networks — ●JOSEPH RUDZINSKI, KURT KREMER, and TRISTAN BEREAU — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

A variety of models, with widely-varying resolution, have contributed to our interpretation of the protein folding process. While atomically-detailed simulations have emerged as an invaluable tool for describing the subtle details which determine particular folding processes, simple physics- and native structure-based coarse-grained (CG) models laid the foundation for current protein folding theories. Despite the success of the latter in describing the essential features of protein folding, the reduced degrees of freedom in CG models inherently obscures the resulting dynamical properties, generally limiting their utility. In this work, we investigate to what extent CG models can describe the precise network of transition pathways for particular protein folding processes. As a model system, we consider the well-studied problem of helix-coil transition kinetics. To elucidate the generic features of the transition, while retaining an accurate description of the transition pathways, we consider a hybrid model with simple, physically-motivated interactions coupled with atomically-detailed sterics. We compare the resulting transition network to networks generated from both an all-atom model and a more sophisticated, transferable CG model. Our results indicate that many features of the transition network are prescribed by rather generic features of the model, motivating further investigation of protein folding kinetics using this approach.

BP 1.12 Mon 12:45 ZEU 250

Mechanism of rhomboid intramembrane proteolysis — ●ANA NICOLETA BONDAR — Department of Physics, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

Intramembrane proteases are membrane-embedded proteins whose substrates are transmembrane protein segments. Reaction mechanisms of intramembrane proteases are important to understand, because these proteins are implicated in essential processes such as cell signalling. A fundamental open question is how specific lipid molecules participate in the reaction coordinate of intramembrane protease. We address this question with extensive all-atom molecular dynamics simulations of the intramembrane rhomboid protease from *Escherichia coli*, GlpG. The computations indicate coupling between lipid binding at the substrate docking-site region and the composition of the lipid membrane, highlighting the importance of lipid interactions for the reaction coordinate of the protease.

Work supported in part by the Excellence Initiative of the German Federal and State Governments provided via the Freie Universität Berlin, and allocation of computing time from the North-German Supercomputing Center, HLRN (bec00076).

References

1. A.-N. Bondar. Biophysical mechanism of rhomboid proteolysis: setting a foundation for therapeutics. Seminars in Cell and Developmental Biology 10.1016/j.semcdb.2016.09.006, Accepted (2016).
2. A.-N. Bondar, C. del Val, and S. H. White. Rhomboid protease dynamics and lipid interactions. Structure 17: 395-405 (2009).

BP 2: Bioimaging and Spectroscopy I

Time: Monday 9:30–12:45

Location: HÜL 386

Invited Talk

BP 2.1 Mon 9:30 HÜL 386

Visualization and Manipulation of the Invisible — ●HEINRICH LEONHARDT — Ludwig Maximilians University Munich, Biocenter, Martinsried, Germany

Fluorescence light microscopy allows multicolor visualization of cellular components with high specificity, but its utility has until recently been constrained by the intrinsic limit of spatial resolution and the lack of specific detection tools. To circumvent these limitations, we applied three-dimensional structured illumination microscopy (3D-SIM, Science, 320, 1332-6) and high-throughput STED microscopy in combination with automated image analysis. For detection of cellular structures, we have generated fluorescent, antigen-binding proteins, termed chromobodies, by combining epitope-recognizing fragments with fluorescent proteins (Nature Methods, 3, 887-9). These chromobodies can be expressed in living cells and used to target or trace epitopes in subcellular compartments providing an optical readout for novel high content analyses and functional studies (Nature Struct. Mol. Biol., 17, 133-139). These antigen-binding fragments can also be recombinantly produced, chemically functionalized and directly used for super-resolution microscopy (Science, 331, 1616-20). To study the dynamics of genome organization we have repurposed prokaryotic DNA binding proteins (TALEs and CRISPR/Cas) for the detection of specific DNA sequences in living cells (NAR 42, e38 and Nucleus, 5, 163-172). This combination of detection tools and microscopy techniques provides new insights into the structure and function of mammalian cells.

BP 2.2 Mon 10:00 HÜL 386

(3+1)D SIM + quantitative analysis for ophthalmologic research — ●FLORIAN SCHOCK^{1,2,3}, GERRIT BEST^{1,3}, NIL CELIK⁴, YANGYI WANG^{2,3}, ALENA BAKULINA⁵, SAADETTIN SEL⁴, UDO BIRK^{1,3}, RAINER HEINTZMANN^{6,7}, JÜRGEN HESSER⁵, STEFAN DITHMAR^{4,8}, and CHRISTOPH CREMER^{1,2,3} — ¹Institute of Molecular Biology, University of Mainz — ²Institute of Pharmacy and Molecular Biotechnology, University of Heidelberg — ³Kirchhoff Institute for Physics, University of Heidelberg — ⁴Department of Ophthalmology, University-Hospital Heidelberg — ⁵Experimental Radiation Oncology, University Medical Center Mannheim, University of Heidelberg — ⁶Institute of Physical Chemistry and Abbe Center of Photonics, University of Jena — ⁷Leibniz Institute of Photonic Technology — ⁸Department of Ophthalmology, HELIOS HSK, Wiesbaden, Germany

While super-resolution-microscopy has become widely available, its application in clinical context is still mostly restricted to cultivated cells. We present the application of (3+1)D(3 excitation/emission spectra) Structured Illumination Microscopy to clinical research on extracted tissues as well as quantitative analysis of over 300 human RPE cells and their granules (intracellular particles) regarding connections to age related macular degeneration. Autofluorescence behaviour is a characteristic hallmark for several chorioretinal conditions, so SIM offers potential for further clinical imaging at illumination powers that allow application to living patients (ongoing clinical study).

BP 2.3 Mon 10:15 HÜL 386

Live-cell super-resolution imaging of intrinsically fast moving flagellates — MARIUS GLOGGER¹, SIMONE STICHLER², INES SUBOTA¹, SARAH BERTLEIN², MARIE-CHRISTIN SPINDLER¹, JÖRG TESSMAR², JÜRGEN GROLL², MARKUS ENGSTLER¹, and ●SUSANNE FENZ¹ — ¹Biocenter: Cell and Developmental Biology, University of Würzburg, Würzburg, Germany — ²Department of Functional Materials in Medicine and Dentistry, University of Würzburg, Würzburg, Germany

Recent developments in super-resolution microscopy make it possible to resolve structures in biological cells at a spatial resolution of a few nm. However, the optimal structural resolution requires repeated illumination cycles and is thus limited to chemically fixed cells. For live cell applications substantial improvement over classical Abbe-limited imaging can already be obtained in adherent or slow moving cells. Nonetheless, a large group of cells are fast moving and thus could not yet be addressed with live cell super-resolution microscopy. These include flagellate pathogens like African trypanosomes. Here, we present an embedding method based on an in situ forming cytocompatible UV-crosslinked hydrogel. The fast cross-linking hydrogel immobilizes trypanosomes efficiently to allow microscopy on the nanoscale. We

characterized both the trypanosomes and the hydrogel with respect to their autofluorescence properties and found them suitable for single-molecule fluorescence microscopy (SMFM). As a proof of principle, SMFM was applied to super-resolve a structure inside the living trypanosome. We present an image of a flagellar axoneme component.

BP 2.4 Mon 10:30 HÜL 386

Coordinate-targeted fluorescence nanoscopy with multiple off-states — ●JOHANN GEORG DANZL^{1,2}, SVEN SIDENSTEIN², CAROLA GREGOR², NICOLAI URBAN², PETER ILGEN², STEFAN JAKOBS², and STEFAN HELL² — ¹Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria — ²Max Planck Institute for Biophysical Chemistry, 37077 Göttingen, Germany

Far-field optical nanoscopy techniques “super-resolve” features residing closer than the diffraction-limit by transiently preparing fluorophores in distinguishable (typically on- and off-) states and reading them out sequentially. In coordinate-targeted superresolution modalities, such as stimulated emission depletion (STED) microscopy, this state difference is created by patterns of light, driving for instance all molecules to the off-state except for those residing at intensity minima. For high resolution, strong spatial confinement of the on-state is required. However, this also subjects fluorophores at intensity maxima to excess light intensities and state cycling. In addition, as spatial confinement of the on-state is increased, state contrast between designated on- and off-regions has to be improved, too. We show that driving fluorophores to a second off-state enables protection of fluorophores and superior state contrast. In a realization that we dubbed “protected STED”, we used reversibly switchable fluorescent proteins as labels and employed both STED and reversible photoswitching as off-transitions. This directly translated into reduced bleaching and enhanced resolution in live-cell nanoscopy (J. G. Danzl, S. C. Sidenstein et al., Nature Photonics 10, 122 (2016)).

BP 2.5 Mon 10:45 HÜL 386

Exploring protein diffusion landscapes in living embryos with SPIM-FCS — ●PHILIPP STRUNTZ, DIRK HOFMANN, and MATTHIAS WEISS — University of Bayreuth, Experimental Physics I, Germany

Macromolecule diffusion in the complex and dynamic environment of living organisms often features spatial variations that report on the cells’ secret life, e.g. during embryogenesis. To explore these spatial heterogeneities one needs to quantify the local diffusion characteristics in extended regions of the sample in a multiplexed fashion. To obtain diffusion maps with high spatiotemporal resolution we have combined single plane illumination microscopy (SPIM) and fluorescence correlation spectroscopy (FCS). By refining a custom-made SPIM setup that was originally designed for long-term in-vivo imaging of early embryos of the small nematode *Caenorhabditis elegans* [1], we were able to acquire pixel-wise FCS curves on spatially extended regions within the embryo. We demonstrate the capabilities of SPIM-FCS by determining the diffusion maps of the peripheral membrane protein PLC1δ1 in the cytoplasm and on the plasma membrane during early stages of embryogenesis [2]. In a next step, we have focused on time-resolved diffusion maps of the protein PIE-1, for which we see the formation of a mobility gradient along the anterior-posterior axis before the first, asymmetric cell division. Our data hence show that SPIM-FCS can be used to explore intracellular transport phenomena even in fragile developmental model organisms.

[1] R. Fickentscher, P. Struntz & M. Weiss, PRL 117, (2016).

[2] P. Struntz & M. Weiss, J. Phys. D 49, 044002 (2016).

30 min break

BP 2.6 Mon 11:30 HÜL 386

Disentangling the effects of viscosity and refractive index mismatch in single-focus FCS — ●JONAS MÜCKSCH, PETRA SCHWILLE, and EUGENE P. PETROV — Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Martinsried, Germany

Fluorescence Correlation Spectroscopy (FCS) is a powerful tool to assess molecular mobilities in various settings ranging from bulk solutions to model lipid membranes, to living cells. The media in which FCS measurements are performed, frequently differ from water with respect to their viscosity and their refractive index. On the other hand, it has

been shown that the refractive index mismatch can severely affect the results of FCS measurements [1]. Here, we explore under which conditions it is possible to disentangle the effects of the solution viscosity and refractive index mismatch on FCS measurements carried out using a standard confocal microscope-based setup and thus employ this experimental technique for reliable determination of diffusion coefficients in various media.

[1] J. Enderlein, I. Gregor, D. Patra, T. Dertinger, and U. B. Kaupp, *ChemPhysChem* **6**, 2324 (2005).

BP 2.7 Mon 11:45 HÜL 386

Investigating DNA binding kinetics by camera-based total internal reflection fluorescence correlation spectroscopy (TIR-FCS) — JONAS MÜCKSCH^{1,3}, PHILIPP BLUMHARDT^{1,3}, MAXIMILIAN STRAUSS^{1,2}, RALF JUNGSMANN^{1,2}, and PETRA SCHWILLE¹ — ¹Max Planck Institute of Biochemistry, Martinsried, Germany — ²Ludwig Maximilian University, Munich, Germany — ³equal contribution

Fluorescence correlation spectroscopy (FCS) has been extensively used to study the kinetics of various *in vitro* and *in vivo* systems on a molecular level. The vast majority of FCS studies is performed using confocal setups, which feature well-defined detection volumes but suffer from low surface selectivity. Combining FCS with total internal reflection fluorescence (TIRF) illumination drastically enhances the spatial selectivity and enables the investigation of reversible binding of fluorescently labeled ligands to surface-confined receptors. So far, this potential to observe and quantify surface binding using TIR-FCS has been used only to minor extent. Here, we present a versatile optical setup for exploring surface-binding kinetics with TIRF illumination and point-(APD) or camera-based (EMCCD) fluorescence detection. In a first application, our camera-based assay facilitated the investigation of the transient hybridization of fluorescently labeled single-stranded DNA to the complementary handles of a surface-immobilized DNA origami scaffold. We varied the nucleotide overlap, yielding different binding times in the range of milliseconds to seconds. Using this highly tunable system, we systematically explored the parameter space accessible to EMCCD-based TIR-FCS.

BP 2.8 Mon 12:00 HÜL 386

A scanning ion conductance microscope (SICM) for large-range imaging — NICOLAS SCHIERBAUM, MARTIN HACK, and TILMAN E. SCHÄFFER — Institute of Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

The scanning ion conductance microscope (SICM) is a high-resolution imaging technique using an electrolyte-filled nanopipette as probe, allowing non-invasive, contact-free topography imaging of soft and fragile biological samples in physiological conditions. The scan range of previously described SICM setups is limited to 200 μm in lateral and 25 μm in vertical direction. We present a SICM setup with a maximum scan range of 25 mm $\times$ 25 mm in lateral and 0.25 mm in vertical direction. The SICM is combined with an optical phase contrast microscope and is equipped with a heated sample stage for live cell imaging. We demonstrate the high versatility of the setup by imaging samples at dif-

ferent length scales: from macroscopic structures such as fingerprints or cell layers to microscopic structures such as small cell protrusions. The large scan range facilitates selecting a region of interest with subsequent high-resolution imaging. We applied the setup to the study of wound healing by time-lapse imaging a live epithelial cell monolayer over 20 hours, demonstrating the long-term imaging stability of the setup.

BP 2.9 Mon 12:15 HÜL 386

Mapping surface charge density of lipid bilayers by quantitative surface conductivity microscopy — LASSE H. KLAUSEN¹, THOMAS FUHS^{1,2}, and MINGDONG DONG¹ — ¹Interdisciplinary Nanoscience Center, Aarhus University, Aarhus, Denmark — ²School of Chemical Engineering and Technology, Harbin Institute of Technology, Harbin, PR China

Local surface charge density of lipid membranes influences membrane-protein interactions leading to distinct functions in all living cells, and it is a vital parameter in understanding membrane-binding mechanisms, liposome design and drug delivery. Despite the significance, no method has so far been capable of mapping surface charge densities under physiologically relevant conditions. Here, we use a scanning nanopipette setup (scanning ion-conductance microscope) combined with a novel algorithm to investigate the surface conductivity near supported lipid bilayers, and we present a new approach, quantitative surface conductivity microscopy (QSCM), capable of mapping surface charge density with high-quantitative precision and nanoscale resolution. The method is validated through an extensive theoretical analysis of the ionic current at the nanopipette tip, and we demonstrate the capacity of QSCM by mapping the surface charge density of model cationic, anionic and zwitterionic lipids with results accurately matching theoretical values.

BP 2.10 Mon 12:30 HÜL 386

High Resolution Imaging of Cellular Signaling Using Fluorescent Nanosensor Arrays — SEBASTIAN KRUSS — Institut für Physikalische Chemie, Universität Göttingen

Intercellular communication via chemical signaling proceeds with both spatial and temporal components, but analytical tools, such as micro-fabricated electrodes, have been limited to just a few probes per cell. In this work, we use a non-photobleaching fluorescent nanosensor array based on single walled carbon nanotubes (SWCNT) rendered selective to the neurotransmitter dopamine to study its release from neuroprogenitor cells at a resolution exceeding 20,000 sensors/cell. This allows the spatial and temporal dynamics of dopamine release, following stimulation, to be measured at exceedingly high spatiotemporal resolution. We observe localized, unlabeled release sites of dopamine spanning 100 ms to seconds that correlate with negative membrane curvature, and not predominately the positive curvature associated with the tips of cellular protrusions as intuitively expected. The results illustrate how directionality of chemical signaling is shaped by membrane morphology, and highlight the advantages of nanosensor arrays that can provide high spatial and temporal resolution of chemical signaling.

BP 3: Mechanics and Dynamics of 3D Tissues - Joint Focus Session (BP/CPP/DY) organized by Peter Loskill

Time: Monday 9:30–13:00

Location: SCH A251

Invited Talk

BP 3.1 Mon 9:30 SCH A251

Cilia-based transport networks — EBERHARD BODENSCHATZ — MPI für Dynamik und Selbstorganisation, Am Fassberg 17, 37077 Göttingen

Cerebrospinal fluid conveys many physiologically important signaling factors through the ventricular cavities of the brain. We investigated the transport of cerebrospinal fluid in the third ventricle of the mouse brain and discovered a highly organized pattern of cilia modules, which collectively give rise to a network of fluid flows that allows for precise transport within this ventricle. Our work suggests that ciliated epithelia can generate and maintain complex, spatiotemporally regulated flow networks. I shall also show results on how to assemble artificial cilia and cilia carpets. This work is in collaboration with Regina Faubel, Gregor Eichele, Christian Westendorf, Azam Gholami, Isabella Guido, Yong Wang, Albert Bae and Marco Tarantola. Support by the Max Planck Society and the BMBF within the MaxSynBio

initiative is gratefully acknowledged.

BP 3.2 Mon 10:00 SCH A251

Quantitative structure-function relationships in 3D tissues — JANNA NAWROTH — Emulate Inc., Boston, MA, USA

Biological tissues are characterized by an organ-specific three-dimensional, multiscale organization of cells and extracellular matrix components. This organization gives rise to organ-specific functions and dysfunctions. Tissue engineering attempts to recapitulate these structure-function relationships *in vitro* to provide models of disease, drug toxicity, and patient-specific responses. One major challenge is to identify and implement quantitative metrics that capture the most relevant structure-function relationships to serve for both quality control and experimental readout of the engineered tissue. Here, I present engineering and analysis strategies for recapitulating and quantifying the cellular organization and mechanical functions in engineered car-

diac muscle and in ciliated epithelia, with a particular emphasis on organ-on-chip technology.

BP 3.3 Mon 10:30 SCH A251

In vivo quantification of spatially-varying mechanical properties in developing tissues — ●FRIEDHELM SERWANE^{1,2}, ALESSANDRO MONGERA¹, PAYAM ROWGHANIAN¹, DAVID KEALHOFFER¹, ADAM LUCIO¹, ZACHARY HOCKENBERRY¹, and OTGER CAMPAS¹ — ¹University of California, Santa Barbara, USA — ²Max Planck Institute for Medical Research, Heidelberg, Germany

We present a technique that allows quantitative spatiotemporal measurements of mechanical properties *in vivo* using biocompatible ferrofluid droplets as local mechanical actuators [1].

The mechanical properties of the cellular microenvironment and their spatiotemporal variations play a central role in controlling cell behavior, including cell differentiation. However, no direct *in vivo* and *in situ* measurement of mechanical properties within developing 3D tissues has been performed yet.

Using our technique we show that vertebrate body elongation entails spatially varying tissue mechanics along the anteroposterior axis. Specifically, we find that the zebrafish tailbud is viscoelastic: elastic below a few seconds and fluid after just one minute. Furthermore, it displays decreasing stiffness and increasing fluidity towards its posterior elongating region.

This method opens the door to study mechanobiology *in vivo*, both in embryogenesis and in disease processes, including cancer.

[1] F. Serwane, A. Mongera, P. Rowghanian, D. Kealhofer, A. Lucio, Z. Hockenberry, O. Campàs. Nature Methods, in press (2016)

BP 3.4 Mon 10:45 SCH A251

Mechanical spectroscopy of retina explants at the protein level employing nanostructured scaffolds — ●MAREIKE ZINK¹ and S. G. MAYR² — ¹Soft Matter Physics Division, University of Leipzig, Leipzig, Germany — ²Leibniz Institute for Surface Modification (IOM), Leipzig, Germany & Division of Surface Physics, Department of Physics and Earth Sciences, University of Leipzig, Germany

The mechanical properties of the retina play a crucial role in function and diseases of the eye. Here we present that nanostructured TiO₂ substrates can be employed as vibrating reed to investigate the mechanical properties of adult mammalian retinæ at the nanometer. Within a self-designed mechanical spectroscopy setup, the reed with the retina on top is excited to perform free damped oscillations. The detected oscillation parameters represent a fingerprint of the frequency-dependent mechanical tissue properties that are derived in combination with sandwich beam analysis and finite element calculations. We found that the Young's modulus of the retina is of the order of a few GPa, much higher than values obtained from experiments in which tissue response is investigated on micrometer length scales. In our study, polymers and proteins on the photoreceptor side of the retina in contact with the nanostructured reed are stretched and compressed during vibration of the underlying scaffold and the acting intramolecular forces are probed at the protein level. To this end, our mechanical spectroscopy approach offers new perspectives in studying mechanical response of individual proteins within the tissue for investigating tissue mechanics, diseases and the effect of drugs.

15 min break

BP 3.5 Mon 11:15 SCH A251

A simulation study on 3D muscle movement: eigen-frequency and force-coupling to the skeleton change with muscle activity — DANIEL F B HAEUFLE, DANIEL WIRTZ, ●KEVIN KRASCHEWSKI, SYN SCHMITT, and OLIVER RÖHRLE — Stuttgart Research Center for Simulation Technology (SimTech), University of Stuttgart, Germany

The muscles in the human body are soft materials coupled flexibly to the rather rigid bones. Due to this flexible coupling, muscles move relative to the bones during movement. The resulting coupling forces of these so-called wobbling masses depend on the neural stimulation of the muscle tissue. It is experimentally very difficult to study the relation between muscle stimulation and coupling forces. Therefore, we developed a 3D continuum-mechanical model of a muscle-tendon complex considering muscle stimulation, elasticity, viscosity, fiber orientation, and tendon stiffness. This model predicts the interaction forces in response to external oscillatory excitations in dependence on excitation frequency and muscle stimulation level. With this approach, the

functional role of wobbling masses in human movement, e.g., energy dissipation and force reduction during the impact in human running, can be studied in more detail.

BP 3.6 Mon 11:45 SCH A251

Electromechanical Turbulence in the Heart — ●JAN CHRISTOPH and STEFAN LUTHER — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The self-organizing pattern forming mechanisms underlying highly life-threatening cardiac fibrillation are still insufficiently understood. High-speed fluorescence imaging provides highly detailed visualizations of the spatio-temporal electrophysiological activity of the heart. During ventricular fibrillation, these visualizations depict complex spatio-temporal electrical patterns including rotating vortices or spiral waves on the heart's surface. However, with limited penetration depths of fluorescence imaging the optically mapped surface dynamics reflect only the superficial projection of three-dimensional wave phenomena that evolve within the depths of the cardiac muscle.

We combined fluorescence imaging with ultrasound to study the coupled electrical and mechanical activity of the fibrillating heart on its surface as well as within the heart wall. We found that during fibrillation electrical activity patterns and elasto-mechanical deformations are highly correlated producing co-localized patterns of electrical and mechanical activation. Specifically, we found that electrical spiral wave rotors can be accompanied by rotational elasto-mechanical patterns, which like fingerprints of vortex activity occur as a characteristic feature within the deformations of the fibrillating muscle. Our data highlights the importance of studying the mechanics and dynamics of 3D cardiac tissues to obtain a better understanding of cardiac arrhythmias and to conceptualize novel diagnostic and therapeutical strategies.

BP 3.7 Mon 12:00 SCH A251

Local rules for robust global transport in liver networks — ●JENS KARSCHAU¹, ANDRE SCHOLICH², MARIUS ASAL¹, HIDENORI NONAKA³, HERNAN MORALES-NAVARRETE³, FABIAN S MIRANDA³, KIRSTIN MEYER³, YANNIS KALAIIDZIS³, MARINO ZERIAL³, FRANK JÜLICHER², and BENJAMIN M FRIEDRICH¹ — ¹cfaed / TU Dresden — ²MPI PKS, Dresden — ³MPI CBG, Dresden

The liver represents a chemical factory that is characterised by intertwined transport networks for toxins and metabolites. Each hepatocyte cell of the liver tissue interacts with two space-filling networks: bile canaliculi and sinusoids which transport bile and blood, respectively. How these networks establish their distinct architecture to supply all hepatocytes, and dynamically adapt to time-varying load as well as to local perturbations remains elusive.

Here, we elucidate design principles of liver tissue structure and self-organisation based on experimental high-resolution imaging data from mice. First, we characterise and quantify liver tissue with tools from liquid-crystal theory that show lobule level patterns of aligned cell polarity and local network anisotropy. Second, we study a simplified flow model to understand the relationship between the spatial structure of the network and robust transport properties. Third, we compare our flow simulations in reconstructed bile canaliculi networks and simulated self-organised networks. Thereby, we establish a connection between local network geometry and properties of global fluid transport, linking tissue structure with function.

BP 3.8 Mon 12:15 SCH A251

Jamming and liquidity in 3D cancer cell aggregates — ●LINDA OSWALD¹, STEFFEN GROSSER¹, JÜRGEN LIPPOLDT¹, STEVE PAWLIZAK¹, ANATOL FRITSCH², and JOSEF KÄS¹ — ¹University of Leipzig — ²MPI CBG Dresden

Traditionally, tissues are treated as simple liquids, which holds for example for embryonic tissue. However, recent experiments have shown that this picture is insufficient for other tissue types, suggesting possible transitions to solid-like behavior induced by cellular jamming. The coarse-grained self-propelled Voronoi (SPV) model predicts such a transition depending on cell shape which is thought to arise from an interplay of cell-cell adhesion and cortical tension. We observe non-liquid behavior in 3D breast cancer spheroids of varying metastatic potential and correlate single cell shapes, single cell dynamics and collective dynamic behavior of fusion and segregation experiments via the SPV model.

BP 3.9 Mon 12:30 SCH A251

Type IV pili govern the internal dynamics of *Neisseria gonorrhoeae* microcolonies. — ●WOLFRAM PÖNISCH¹,

CHRISTOPH WEBER², KHALED ALZURQA³, HADI NASROLLAHI³, KELLY ECKENRODE³, NICOLAS BIAIS³, and ZABURDAEV VASILY¹ — ¹Max Planck Institut für Physik Komplexer Systeme, Dresden — ²Harvard University, Cambridge — ³Brooklyn College, New York

An important step in the evolution of biofilms is the formation of microcolonies, agglomerates of cells that can consist of several thousands of cells. For many pathogenic bacteria, i.e. *N. gonorrhoeae* or *P. aeruginosa*, the attractive cell-cell-interactions required for microcolonies to form are mediated by micron-long and thin appendages, the called type IV pili. We are interested in the pili-mediated dynamics of individual bacteria within microcolonies and how they affect the properties of the agglomerates. In experiments, we observe a gradient of motility of cells of *N. gonorrhoeae*, depending on their position within a colony. We will present a computational model of cells interacting via individual pili. It allows us to model microcolonies on biologically relevant temporal and spatial scales and is able to reproduce the differential motility of cells within a colony. Furthermore, it enables us to study quantities that are not yet accessible by experiments, e.g. the cell density within a colony, the pili-mediated cell forces and force fluctuations

and the internal structure of the colonies. Finally, we will present how the assembly and morphology of microcolonies is affected by the pili properties, particularly for mixtures of cell populations characterized by mutations of their pilus apparatus.

BP 3.10 Mon 12:45 SCH A251

Growth Dynamics of Biofilms — •BENEDIKT SABASS^{1,2}, JING YAN², HOWARD A. STONE², and NED S. WINGREEN² — ¹Forschungszentrum Jülich — ²Princeton University

Bacteria can form tight communities that are called biofilms. Although biofilms are ubiquitous and ecologically important, little is known about the physics of biofilm growth. Here, we focus on rod-shaped *V. cholerae* bacteria that form hemispherical biofilms when growing on a surface. Using high-resolution microscopy data, we measure cell density, cell orientation, and shape evolution of the biofilm. We quantitatively explain the density and cell orientation inside the biofilm by minimization of elastic energies. The evolution of the whole biofilm shape is governed by apparent viscous relaxation. We find that the shape parameters of biofilms follow rather simple, generic scaling laws.

BP 4: Systems Biology & Gene Expression and Signalling

Time: Monday 15:00–17:30

Location: ZEU 250

Invited Talk BP 4.1 Mon 15:00 ZEU 250
Antibiotic-induced gene expression noise and cross-protection at the single-cell level — •TOBIAS BOLLENBACH — University of Cologne, Germany

Antibiotics elicit drastic changes in microbial gene expression, including the induction of stress response genes. While certain stress responses are known to 'cross-protect' bacteria from other stressors, it is unclear if cellular responses to antibiotics can have a similar protective role. By measuring the dynamic genome-wide transcriptional response of *Escherichia coli* to four antibiotics, we found that trimethoprim induces a rapid and strong acid stress response pulse which protects bacteria from subsequent exposure to acid. We then combined microfluidics and time-lapse imaging to monitor survival and the dynamics of acid stress response induction in single cells. The fraction of surviving cells followed a simple exponential decay and thus appeared consistent with a memoryless Poisson process. Interestingly, however, the noisy expression of one of the major acid resistance genes explained the great spread in single-cell survival times. Simultaneous measurements of gene expression and pH using a ratiometric sensor revealed that cells with higher expression of acid resistance genes upon trimethoprim exposure maintain higher intracellular pH and survive the acid shock better. The seemingly stochastic single-cell survival times under acid stress therefore become predictable once their underlying molecular cause is identified. Overall, this work provides a roadmap for the systematic identification of molecular mechanisms behind single-cell cross-protection between antibiotics and other stressors.

BP 4.2 Mon 15:30 ZEU 250

Origin and consequences of the exponential decay of viability of *Escherichia coli* during starvation — •SEVERIN SCHINK¹, ELENA BISELLI¹, CONSTANTIN AMMAR^{1,2}, and ULRICH GERLAND¹ — ¹Technische Universität München, Physik Department — ²Ludwig-Maximilians-Universität München, Institut für Informatik

Surviving nutrient limitation is an important part of the microbial life cycle. When carefully starved of all energetic substrates, *Escherichia coli* shows an exponential decay of viability, with the rate depending on environment and genetics. In this work we identify the exponential decay to be a consequence of the energetic needs of the cell for maintenance. When no carbon resources are available in the medium, the only external possibility for energy production are resources freed by lysed cells in the population. Such a cannibalistic process, in which dying cells release resources that can sustain the remaining live cells, naturally leads to an exponential decay of viability. The death rate of a starved population is thus a measure for the maintenance rate, and allows quantitative studies of environmental and genetic perturbation, as exemplified by the study of knock-outs of the stress response sigma factor rpoS.

BP 4.3 Mon 15:45 ZEU 250

Magnetogenetic Manipulation of Intracellular Signalling —

•CORNELIA MONZEL¹, CHIARA VICARIO¹, DOMENIK LISSE², MATHIEU COPPEY¹, JACOB PIEHLER², and MAXIME DAHAN¹ — ¹Laboratoire Physico-Chimie, Institut Curie, CNRS UMR168, 75005 Paris, France — ²University of Osnabrück, Department of Biology, 49076 Osnabrück, Germany

Many cell functions rely on the coordinated activity of signalling pathways at a subcellular scale. However, there are few tools capable of probing and perturbing signalling networks with a spatial resolution matching the intracellular dimensions of their activity patterns. Here, we develop a generic magnetogenetic approach based on functionalized magnetic nanoparticles (MNPs) targeting an intracellular protein of interest. Upon protein recruitment the MNP-protein complexes act as nanoscopic hot spots that can be displaced by magnetic forces to provide molecularly graded information to the cell and to trigger a signal transduction pathway that brings about a cellular response. We demonstrate that magnetic nanoparticles based on the natural iron storage protein ferritin are ideally suited for intracellular applications. We use these ferritin MNP to manipulate Rho-GTPases - a set of molecular switches known to regulate cell morphology via complex spatiotemporal patterns of activity. The MNP-Rho-GTPase mediated stimulus is then shown to trigger morphological and signalling activity.

BP 4.4 Mon 16:00 ZEU 250

Cause and Cure of Sloppiness in Ordinary Differential Equation Models — •CHRISTIAN TÖNSING¹, JENS TIMMER^{1,2,3}, and CLEMENS KREUTZ^{1,2} — ¹Institute of Physics, University of Freiburg, Germany — ²Center for Biosystems Analysis (ZBSA), University of Freiburg, Germany — ³BIOSS Centre for Biological Signalling Studies, University of Freiburg, Germany

For the purpose of mathematical modeling of biochemical reaction networks by the frequently utilized nonlinear ordinary differential equation (ODE) models, parameter estimation and uncertainty analysis is a major task.

In this context the term sloppiness has been introduced recently for an unexpected characteristic of nonlinear ODE models. In particular, a broadened eigenvalue spectrum of the Hessian matrix of the objective function covering orders of magnitudes is observed, although no such hierarchy of parameter uncertainties was expected a priori.

In this work, it is shown that sloppiness originates from structures in the sensitivity matrix arising from the properties of the model topology and the experimental design. It will be clarified that the intensity of the sloppiness effect is controlled by the design of experiments, i.e., by the data. Thus, we conclude that the assignment of sloppiness to a model as a general characteristic is incomplete without discussing experimental design aspects. Furthermore, we validate this proposition by presenting strategies using optimal experimental design methods in order to circumvent the sloppiness issue and show results of non-sloppy designs for a benchmark model.

BP 4.5 Mon 16:15 ZEU 250

Engineering orthogonal synthetic timer circuits in bacteria — ●MARCO MAURI¹, DANIELA PINTO², STEFANO VECCHIONE¹, HAO WU¹, THORSTEN MASCHER², and GEORG FRITZ¹ — ¹LOEWE-Center for Synthetic Microbiology (SYNMIKRO), Philipps-University Marburg, Germany — ²Institut für Mikrobiologie, Technische Universität Dresden, Germany

The rational design of synthetic circuits in bacteria is often restricted by cross-reactions between circuit components and physiological processes within the heterologous host. Here, we present a strategy to overcome these restrictions by using extracytoplasmic function sigma factors (ECFs). These are reversible binding subunits of the bacterial RNA polymerase, which are activated upon environmental stress conditions. ECFs represent ideal orthogonal regulators because there exist over 90 phylogenetic ECF groups recognizing distinct target promoters. To explore their potential for synthetic circuit design, we evaluate several heterologous ECFs in *Escherichia coli* and *Bacillus subtilis*. After a quantitative study of simple switches, we use a computational model to predict the behaviour of a cascade with two and three ECFs, which we find in excellent agreement with experimental data. We show that in both organisms these "autonomous timers" sequentially activate a series of genes with a defined time delay. These results not only serve as a proof of concept for the application of ECFs as organism-independent building blocks for synthetic biology, but could also be used to introduce a timing hierarchy among the expression of biosynthetic pathway components in biotechnological applications.

BP 4.6 Mon 16:30 ZEU 250

Local Riemannian geometry of model manifolds and its implications for practical parameter identifiability — ●DANIEL KASCHEK¹, DANIEL LILL², and JENS TIMMER¹ — ¹Physikalisches Institut, Universität Freiburg — ²Systems Biology Ireland, University College Dublin

When dynamic models are fitted to time-resolved experimental data, parameter estimates can be poorly constrained albeit being identifiable in principle. This means that along certain paths in parameter space, the negative log-likelihood does not exceed a given threshold but remains bounded.

This situation, denoted as practical non-identifiability, can only be detected by Monte Carlo sampling or systematic scanning by the profile likelihood method. In contrast, the Fisher information matrix which is based on second-order model sensitivities in the optimum reveals no information about the boundedness at all.

Here, we show that for some dynamic models the information about the bounds is already contained in the Christoffel symbols, which are also computed from model sensitivities up to order two at the optimum. Assuming constant Christoffel symbols in the geodesic equation, approximate Riemannian normal coordinates are constructed. The new coordinates give rise to an approximative log-likelihood, featuring flat directions and bounds similar to that of the original log-likelihood.

BP 4.7 Mon 16:45 ZEU 250

Cellular memory couples sporulation and spore revival — ALPER MUTLU^{1,2}, STEPHANIE TRAUTH^{1,2}, MARIKA ZIESACK², JAN-PHILIP BERGEEST², KARL ROHR^{2,3}, NILS BECKER^{2,3}, THOMAS HÖFER^{2,3}, and ●ILKA BISCHOF^{1,2} — ¹MPI for Terrestrial Microbiology — ²University of Heidelberg — ³DKFZ Heidelberg

In bacteria, entry into and exit from dormancy are controlled by reg-

ulatory networks with little known overlap, indicating that the two processes operate independently from each other. Using *B. subtilis* as a model we developed an advanced time-lapse microscopy assay and a fluorescent marker that reports on a spore's differentiation history to study the effect of variable sporulation timing on nutrient-induced spore revival. We find that spores exhibit long-term phenotypic memory of their differentiation history. Modeling and experiments with re-programmed cells suggest that this memory creates a quantity versus quality trade-off to generate fewer but more efficient spores. We therefore suggest that phenotypic memory contributes to the emergence of complex adaptive traits.

BP 4.8 Mon 17:00 ZEU 250

Inflammatory diseases from the network perspective — ●PIOTR NYCZKA¹, AMKE CALIEBE², SILKE SZYMCAK², CAROLIN KNECHT², KRISTINA SCHLICHT², MICHAEL KRAWCZAK², and MARC-THORSTEN HÜTT¹ — ¹Jacobs University Bremen, Germany — ²Christian Albrechts University of Kiel, Germany

We have studied gene expression patterns (provided to us by the KORA study within the framework of the sysINFLAME systems medicine consortium) of human patients with inflammatory diseases with respect to the gene centric metabolic networks.

Despite the fact of dealing with very noisy data we were able to find clear evidence of prominent differences between two inflammatory diseases: Psoriasis and Inflammatory Joint Disease, from the perspective of these networks. This difference was clearly visible even on purely topological level and result was robust across two different human metabolism models, and different parameter values.

This is definitely important result and could be a serious step forward in further understanding of these diseases, from the network perspective. We will also discuss results regarding protein network perspective and give some more details about human metabolism and methods we use.

BP 4.9 Mon 17:15 ZEU 250

Designing Synthetic Networks and Experimentation in silico: A Generalized Evolutionary Algorithm Approach — ●CHRISTIAN FLECK — Laboratory of Systems and Synthetic Biology, Wageningen University, The Netherlands

Evolution has led to the development of biological networks that reliably respond to environmental signals. Elucidating, understanding and then reconstructing important network motifs is one of the principal aims of Systems & Synthetic Biology. In this work we present a generalised in silico evolutionary algorithm that simultaneously finds network structures and reaction rates that satisfy defined objectives. By using a schema description of model properties and employing recombination between pairs of networks, the algorithm is able to explore large regions within the search space. We show the utility of our algorithm by finding robust synthetic oscillators, and, by using multi-objective optimisation to find a set of oscillators and feed-forward loops that are optimal at balancing competing objectives. Notably, we highlight that protein dimerisation is an important aspect of oscillating networks. We go on to discuss our results in the context of understanding network evolution in nature and in the laboratory. Furthermore, we suggest how in silico evolution can aid the efficiency of directed evolution experiments for designing synthetic circuits. The use of optimisation algorithms to design robust networks should enable synthetic biologists to construct new systems that produce increasingly complex responses.

BP 5: Single Molecule Biophysics

Time: Monday 15:00–17:30

Location: HÜL 386

Invited Talk

BP 5.1 Mon 15:00 HÜL 386

Metal Induced Energy Transfer — ●JÖRG ENDERLEIN — 3. Physikalisches Institut, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077 Göttingen

Classical fluorescence microscopy is limited in resolution by the wavelength of light (diffraction limit) restricting lateral resolution to ca. 200 nm, and axial resolution to ca. 500 nm. However, recent years have seen a tremendous development in super-resolution techniques, such as Photoactivatable Localization Microscopy (PALM) or STochastic Optical Reconstruction Microscopy (STORM), pushing the lateral resolution down to a few nanometers. However, even with these methods, the resolution along the optical axis is typically a factor 3 to 5 worse than the lateral resolution. Recently, we have developed a new method for localizing fluorescent emitters along the optical axis with nanometer accuracy. The method is based on the energy transfer of the excited fluorophore into surface plasmons of a thin metallic film, which is extremely sensitive on the distance between the fluorophore and the metal surface. We call this method Metal Induced Energy Transfer or MIET imaging. I will explain the physical foundations of MIET, and will present numerous of its applications.

BP 5.2 Mon 15:30 HÜL 386

Dynein's direction-dependent microtubule-binding strength is controlled via a tension-induced sliding of dynein's stalk helices mediated by the coiled-coil strut — LU RAO¹, FLORIAN BERGER², MATTHEW NICHOLAS¹, and ●ARNE GENNERICH¹ — ¹Albert Einstein College of Medicine, Bronx, USA — ²Rockefeller University, New York, USA

Cytoskeletal motor protein motility requires coordination of ATPase and filament-binding cycles. Mechanical tension strongly influences these processes, and likely regulates motor stepping as external forces resist motor movement and intramolecular tension develops between motor domains. In cytoplasmic dynein, an AAA+ ATPase, applied tension affects microtubule (MT)-binding strength anisotropically - backward tension induces stronger binding- while in the absence of tension, reconfiguration of the coiled-coil 'stalk' (which connects the AAA+ and MT-binding domains) is known to alter MT affinity. Using optical tweezers, mutagenesis, and chemical cross-linking, we show that preventing relative motion of the stalk helices or deleting the 'strut' (which emerges from the AAA+ domain and contacts the stalk) both eliminate tension-based regulation of MT-binding strength. Thus, tension alters dynein's MT-binding strength by inducing sliding of the stalk helices, and the strut is a key mediator of this process.

BP 5.3 Mon 15:45 HÜL 386

Coiled Coils as Mechanical Building Blocks — MELIS GOKTAS, PATRICIA LOPEZ-GARCIA, RUBY M. A. SULLAN, and ●KERSTIN G. BLANK — Max Planck Institute of Colloids and Interfaces

Coiled coils (CCs) are ubiquitous structural motifs found in many different proteins. They are made of α -helices that self-assemble into helical superstructures such as dimers, trimers and tetramers. CCs are important components of cytoskeletal and extracellular matrix proteins, highlighting their crucial role as mechanical building blocks. Despite their widespread appearance, the general structural determinants that define their molecular mechanical properties in different pulling geometries ('shear' vs. 'unzip') are largely unknown. With the goal of shedding light on the structure-to-mechanics relationship, we are applying AFM-based single molecule force spectroscopy to a set of CCs characterized by differences in CC length and sequence. We show that a 28-amino-acid-long, heterodimeric CC ruptures at a most probable force of >40 pN when loaded in shear geometry, while the rupture force for the unzip geometry is below the detection limit of AFM. In the shear geometry, we observe a clear dependence on CC length and helix propensity, showing that the rupture force of CCs in the shear geometry can be tuned by a number of parameters. Our final goal is to develop a library of CCs for the synthesis of CC-based materials with tunable mechanical properties for applications in tissue engineering.

BP 5.4 Mon 16:00 HÜL 386

3D Light microscopy of protein structure with Angstrom resolution — ●DANIEL BÖNING¹, SIEGFRIED WEISENBURGER¹, BENJAMIN SCHOMBURG², KARIN GILLER², STEFAN BECKER², CHRISTIAN

GRIESINGER², and VAHID SANDOGHDAR¹ — ¹Max Planck Institute for the Science of Light, 91058 Erlangen, Germany — ²Max Planck Institute for Biophysical Chemistry, 37077 Goettingen, Germany

Insight into the atomic and molecular structure of proteins and other biomolecular assemblies is highly desirable in many areas of life sciences, and several physical techniques such as x-ray crystallography, electron microscopy (EM) and magnetic resonance spectroscopy have been employed over decades to arrive at such information. However, due to limitations in each method the structures of the great majority of the proteins and larger biomolecules remain unknown to us. Here, we present a novel optical microscopy technique, termed Cryogenic Optical Localization in three Dimensions (COLD), which reaches Angstrom resolution in deciphering the positions of several fluorescent sites within a single small protein. The key mechanism for reaching this limit is the enhanced photostability at low temperatures, thus providing a much higher shot-noise-limited signal-to-noise ratio than in room temperature super-resolution microscopy. As an example of the application of this method, we show how we resolve the four sites where biotin binds to streptavidin in three dimensions. COLD opens new doors for obtaining quantitative structure information from small to medium sized biomolecules at the Angstrom scale and can complement other existing techniques such as magnetic resonance spectroscopy.

BP 5.5 Mon 16:15 HÜL 386

Biased side-stepping enables single molecules of yeast kinesin-8 to avoid roadblocks on microtubules — ANIRUDDHA MITRA^{1,2}, ●FELIX RUHNOW¹, and STEFAN DIEZ^{1,2} — ¹B CUBE - Center for Molecular Bioengineering, TU Dresden, Germany — ²Center for Advancing Electronics Dresden (cfaed), TU Dresden, Germany

During mitosis, kinesin-8 motors regulate spindle length based on their depolymerization activity at microtubule plus-ends. Remarkably, depolymerization occurs in a length-dependent manner, the underlying mechanism of which has been described by an antenna model where motors bind along the entire lengths of the microtubules and subsequently walk to the plus-ends relying on their extremely high processivity. During such long runs, motors in vivo are expected to frequently encounter roadblocks, such as microtubule-associated proteins. It has therefore been speculated that kinesin-8 motors may use protofilament switching on the microtubules lattice to bypass such obstacles. Whereas recent reports agree that kinesin-8, quite in contrast to kinesin-1, is indeed capable of switching protofilaments, it has not been clear if the underlying side-stepping occurs in a directionally-biased manner. To resolve this controversy, we tracked the 3D-motion of single QD-conjugated kinesin-8 motors stepping along freely suspended microtubules. We observed a spiraling motion with leftward pitches in the order of 1 μ m, indicating that the motors do switch protofilaments in a biased manner. Assays under limiting ATP conditions and in the presence of roadblocks reveal that side-stepping is a robust phenomena, which is not directly coupled to the forward stepping rate.

BP 5.6 Mon 16:30 HÜL 386

Controlling the translocation of polymers through by selective nanopore modifications — ●ADWAIT DATAR¹, UMBERTO MARINI BETTOLO MARCONI², SIMONE MELCHIONNA³, and MARIA FYTA¹ — ¹Institute for Computational Physics, University of Stuttgart, Germany — ²School of Sciences and Technologies, University of Camerino, 62032 Camerino Italy — ³ISC - CNR, Institute for Complex Systems, Consiglio Nazionale delle Ricerche, Università La Sapienza, P.le A. Moro 2, 00185 Rome, Italy

The focus of this work is the process of charged polymer translocation through nanometer-sized nanopores. These nanopores are placed in a salt solution and can electrophoretically thread charged molecules. Our aim is to control the polymer dynamics throughout the translocation process and optimize the translocation speed. In order to achieve this, we attempt to tune the specific polymer-nanopore interactions by changing the pore characteristics. Specifically, we investigate the influence of a variety of different patterns of the charge distribution within the nanopore on guiding the polymer dynamics. Our work is based on a multiscale computational approach seamlessly coupling the dynamics of the polymer with an electrokinetic description for the salt solution in which the translocation process takes place. Our results are evaluated with respect to different sensors characteristics in the nanopore,

the flow patterns within the pore, and the velocity of the translocated polymer, as well as the cooperativity of solution, flow, and nanopore. We discuss the impact of our work in selectively engineering nanopores for single molecule experiments and DNA sequencing.

BP 5.7 Mon 16:45 HÜL 386

Single-Molecule Biophysics: The Challenge of Reproducibility — ●FABIAN CZERWINSKI¹, LENE ODDERSHEDE², and OLIVER OTTO¹ — ¹Universität of Greifswald, Greifswald, Germany — ²Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark

Resolving dynamic processes within inherently fluctuating systems often sets the biophysical agenda to employ novel analysis methods as well as to develop cutting-edge technology. Thus, single-molecule experiments and their vastly evolving data are faced with the scientific demands of consistency and reproducibility. This requirement is reinforced as single-molecule biophysics assesses more and more tasks of quantitative biology.

Here, we discuss three measures that allow for consistent comparison of single-molecule data: i) Bayesian likelihood, ii) Allan variance, and iii) editorial standardization. In a retrospective way, we review examples of force spectroscopy and super-resolution fluorescence microscopy. The examples are confronted with NATURE's editorial checklist for life sciences articles [1, 2]. We argue that the further growing interest in biophysical single-molecule data mandates rigorous, transparent and comprehensive effort from scientists and institutions.

[1] Reducing our irreproducibility. NATURE 2013, 496:398

[2] <http://www.nature.com/authors/policies/checklist.pdf>

BP 5.8 Mon 17:00 HÜL 386

Analytical catch-slip bond model for arbitrary forces and loading rates — ●JAKOB TÓMAS BULLERJAHN and KLAUS KROY — Universität Leipzig, Institut für Theoretische Physik, Leipzig, Germany

Some biological bonds exhibit a so-called catch regime, where the

bond strengthens with increasing load. We build upon recent advances in slip-bond kinetics [1] to develop an analytically tractable, microscopic catch-slip bond model [2]. To facilitate the analysis of force-spectroscopy data, we calculate the bond's mean lifetime and the rupture-force distribution for static loading and linear force ramps. Our results are applicable for arbitrary forces and loading rates, covering the whole range of conditions found in experiments and all-atom simulations. A generalization to account for force transducers of finite stiffness is also provided.

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

[2] J. T. Bullerjahn & K. Kroy, *PRE* **93**, 012404 (2016).

BP 5.9 Mon 17:15 HÜL 386

In vitro study of the regulation and the mechanism of the MKLp2 mitotic kinesin — ●AMNA ABDALLA MOHAMMED KHALID¹, I-MEI YU², CHRISTOPH SCHMIDT¹, and ANNE HOUDUSSE² — ¹Third Institute of Physics - Biophysics, Georg August University, Germany — ²Institut Curie Paris, France

The mitotic kinesin-like protein 2 (MKLp2), is a N-terminal kinesin of the Kinesin-6 family with unique features. It plays critical roles for the metaphase to anaphase transition and for cytokinesis in cell division. Previous studies have shown that MKLp2 inhibitors reduced the cell growth in pancreatic adenocarcinoma cells and can kill tumour stem cells. On the other hand, MKLp2 is overexpressed in variety of cancers. Therefore it is considered as a good candidate for new cancer therapies. High-resolution single-molecule studies are fundamental to understand the regulation and mechanism of MKLp2 at the molecular level. We are studying truncated MKLp2 constructs to explore basic motor functions and to understand the influence the domains on motor properties. Here I present single-molecule studies of a dimeric truncated MKLp2, in vitro using total internal reflection fluorescence microscopy (TIRFM). Our data confirm that the dimeric truncated MKLp2 motors are active. A conspicuous feature of this motor is its microtubule bundling activity.

BP 6: Cell Mechanics (Joint Session BP/DY)

Time: Monday 15:00–16:45

Location: SCH A251

Invited Talk

BP 6.1 Mon 15:00 SCH A251

Quantifying and modelling active motion in biological systems — ●TIMO BETZ — Institute of Cell Biology, ZMBE, University Münster, Germany

Living biological systems are continuously reorganizing their structure to perform their function. The mechanical activity plays here an important role, as the constant generation of forces drives fluctuations as well as controlled motion of intracellular particles, membranes and cells. From a physical point of view, this active motion drives the system far away from thermodynamic equilibrium, which can be measured as a violation of equilibrium quantities such as the fluctuation dissipation theorem.

Quantifying the out-of-equilibrium components provides the possibility to model the active molecular processes. We measure the energy and the forces actively applied on membranes as well as cellular granules and model these with an active Langevin approach. By comparing the predictions of forces and mechanics with the measurement of the fluctuations and viscoelastic properties we can extract molecular parameters from mesoscopic measurements. This gives timescales and chemical reaction parameters such as forces, binding states and velocities of the underlying proteins using a simple average measurement of the active motion.

BP 6.2 Mon 15:30 SCH A251

Feeling for Phenotype: Real-Time Deformability Cytometry for Label-Free Cell Functional Assays — ●OLIVER OTTO^{1,2,3}, PHILIPP ROSENDAHL^{1,3}, MAIK HERBIG¹, ANGELA JACOBI^{1,4}, MARTIN KRÄTER^{1,4}, NICOLE TÖPFNER¹, MARTA URBANSKA¹, MARIA WINZI¹, KATARZYNA PLAK¹, ALEXANDER MIETKE⁵, CHRISTOPH HEROLD³, DANIEL KLAUE³, EDWIN CHILVERS⁶, REINHARD BERNER⁴, MARTIN BORNHÄUSER⁴, and JOCHEN GUCK¹ — ¹Technische Universität Dresden, Dresden, Germany — ²Universität Greifswald, Greifswald, Germany — ³Zellmechanik Dresden, Dresden, Germany — ⁴Universitätsklinikum Dresden, Dresden, Germany — ⁵Max-Planck-Institut für Molekulare Zellbiologie und Genetik, Dresden, Germany

— ⁶University of Cambridge, Cambridge, United Kingdom

By real-time deformability cytometry (RT-DC), we have introduced a high-throughput method for continuous mechanical single-cell classification of heterogeneous cell populations at rates of several hundred cells per second. Here, we demonstrate the extension of this method towards a multi-parameter biological assay where phenotyping is based on quantitative image analysis. Performing RT-DC on whole blood we highlight its potential to identify subsets in heterogeneous cell populations without any labelling and extensive sample preparation. We also demonstrate its capability to detect lineage-, source- and disease-specific mechanical phenotypes in primary human hematopoietic stem cells and mature blood cells. In summary, RT-DC enables marker-free, quantitative phenotyping of heterogeneous cell populations with a throughput comparable to standard flow cytometry.

BP 6.3 Mon 15:45 SCH A251

Light-driven intracellular flow perturbations to unravel transport processes in cells and developing embryos — ●MATTHÄUS MITTASCH^{1,4}, PETER GROSS², MICHAEL NESTLER³, MATHIAS MUNDER¹, AXEL VOIGT^{3,4}, SIMON ALBERTI¹, STEPHAN GRILL^{2,4}, and MORITZ KREYSING^{1,4} — ¹MPI-CBG, Dresden — ²Biotechnology Center, Technische Universität Dresden — ³Department of Mathematics, TU Dresden — ⁴Center for Systems Biology Dresden

Throughout the last decades, advances in molecular and cell biology have allowed for a precise control of molecular reactions inside cells. The complex interplay of molecular reactions with physical transport processes was suggested to control the spatiotemporal organization of cells and developing embryos. However, unravelling the function of physical transport during morphogenesis and cellular homeostasis remains a challenge due to the lack of suitable perturbation methods for in vivo systems. Here, we exploit thermoviscous pumping (Weinert & Braun) to perform light-driven intracellular flow perturbations. Thereby, we show the causal implications of intracellular flows during PAR polarization of the *C. elegans* zygote. Finite element simulations in 3D of the Stokes equation with time-dependent source terms reca-

pitulated the experimental findings nearly identical. Furthermore, we utilize flow perturbations for active and probe-free micro-rheology measurements in yeast cells. Hence, we revealed a fluid-to-solid transition of the cytoplasm in energy-depleted cells. Light-driven intracellular flow perturbations lay the foundation to dissect the design principles of transport-dependent organization of living systems.

BP 6.4 Mon 16:00 SCH A251

Biophysics of neutrophil extracellular trap (NET) formation — •DANIEL MEYER¹, ELSA NEUBERT^{1,2}, ANJA KWACZALA-TESSMANN², SUSANNE SENER-SANDER², MICHAEL P. SCHÖN², LUISE ERPENBECK², and SEBASTIAN KRUS¹ — ¹Institute of Physical Chemistry, Göttingen University, Germany — ²Dermatology, Venerology and Allergology, University Medical Center Göttingen, Germany

Neutrophils are the most abundant type of immune cells in the human blood system and central for immune defense. Recently, it was found that neutrophils and other cells are able to catch and kill pathogens by expelling a fibril network made from their own DNA (neutrophil extracellular traps, NETs). During this process (NETosis), a massive rearrangement of the materials inside the cell takes place which is still poorly understood. Our results show that NETosis can be divided into three distinct phases. The chromatin decondenses out of the disassembled nucleus until it fills the complete cell lumen. Simultaneously, the cytoskeleton decomposes and the cells become softer. In the final phase the cell body rounds up yet stays adherent to the surface, and the cytoplasmic membrane ruptures releasing the NET to the extracellular space. Using Atomic Force Microscopy (AFM) together with fluorescence microscopy methods, we demonstrate how the NETs-release is temporarily regulated by chromatin swelling, changes within the cytoskeletal components as well as the mechanical properties of the cell.

BP 6.5 Mon 16:15 SCH A251

Building up and force probing the microtubule cytoskeleton from scratch — •MATTHIAS KOCH^{1,2} and ALEXANDER ROHRBACH¹ — ¹IMTEK, University of Freiburg, Germany — ²Lewis-Sigler Institute, Princeton University, USA

Eukaryotic cells are exposed to and driven by a large variety of forces or mechanical stimuli on a brought range of times scales. Due to their mechanical rigidity, microtubules are able to transport such stimuli enabling instantaneous mechanical integration of distant regions of a cell. However, only equilibrium mechanical properties of single micro-

tubules have been characterized so far. We fill this void by using an in vitro bottom-up approach to determine the frequency response of single microtubules and small networks thereof that mimic the basic cytoskeletal structure. We combine a new scanned darkfield imaging technique with multiple time-shared optical tweezers to flexibly construct and force probe such networks with a well-defined, user-selected geometry over a broad frequency range. We report on a length dependent stiffening of individual microtubules above a physiologically relevant transition frequency between 1-30Hz due to the excitation of higher order bending modes which displays a mechanical high-pass filter with a tunable cutoff frequency. Furthermore, we identify and relate different mechanical responses of different network geometries to different functions inside the cell. The mechanistic comparison of basic network geometries to the known cytoskeletal topologies and the general function of different cell lines will substantially strengthen our understanding of the function and structure of the cytoskeleton.

BP 6.6 Mon 16:30 SCH A251

Theory for forces that slide k-fibers and bridging microtubules to move chromosomes — •AGNEZA BOSILJ¹, KRUNO VUKUSIC², RENATA BUDA², ANA MILAS², IVA TOLIC², and NENAD PAVIN¹ — ¹Department of Physics, Faculty of Science, University of Zagreb, Bijenicka cesta 32, 10000 Zagreb, Croatia — ²Division of Molecular Biology, Ruder Boskovic Institute, Bijenicka cesta 54, 10000 Zagreb, Croatia

During cell division forces on chromosomes are exerted by k-fibers, bundles of microtubules which extend from the opposite spindle poles and attach to chromosomes. Recently we have shown that in metaphase microtubules which extend between sister chromatids, termed bridging fibers, bridge sister k-fibers and balance the tension between sister chromatids [Kajtez et al, Nat Commun 2016]. However, a theoretical description of forces driving chromosome segregation in anaphase is still missing. Here we introduce a theoretical model which includes motor proteins that connect antiparallel microtubules, as well as passive cross-linkers that connect parallel microtubules. Our model shows that motor proteins generate forces that slide antiparallel bridging microtubules apart, thereby sliding sister k-fibers apart. This implies that forces at chromosomes are balanced by bridging fibers, which we confirmed experimentally by laser ablation of (i) k-fibers close to the spindle pole and (ii) bridging fibers. Our model also predicts that non-motor cross-linkers in regions of parallel overlap allow for movement of k-fibers and chromosomes together with the bridging fiber.

BP 7: Posters - Mechanics and Dynamics of 3D Tissues (Focus Session)

Time: Monday 17:30–19:30

Location: P3

BP 7.1 Mon 17:30 P3

Contractile performance of cardiac tissues under synchronized mechanical and electrical stimulation — •DOLF KAH¹, INGO THIEVESEN¹, CLAIRE AMADO², JULIA KRAXNER¹, MARINA SPÖRRER¹, SANDRA WIEDENMANN¹, WOLFGANG GOLDMANN¹, and BEN FABRY¹ — ¹Department of Physics, Biophysics Group, Friedrich-Alexander-University Erlangen-Nuremberg, D-91052, Erlangen, Germany — ²Laboratoire de Physique de la Matière Condensée, URA 792 du CNRS, Collège de France, 75231 Paris Cedex 05, France

In vitro engineered cardiac tissue grafts are of growing interest either as substitutes for scarred myocardial tissue after infarction or chronic cardiomyopathies, or as a drug testing platform. To investigate how mechanical and electrical conditioning influences the maturation and contractility of engineered cardiac tissue, we developed a stretchable and electrically paceable bioreactor consisting of an array of 4x2 mm microwells with two elastic pillars that serve as force sensors. Cardiac cells mixed with monomeric collagen are added to the microwells and, after polymerization and compaction of the collagen matrix, form an aligned tissue that spans between the pillars. Mechanical stretching with a linear stepper motor, electrical pacing with carbon electrodes, and microscopic imaging of the tissue is synchronized by a microcontroller, allowing us to study isotonic, isometric or eccentric contractions for various pacing protocols. Maximum contractile forces and electrical field strength threshold increased with increasing isotonic load, or pillar stiffness, indicating a pronounced mechanical responsiveness of the cardiomyocytes during the tissue maturation process.

BP 7.2 Mon 17:30 P3

Morphogenesis control using mechanical stress — •JASON KHADKA, JEAN-DANIEL JULIEN, and KAREN ALIM — Max Planck Institute for Dynamics and Self-Organization

A major question in developmental biology is to understand how reproducible shapes arise from the collective behaviour of individual cells. Can mechanical interaction of cells within a tissue counteract randomness? We address this question in the shoot tip of plants. It has been shown that cortical microtubules in plant cells respond to mechanical stresses within a tissue. Cortical microtubules pattern down cell wall mechanics and thus mechanical stresses feed back on the mechanics of cell wall and cell growth. Here, we study how this mechanical feedback counteracts randomness in cell growth and thus gives rise to robust shape formation in the shoot tip. We present a three dimensional vertex model of plant tissue growth. Evaluating this model at different mechanical feedback strengths we assess the role of mechanics for reproducible three-dimensional shape formation.

BP 7.3 Mon 17:30 P3

Dynamics of fluid pumping through a thick epithelium — •NILADRI SARKAR¹, JACQUES PROST^{2,3}, and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems — ²Institut Curie/CNRS — ³MBI, National University of Singapore

We study the dynamics of a thick epithelial tissue which pumps an interstitial fluid. We consider a tissue with average cell polarity normal to the tissue layer. The cell pumps fluid against a pressure difference. Using a two-component hydrodynamic continuum theory, we study the dependence of tissue stress, cell velocity and fluid flow on the ex-

ternal fluid pressure and the cell pumping activity. We find that the existence of steady states depend strongly on the external pressure difference, the pumping activity and the properties of the interface separating the tissue from the surrounding fluid.

BP 7.4 Mon 17:30 P3

Non-Linear Compliance of Elastic Layers to Indentation — ●ADRIAN FESSEL and HANS-GÜNTHER DÖBEREINER — Universität Bremen, Bremen, Deutschland

We present a single-exponent scaling model for description of large, non-linear deformations in elastic layers, based on analytical analyses and approximations of asymptotic behavior for small and large indentation upon variation of layer thickness. For very thin layers, the scaling model arises as an extension of an analytically exact model for small indentation. In conjunction with data from finite element simulations, investigation with the model leads to the conclusion that when drafting experiments, it is essential to recognize that separation of non-linear material properties from effects of geometrical confinement is conveniently possible only with thin layers. Furthermore, partition of strain-energy into parts associated with specific asymptotic regimes motivates introducing a scalar which we define in analogy to Poisson's ratio but for the ratio of principal strains in the layer geometry. Numerically, we find quantitative agreement between the scalar and the exponent characterizing the scaling model in the case of a thick, linear-elastic layer, and qualitative agreement in the non-linear case. We conjecture this effect to be due to higher-order contributions of geometrical confinement present even in linear-elastic settings.

BP 7.5 Mon 17:30 P3

Time-dependent tension drives collective cell migration in zebrafish — ●BERNHARD WALLMEYER¹, SARAH TRINSCHKE², SARGON YIGIT¹, UWE THIELE², and TIMO BETZ¹ — ¹Institute of Cell Biology, Center for Molecular Biology of Inflammation, Von-Esmarch-Str. 56, 48149 Münster, Germany — ²Institute for Theoretical Physics, University of Münster, 48149 Münster, Germany

Collective cell migration is a fundamental process during embryogenesis and adult life. An in vivo model for collective cell migration is epiboly. Epiboly is an event occurring in early zebrafish development, where the cells that initially form a cluster at one pole of the spherical yolk, spread towards the other pole in a continuous movement to eventually fully cover the yolk. Inspired by the physics of wetting we determine the contact angle between the cells and the yolk during epiboly. Similar to the situation of a liquid drop on a surface there are three interfaces, namely, between cells-medium, yolk-cells and yolk-medium that carry mechanical tension. By assuming that the origin of interface tension lies in cell-cell adhesion we propose a time-dependent tension due to the dynamics of adhesive contacts. Using the classical physics of wetting this model accurately characterizes the contact angle measured in our experiments. We are thus able to describe the fundamental and complex developmental mechanism of morphogenesis onset by three main parameters – the static tension strength α , the

offset angle δ and the time scale λ .

BP 7.6 Mon 17:30 P3

A new method for analyzing high-frequency microrheology data — ●KENGO NISHI¹, MARIA KILFOIL², FRED MACKINTOSH³, and CHRISTOPH SCHMIDT¹ — ¹Goettingen University, Goettingen, Germany — ²University of Massachusetts Amherst, Massachusetts, USA — ³Rice University, Houston, USA

Passive microrheology is an experimental technique used to measure the mechanical response of materials from the fluctuations of micron-sized beads embedded in the medium. In one common approach, one uses the fluctuation-dissipation theorem to obtain the imaginary part of the material response function from the power spectral density of bead displacement fluctuations, while the real part of the response function is calculated using a Kramers-Kronig integral. The high-frequency cut-off of this integral strongly affects the real part of the response function in the high frequency region. To moderate this high-frequency cut-off, we recently proposed a new analysis method for passive microrheology by using the fluctuation-dissipation theorem in time domain, i.e., Fourier transforming the time derivative of the mean squared displacement or the auto correlation function. To see the validity of this method, we conducted one- and two-particle microrheology experiments, and the systematic error analysis by synthetic data.

BP 7.7 Mon 17:30 P3

Organs-on-a-chip: Microphysiological platforms as in vitro models of cardiac and adipose tissue — ●OLIVER SCHNEIDER, JULIA ROGAL, CHRISTOPHER PROBST, and PETER LOSKILL — Department of Cell and Tissue Engineering, Fraunhofer Institute for Interfacial Engineering and Biotechnology IGB, Stuttgart, Germany

Drug discovery and development to date relies on animal models, which are useful, but fail to resemble human physiology. The discovery of human induced pluripotent stem (iPS) cells has led to the emergence of drug screening using human disease-specific organ-models. One promising approach are microfluidic devices, simulating 3D tissue structure and function. Using microfabrication techniques we have developed two microphysiological platforms (MPSs) incorporating in vitro models of human cardiac and adipose tissue. Both MPSs consist of three functional components: a tissue culture chamber mimicking organ-specific geometrical in vivo properties; 'vasculature-like' media channels enabling a precise delivery of compounds (nutrients, drugs); *endothelial-like* barriers protecting the tissues from shear forces while allowing diffusive transport. We developed and deployed a novel biocompatible membrane as barrier, matching the desired organ-specific properties by varying its porosity. Both organ-chips manage to create physiological micro-tissues that are viable and functional for multiple weeks. The developed chips are the first systems that combine human genetic background, physiologically relevant tissue structure and 'vasculature-like' perfusion. Both MPSs are extremely versatile and can be applied for drug toxicity screening and mechanistic research on tissue dynamics.

BP 8: Posters - Bioimaging and Spectroscopy

Time: Monday 17:30–19:30

Location: P3

BP 8.1 Mon 17:30 P3

Adjustment of pulsed laser radiation for stroboscopic experiments — ●BENEDIKT KAMP¹, TOBIAS LÖFFLER¹, JULIA KRISTIN², and MATHIAS GETZLAFF¹ — ¹Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf — ²Hals-Nasen-Ohrenklinik, Universitätsklinikum Düsseldorf

This contribution aims to adjust the pulsed laser radiation of a fluorescence microscope depending on an electrical voltage. Through this a stroboscopic effect can be achieved and the periodic movement of an observed probe can be researched in even more detail. The described microscope already has an integrated array of shutters, which are operated by TTL-signals. First the incoming alternating voltage is regulated in amplitude and filtered. The resulting sine wave is converted into a rectangular voltage of 5V by a comparator, so that it can be used as a TTL-signal. This signal runs through monostable multivibrators, in which the time ratio of the logic "high" and "low" can be changed with external potentiometers without changing the frequency. It results in a device that can change the time length and phase of the "high", in

order to be able to control the shutters accordingly. Furthermore the device possesses overvoltage protection, so that the microscope cannot suffer damage. In future, for even better usage of the stroboscopic effect, a counter can be implemented for limiting the frequency the shutters have to work at.

BP 8.2 Mon 17:30 P3

Luminescence characterisation of fluorescent Nanodiamond — ●FREDERIKE ERB¹, BORIS NAYDENOV², ULLA NOLTE¹, FEDOR JELEZKO², and KAY-E. GOTTSCHALK¹ — ¹Institute of Experimental Physics, Ulm University, Germany — ²Institute of Quantum Optics, Ulm University, Germany

Fluorescent nanodiamonds (FNDs) offer various new imaging and metrology approaches, especially in the life sciences. Nanodiamonds containing nitrogen-vacancy centers as fluorophores emit light in the near-infrared window of bioimaging [1]. Their luminescence properties depend on the environment and thus FNDs can not only be used for bioimaging but also find an application as part of various biosensors. In contrast to dye molecules, FNDs neither blink nor bleach.

Moreover, as they are biocompatible, non cytotoxic and do not affect proliferation, they can be used for longtime experiments in live cells [1].

We present luminescence properties of FND and their performance as markers in cells.

References:

[1] Hsiao, Wesley Wei-Wen; Hui, Yuen Yung; Tsai, Pei-Chang; Chang, Huan-Cheng (2016): Fluorescent Nanodiamond: A Versatile Tool for Long-Term Cell Tracking, Super-Resolution Imaging, and Nanoscale Temperature Sensing. In: Accounts of chemical research 49 (3), p. 400-407.

BP 8.3 Mon 17:30 P3

Staining of squamous cell carcinoma cells and dysplastic oral keratinocytes — •JAN LIETZ¹, MAJA STRUGACEVAC¹, AYSE ALMACI¹, JULIA KRISTIN², MARCEL GLAAS², JÖRG SCHIPPER², and MATHIAS GETZLAFF¹ — ¹Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf — ²Hals-Nasen-Ohrenklinik, Universitätsklinikum Düsseldorf

The goal of this research is to investigate the differences between oral carcinoma cells (UD-SCC-1) and dysplastic oral keratinocytes (DOK). In order to obtain more information about cell properties confocal laser scanning microscopy is used.

The cell membrane as well as the cytoskeleton, mitochondria and nucleus of both, squamous cell carcinoma cells and oral keratinocytes, were stained with CellMask green, SiR-tubulin and SiR-actin, Mito-Tracker orange and Hoechst 33342, respectively.

This contribution focuses on combining two, three and four different fluorescent dyes and optimizing the staining process accordingly. In addition, we acquired z-stacks and present reconstructed 3D images for each of the two cell lines.

BP 8.4 Mon 17:30 P3

An integrated platform for rapid semi-confocal imaging and spatially resolved fluctuation microscopy — •ADAL SABRI, ANDREAS VERES, and MATTHIAS WEISS — Experimental Physics 1, University of Bayreuth

Fluorescence imaging is a key method to study the dynamics of biological specimen. Due to the common trade-off between spatial and temporal resolution, rapid high-quality data acquisition often comes at the cost of complex and technically challenging methods.

We report on a technique that increases the temporal resolution of image acquisition by more than an order of magnitude as compared to standard confocal microscopy approaches. Large areas (up to 450 μm edge length) can be imaged rapidly with a resolution close to the diffraction limit. To this end, multiple cylindrical lenses shape a thin light sheet so that effectively only a line within a thin specimen (oriented perpendicular to the optical axis) is illuminated. This line of illumination is scanned in one spatial direction with a Galvo mirror. A slit aperture in the detection path yields an axial discrimination, thus creating a semi-confocal setup.

Swift switching to a second excitation/detection path allows for alternating between advanced rapid image acquisition and two-point fluctuation spectroscopy on smaller scales. The setup allows one to correlate fluorescence fluctuations at two selectable, spatially separated foci over time to determine local transport coefficients, hence supports the combination of a rapid imaging and the analysis of dynamic intracellular events on a subcellular scale.

BP 8.5 Mon 17:30 P3

Photothermal detection of single gold nanoparticles in living fibroblasts — •ALICE ABEND, ROMY SCHACHOFF, and FRANK CICHOS — Universität Leipzig

Live cell bioimaging allows for the observation of cellular processes and their dynamics and provides insight into functions of cells such as metabolism, replication and movement. Modern nanotechnology enables manufacturing of nanometer sized objects with tailored optical properties and specific functionalization which turns them into ideal optical probes for several imaging techniques. We deliver gold nanoparticles (AuNPs) to the cells (NIH/3T3) as they are photostable and allow for long term imaging and seem to be less toxic to living organisms in comparison to semiconductor quantum dots. Our imaging method, photothermal optical microscopy, provides sensitive detection of AuNPs and is therefore suitable to prove the presence of AuNPs in the fibroblasts' interior. As photothermal microscopy is based on heating of the contrast agent, AuNPs can double as heat sources for inducing local intracellular temperature fields which could be useful to manipulate cellular functions such as protein synthesis, metabolism

processes and cell motility.

BP 8.6 Mon 17:30 P3

Quantitative Phase Microscopy with a Single Shot Measurement Technique — •TOBIAS NECKERNUSS¹, JONAS PFEIL¹, CHRISTOPH KOCH², and OTHMAR MARTI¹ — ¹Institute of Experimental Physics, Ulm University — ²Department of Physics, Humboldt University of Berlin

In cellular biophysics, there are numerous interesting questions concerning the height of cells under different conditions. However, using classical microscopy techniques recovering the height of an object is related to determine the phase change of the light and is a tough task. Most of the common phase retrieval methods require a stack of images and hence are limited to nonmoving cells since it takes several seconds to capture all images. A second possibility is interferometry where the most critical point is the mechanical stability of the setup so that it is often not applicable in normal laboratories. We introduce an inline holography setup where we use the transport of intensity equation (TIE) to recover the optical path length of the sample from two differently focused pictures. The pictures are taken simultaneously which means that camera speed is the only limitation and therefore changes up to 100Hz can be resolved. Several refinements had to be applied to the reconstruction algorithm in order to get it working since it was originally designed for electron microscopy using more than two pictures. We use a partially coherent LED lamp to avoid common artifacts emerging from laser illumination. Data of polystyrene beads on surfaces as well as of adherent cells in medium is shown. We will compare the reconstructed height with the real ones measured by AFM.

BP 8.7 Mon 17:30 P3

Fluorescent Gold Nanoparticles on/in Cells Visualized by Fluorescence-Lifetime Imaging Microscopy — •MARINA MUTAS, TIM HADLER, CHRISTIAN STRELOW, TOBIAS KIPP, and ALF MEWS — Institut für Physikalische Chemie, Universität Hamburg

Fluorescence-Lifetime Imaging Microscopy (FLIM) is a powerful method to discriminate emitters with different fluorescence lifetimes. Gold nanoclusters with mercaptoundecanoic acid as stabilizing ligand (MUA-AuNCs) show a fluorescence emission that peaks at a wavelength around 525 nm with decay times longer than 100 ns. The autofluorescence of biological cells is in the same wavelength region but the fluorescence decay time, which is about 3 ns, is much shorter. We are able to specifically biofunctionalize these MUA-AuNCs with an aptamer which binds to a receptor expressed on the cells' membrane. To get an image of the whole cell we use cross-sectional FLIM scans in axial direction at different heights through the cell. With this technique we are able to visualize specifically bound aptamer-MUA-AuNCs on the cells' membrane using three FLIM methods and reflection images.

BP 8.8 Mon 17:30 P3

Robust control of spins in nanodiamonds in complex environments — •PHILIPP KONZELMANN¹, TORSTEN RENDLER¹, ANDREA ZAPPE¹, SEBASTIAN ZAISER¹, MATTHIAS WIDMANN¹, SANG YUN LEE², PHILIPP NEUMANN¹, JÖRG WRACHTRUP¹, and FLORIAN DOLDE³ — ¹3rd Institute of Physics, IQST and SCOPE, Stuttgart — ²Korea Institute of Science and Technology — ³DNT Inc.

Nanodiamonds (ND) had been shown to be of excellent biocompatibility and additionally can host color centers. One of the most prominent representatives is the so-called nitrogen vacancy center (NV) that features, due to its unique spin system, the intrinsic capacity to sense for example magnetic or electric fields, pressure and temperature [1]. Furthermore, intense progress in functionalization of ND surface in past years promises a manifold of different applications in life science [2]. However, keeping control of the NV spin sublevel, especially in complex environments, remains challenging. If a ND changes for example its orientation, variations in excitation strength and shifts of the NV spin transitions are expectable. To overcome this obstacle several techniques had been developed exhibiting a certain robustness against such fluctuations [3,4,5]. To this end, we utilize optimum control theory in combination with so-called cooperative pulse schemes [5]. In our work, we present a systematical study exploring the efficiency of such pulses for NVs in NDs. [1] R. Schirhagl et al., *ARPC* 65: 83-105 (2014) [2] D.G. Lim et al., *Int. J. Pharm.* 514: 41-51 (2016) [3] M. Garwood et al., *JMR.* 153: 155-177 (2001) [4] A. M. Souza et al., *PRL* 106: 240501 (2011) [5] M. Braun et al., *NJP* 16 (2014)

BP 8.9 Mon 17:30 P3

Improving tissue transparency by combinatorial expression of

crystallins — ●SAMET KOCABEY, HEIKE PETZOLD, KAUSHIKARAM SUBRAMANIAN, and MORITZ KREYSING — MPI-CBG, Dresden, Germany

The optical access to biological tissues has long been a goal for scientists to get physiological information. Most tissues show poor optical quality due to the light scattering emerging from heterogeneous refractive index distribution. There are few exceptions including the eye-lens where the cells in the light path leading to the retina have evolved to be transparent that allows minimal light scattering before sensed by retina.

The lens fiber cells are largely comprised of crystallin proteins assembled into a highly ordered macro-structure essential for tuning the refractive index and thus lens transparency. The crystallin proteins have chaperone-like activity and mutations in crystallins cause protein aggregation that leads to cataract formation. However, the precise mechanism by which crystallin proteins maintain the lens transparency is poorly understood. In this study, we aim to find the genetic determinants of lens tissue transparency and ultimately enhance the optical properties of other tissues by combinatorial expression of crystallins and crystallin-related proteins in cells from different tissues.

BP 8.10 Mon 17:30 P3

Beyond the beaten track: Pushing the limits of fluorescence microscopy — ●HANNAH S. HEIL¹, BENJAMIN SCHREIBER¹, SI-YUN LIU¹, MARTIN KAMP², MARKUS SAUER³, and KATRIN G. HEINZE¹ — ¹Rudolf Virchow Center, Research Center for Experimental Biomedicine, University of Würzburg — ²Technische Physik, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — ³Department of Biotechnology and Biophysics, Biozentrum, University of Würzburg

Combining optical with plasmonic approaches opens exciting perspectives for fluorescence microscopy: So called surface plasmons in specially designed nanostructures can generate extremely high photon densities in a nanoscopic volume that is much lower than the Abbe criteria usually allows. The interaction of fluorophores with plasmonic surfaces enables amplified fluorescence, increased photostability and distance dependent dynamical and spectral emission shifts. All of these effects are very welcome in pushing the two fundamental limits of fluorescence microscopy: contrast and resolution, particularly in the axial dimension. The strength of the approach is that - except for special cover glasses - no special microscope setup is required. Here we show that biocompatible plasmonic nanostructures fabricated on microscopy slides can improve the resolution of the super-resolution technique dSTORM by boosting the signal and thus the localization precision by a factor of two. Finally we give an outlook on how the plasmonic effects could allow 3D reconstructions of molecular distributions and interactions in live cells with nanometer precision.

BP 8.11 Mon 17:30 P3

GPU-based 3D statistical multi-resolution estimators for image reconstruction — ●STEPHAN KRAMER¹, JOHANNES HAGEMANN², and SIMON STEIN³ — ¹Fraunhofer ITWM, Kaiserslautern — ²Institut für Röntgenphysik, Universität Göttingen — ³III. Institut für Physik, Universität Göttingen

We extend our previous work [1] on statistical multiresolution estimators (SMRE) to 3D. SMREs are a recent development for the deconvolution of noisy images. Their main feature is the replacement of unphysical regularization parameters by only one which represents the probability that the reconstructed image fulfills the hypothesis test for being the correct one. Their convergence does not degrade with increasing noise. In each iteration step of an SMRE the reconstructed noise is tested whether it obeys a pre-defined distribution on all subsets of the input image. Since the number of possible subsets of an image grow exponentially with its size SMREs are computationally expensive. Reasonable runtimes can only be achieved by a careful parallelization [1] and a proper choice of the image subsets on which the statistical tests are performed. Our implementation is based on our SciPAL library [2] and CUDA. As sample application we discuss preprocessing the time series needed in super-resolution optical fluctuation imaging (SOFI) methods for 3D stacks of images from fluorescence microscopy.

[1] Kramer, S.C., Hagemann, J., Künneke L. and Lebert, J., 2016. SIAM Journal on Scientific Computing, 38(5), pp.C533-C559.

[2] Kramer, S.C. and Hagemann, J., 2015. ACM TOPC, 1(2), p.15.

BP 8.12 Mon 17:30 P3

Network properties and dynamics of the endoplasmic reticulum — ●LORENZ STADLER, KONSTANTIN SPECKNER, and MATTHIAS

WEISS — University of Bayreuth, Bayreuth

The endoplasmic reticulum (ER) is an essential cellular organelle that assumes the shape of an extended network of interconnected membrane tubules and sheets. Being responsible for crucial cellular functions, e.g. protein folding and lipid synthesis, malfunctions of the ER are linked to severe diseases. To gain insights into the dynamic ER morphogenesis, we have used fluorescence imaging with high spatiotemporal resolution. ER images taken in cells at different states were skeletonized in a custom-made procedure, hence reducing the organelle's shape to planar graphs composed of edges and nodes. These graphs were analyzed via a set of network measures to quantify topological and geometrical features. Moreover, the motion of network nodes as well as the motion of membrane domains on the ER were analyzed in the presence and absence of cytoskeletal elements. These data highlight the role of active fluctuations for the ER's dynamic morphogenesis in the crowded interior of living cells.

BP 8.13 Mon 17:30 P3

Direct characterization of the evanescent field in objective-type total internal reflection microscopy — ●CHRISTIAN NIEDERAUER, PHILIPP BLUMHARDT, JONAS MÜCKSCH, MICHAEL HEYMANN, ARMIN LAMBACHER, and PETRA SCHWILLE — Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Martinsried, Germany

Total internal reflection fluorescence microscopy (TIRFM) is a powerful tool to study the interaction of molecules in close proximity to a surface. Usually, the axial TIRFM excitation profile is assumed to be a single-exponential with a characteristic penetration depth. Exploiting the full potential of TIRFM data requires a precise knowledge of the excitation profile. In a first approximation, the depth of the evanescent field can be estimated from geometrical considerations. However, significant deviations from the assumed theoretical single-exponential profile have been observed in objective-type TIRFM [1]. Available methods to characterize the precise shape of the axial excitation profile require special instrumentation [2,3], sophisticated sample preparation [3] or are not applicable at typical refractive indices [1]. Here, we present our work on a new approach to quantify the axial TIRFM excitation profile. Our goal is to fabricate a robust and user-friendly micropatterned slide for in situ calibration.

[1] A.L. Mattheyses, D. Axelrod, J. of Biomed. Optics **11**, 140060 (2006).

[2] Sarkar, A., et al., PNAS **101**, 12882–12886 (2004).

[3] Gell, C., et al., J. of Microscopy **234**, 38–46 (2009).

BP 8.14 Mon 17:30 P3

PDMS micro-moulds as test samples for Scanning Ion Conductance Microscopy — ANNELIE MARX¹, ●REGINA LANGE¹, HENRIKE REBL², BARBARA NEBE², INGO BARKE¹, and SYLVIA SPELLER¹ — ¹University of Rostock, Institute of Physics, 18059 Rostock — ²University Medical Center Rostock, Dept. of Cell Biology, 18057 Rostock

Scanning Ion Conductance Microscopy (SICM) is a less known scanning probe method that uses a nanopipette with an opening diameter below 100 nm as probe. The topography of a soft non-conducting material placed in a (conducting) liquid is measured on the nanoscale, avoiding direct forces between the sample and the probe. Hence, SICM represents a good choice for in vitro high resolution imaging of living cells in physiologic medium. Therefore, among others, the influence of the substrate structure and of potential, or of light on the cell behaviour can be studied in real time.

For testing the SICM method and for making available prospective substrates for cell adhesion experiments we prepare PDMS (polydimethylsiloxane) micro-moulds of various samples. For instance moulds of dry etched glass structures exhibiting equidistant grids and pillars of different aspect ratios with vertical side walls are produced. To compare the replica with their original both were studied by AFM. A decent reproduction quality was obtained with 2 micrometer deep grooves and unity aspect ratio.

BP 8.15 Mon 17:30 P3

Investigating the temperature dependence of lipid mobility in free-standing membranes using circular scanning fluorescence correlation spectroscopy — ●ARACELI SEBASTIÁN, JONAS MÜCKSCH, PHILIPP BLUMHARDT, LAURA KACENAUŠKAITE, CHRISTIAN NIEDERAUER, EUGENE P. PETROV, and PETRA SCHWILLE — Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Mar-

tinsried, Germany

Circular scanning Fluorescence Correlation Spectroscopy (csFCS) is a calibration-free alternative to conventional static point FCS [1,2]. Not only does csFCS allow for the direct determination of the diffusion coefficient, but, in case of quasi-planar membranes, also avoids potential errors originating from imprecise axial positioning. Previously, csFCS has been used to measure diffusion in giant unilamellar vesicles (GUVs), serving as a model of free-standing lipid membranes [3]. Despite the immanent importance of model membranes, their temperature-dependent lipid mobility has been subject to only few studies. Here, we report on our progress of employing csFCS to systematically characterize the diffusion in GUVs over a wide range of temperatures.

[1] K. M. Berland, P.T.C. So, Y. Chen, W.W. Mantulin, and E. Gratton, *Biophys. J.* **71**, 410 (1996).

[2] Z. Petrášek and P. Schuille, *Biophys. J.* **94**, 1437 (2008).

[3] Z. Petrášek, S. Derenko, and P. Schuille, *Opt. Express* **19**, 25006 (2011).

BP 8.16 Mon 17:30 P3

Super-Resolution by Structured-Illumination-Axial-Tomography (SIAT) — •FLORIAN SCHOCK^{1,2,3}, VERENA RICHTER⁴, THOMAS BRUNS⁴, UDO BIRK^{1,3}, RAINER HEINTZMANN^{5,6}, HERBERT SCHNECKENBURGER⁴, and CHRISTOPH CREMER^{1,2,3} —

¹Institute of Molecular Biology, University of Mainz — ²Institute of Pharmacy and Molecular Biotechnology, University of Heidelberg — ³Kirchhoff Institute for Physics, University of Heidelberg — ⁴Aalen University of Applied Sciences, Institute of Applied Research, Aalen, Germany — ⁵Institute for Physical Chemistry and Abbe Center of Photonics, University of Jena — ⁶Leibniz Institute of Photonic Technology, Jena, Germany

Since the first developments of super-resolution-microscopy (SRM), methods allowing to circumvent (“break”) the Abbe limit of optical resolution, a variety of different complementary SRM techniques were discovered. Due to differences in the mode of operation, a further optimization of super-resolution imaging can be achieved by appropriate combinatorial strategies. One of these is the combination of Structured-Illumination-Microscopy (SIM) and Micro-Axial-Tomography (AT). Both of them operate in the visible range spectra and are usable for live-cell imaging. While SIM allows for a resolution-improvement of a factor 2 in all spatial directions (3D), together with appropriate image processing, SIM-AT makes it possible to achieve a homogeneous effective resolution down to 100nm in all directions.

BP 8.17 Mon 17:30 P3

Coherent imaging of biological systems with ultrabright electron pulses — •ROBERT BÜCKER¹, PHILIPP PELZ¹, GOPAL SINGH¹, CHIWON LEE¹, NARIMAN KHAZAI², PASCAL HOGAN^{1,2}, SERCAN KESKIN¹, SANA AZIM¹, ALBERT CASANDRUC¹, EIKE SCHULZ¹, GÜNTHER KASSIER¹, and R. J. DWAYNE MILLER^{1,2} — ¹Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ²Departments of Chemistry and Physics, University of Toronto, Toronto, Canada

High-brightness electron pulses as an ideal probe for structural dynamics are employed in a variety of experimental schemes spanning orders of magnitude in their accessible spatial and temporal scales, from mapping atomic motions driving phase transitions to real-space movies on the nano scale. Further extending this scope - in particular into the realm of complex and fragile biomolecules - will require improvement of electron sources in terms of current and coherence, as well as exploration of imaging techniques that maximize the information gathered from each scattered particle, hence minimizing beam-induced damage.

In this contribution, we present concepts of and first results from experimental setups designed for coherent imaging and protein crystallography using electron pulses in the nanoseconds to milliseconds regime. These comprise different electron energies, imaging modalities, and electron source technologies. Also methods for interferometric beam characterization, and theory developments for optimal reconstruction of the sample from diffracted intensities will be shown.

BP 8.18 Mon 17:30 P3

A theoretical framework for spatiotemporal chemical imaging with nanosensors — •DANIEL MEYER, ANNIKA HAGEMANN, and SEBASTIAN KRUSS — Institute of Physical Chemistry, Göttingen University, Germany

Fluorescent nanosensors provide many beneficial properties and are often used to gain precise single-molecule data from biological system. The collective imaging of many sensors can, moreover, supply spatial and temporal information about the local concentration of a given analyte and thus is able to identify fast changing processes on a nanoscale. This idea of chemical imaging with nanosensors becomes attractive when studying chemical signaling between cells. We developed a theoretical framework to simulate the fluorescence image of arrays of nanosensors in response to a spatiotemporal concentration profile. We especially focus on the role of sensor kinetics as it determines how fast sensors can report about concentration changes. For that purpose, the (fluorescence) response of each single nanosensor is modeled with a Monte-Carlo simulation that describes the binding/debinding of the analyte and the respective fluorescence change. Multiple nanosensors are arranged on a surface and exposed to a concentration pattern $c(x,y,t)$ of an analyte. We account for the Abbe-limit and the acquisition speed and resolution of the optical setup and determine the resulting sensor array response images $I(x,y,t)$. Consequently we introduce terms for the spatial and temporal resolution and simulate phase diagrams that allow us to predict the best binding properties of our nanosensors for fast release events such as neurotransmitter releases.

BP 8.19 Mon 17:30 P3

Wavefront-shaping for flow-field measurements — •BOB FREGIN¹, NEKTARIOS KOUKOURAKIS², JÖRG KÖNIG³, JÜRGEN CZARSKÉ², and OLIVER OTTO¹ — ¹Universität Greifswald, Greifswald, Germany — ²Technische Universität Dresden, Dresden, Germany — ³IFW Dresden, Dresden, Germany

Flow-field measurements within (non)-stationary fluid systems are important for several applications in process engineering and biomedical sciences. However, there are environments like biological tissues where experimental assays are impeded by aberrations or scattering. The latter could lead to a strong increase in measurement uncertainty. Supported by the technological progress of spatial light modulators (SLM) and wave front sensing techniques, sensor-based adaptive optics enables to overcome these limitations, as it allows for flexible and dynamic control of light-fields.

In this contribution we analyze the usage of time-reversal and wave front shaping techniques for both turbidity suppression and aberration correction. The effect of scattering or fluctuating media, e.g. inside a microcapillary, on the measurement accuracy of image-correlation based flow-field measurements is investigated and results of first measurements and simulations are presented and limitations are discussed. We show that time-reversal, digital holography and wavefront shaping techniques have the potential to strongly improve the quality of disturbed flow-field measurements with application inside Biology and Biochemistry.

BP 8.20 Mon 17:30 P3

X-Band Electron Paramagnetic Resonance (EPR) Measurements of Absorbed Dose by Gamma Irradiated Fossil Tooth Enamel — •OZGUL KARATAS^{1,2}, REFIK KAYALI¹, and VLADISLAV KATAEV² — ¹Omer Halisdemir University, Faculty of Science and Letters, Physics Department, Nigde, Turkey — ²Leibniz Institute for Solid State and Materials Research IFW, Institute for Solid State Research, Dresden, Germany

The measurement of the concentration of stable free radicals in the calcified tissues, such as tooth, due to the radiation is directly related to absorbed dose and it has been used for dose assessment in retrospective dosimetry and dating studies. When tooth enamel is exposed to the ionizing radiation, radicals are formed, which can be detected using Electron Paramagnetic Resonance (EPR) technique. EPR using tooth enamel is based on the correlation between the intensity or amplitude of some of the radiation-induced with the dose absorbed in the enamel. In this study, teeth samples, which were extracted from archaeological site in Nigde, Turkey, were used in the experimental studies. Five animal teeth were selected to obtain an enamel sample formed and then this resultant sample was prepared with combined processes of mechanical and chemical treatment of teeth. This tooth enamel sample was irradiated by ⁶⁰Co gamma-ray source in dose range of 0-9 kGy at Turkish Atomic Energy Agency (TAEK), ÇNAEM in Istanbul, Turkey and then EPR spectra were recorded by using Bruker EMX X-Band EPR spectrometer between 4K-300K temperatures, in Leibniz Institute for Solid State and Materials Research in Dresden, Germany. Radiation induced paramagnetic centers and radicals in this enamel were investigated and interpreted by obtained X-band EPR results.

BP 9: Posters - Cell Mechanics

Time: Monday 17:30–19:30

Location: P3

BP 9.1 Mon 17:30 P3

Characterization of the power and thermic behaviour of an ultrasonic probe — •TOBIAS LÖFFLER¹, MIKE HUWER¹, JULIA KRISTIN², and MATHIAS GETZLAFF¹ — ¹Institute of Applied Physics, University of Düsseldorf — ²Hals-Nasen-Ohrenklinik, Universitätsklinikum Düsseldorf

We want to use an ultrasonic probe to transfer energy to biological samples in liquid. For a better understanding of the influence of the ultrasound, we need a detailed characterization of its properties in the liquid environment.

In order to determine the temperature-profile in the vicinity of our ultrasonic probe, measurements of the temperature at different distances in direction of oscillation and additionally as a function of time have been performed. The displacement of the probe head was measured with an optical microscope.

The characterization of the output energy was performed with calibrated ultrasonic-power-detectors at different distances in the direction of propagation.

BP 9.2 Mon 17:30 P3

Development of a mechanically stable cell stretcher for measuring the influence of external strain on cell mechanics with the AFM — •FABIAN PORT, PATRICK PAUL, and KAY-E. GOTTSCHALK — Institute of Experimental Physics, Ulm University

In the last few decades the correlation between cell mechanics and different physiological or pathophysiological conditions, like stem cell differentiation [1] or cancer [2], has been a growing aspect of biophysical research. To understand the underlying mechano-chemical feedback cycles, it is important to understand the mechanical properties of cells under varying conditions. Such conditions could be the effect of strain on cells, which is particularly important for a variety of cell types like endothelial cells in the lung, in arteries or in the bladder. The impact of such conditions on the cell mechanics is not yet well understood on the cellular and subcellular level. For a detailed analysis of the cells response to stretch, we present here a self-developed cell stretching device, which is compatible with correlative AFM and FLIM Measurements.

[1] Suresh, S., Spatz, J., Mills, J. P., Micoulet, A., Dao, M., Lim, C.T., and Seufferlein, T. (2005). Connections between single-cell biomechanics and human disease states: gastrointestinal cancer and malaria. *Acta Biomaterialia*, 1(1), 15-30.

[2] Sokolov, I. (2007). Atomic force microscopy in cancer cell research. *Cancer Nanotechnology*, 1-17.

BP 9.3 Mon 17:30 P3

Cooperative microtubule dynamics in closed elastic compartments — •JONAS HEGEMANN and JAN KIERFELD — TU Dortmund, 44221 Dortmund, Germany

Microtubules are an essential part of the cytoskeleton and interact mechanically with cell cortex and membrane. Since local polymerization forces on the cell boundary can affect its global shape, this generates a coupling between different microtubules. We propose a model, which describes the polymerization dynamics of a microtubule ensemble confined in a closed elastic compartment in two dimensions and growing radially outwards. This serves as a simple model for microtubules in an elastic cell cortex, which can change its shape. Microtubules are coupled via their growth velocities, which depend on local forces derived from an elastic energy functional. The cell cortex dynamically reacts to stochastic displacements produced by the microtubules. We investigate synchronization effects and polarization mechanisms.

BP 9.4 Mon 17:30 P3

Adhesive dynamics of Plasmodium falciparum-infected red blood cells — •ANIL K. DASANNA, CHRISTINE LANSCHKE, MICHAEL LANZER, and ULRICH S. SCHWARZ — Heidelberg University

The clinical symptoms of the malaria disease appear when healthy red blood cells (RBC) are invaded by the malaria parasites during the blood stage of the life cycle. The whole infection of RBC takes about 48 hrs and proceeds through the three stages of ring, trophozoite and schizont. During these stages, infected RBC increasingly develop adhesive protrusions, so-called knobs, on their surface. These knobs cause iRBCs to adhere to endothelial cells in the microvascula-

ture, preventing their clearance by spleen and liver, but also leading to capillary obstruction. We first present how exactly the shape of iRBCs change during the time course along with their geometrical features such as volume and surface area using confocal microscopy and image processing. We then discuss how these changes in shape and knob details through out the blood stage affect the rolling adhesion of iRBCs on endothelial cells using flow chamber experiments. Results from these flow chamber experiments are complemented with adhesive dynamics of deformable RBC simulations. Hydrodynamics is implemented with multiparticle collision dynamics (MPCD). In particular using simulations, we will discuss how does the combination of iRBC shape or different infectious stage cell along with different knob density give rise to different adhesive dynamics such as flipping motion or stable rolling. We will show how does membrane elasticity play role in adhesive dynamics.

BP 9.5 Mon 17:30 P3

Functional analysis of chordotonal organ mechanics in vivo — •CHONGLIN GUAN¹, MARTIN GÖPFERT², and CHRISTOPH SCHMIDT¹ — ¹Faculty für Physics, Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — ²Department of Cellular Neurobiology, Schwann-Schleiden-Centre for Molecular Cell Biology, Georg-August-University, Göttingen, Germany

Most if not all higher organisms require reliable mechanosensation for various biological processes including hearing, balance, proprioception and touch. Vertebrates and invertebrates have evolved specialized mechanosensory devices and strategies to manage this immense challenge. Vertebrates possess multiple organs, which are typically adapted to particular mechanical stimuli. In contrast, *Drosophila* is equipped with a polymodal sensor * the chordotonal organ (ChO) through which they are capable to perceive different mechanical stimuli including sound, touch and proprioception. Previously, I have developed a preparation to directly record from the sensory neurons of larval ChOs and managed to correlate defined mechanical inputs with the corresponding electrical outputs (Scholz et al., 2015). Our in vivo model established ChOs as interesting sites to study the molecular machinery involved in the perception of mechanical stimuli. However, genetic and functional dissection of ChO mechanics in vivo has been challenging. Here, we aim to obtain a deeper mechanistic understanding and provide new insights into the biophysics of ChOs. We correlate mechanical properties and active manipulation with neuronal activity. We focus on cytoskeleton structures and force generation.

BP 9.6 Mon 17:30 P3

A Protein Flux-based Mechanism for Midcell Sensing in Bacteria — •SILKE BERGELER¹, DOMINIK SCHUMACHER², LOTTE SØGAARD-ANDERSEN², and ERWIN FREY¹ — ¹ASC for Theoretical Physics, Ludwig-Maximilians-Universität, München, Germany — ²Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

Precise positioning of the cell division site is essential for the correct separation of the genetic material into the two daughter cells. In myxobacteria, a protein cluster is formed on the nucleoid that performs a biased random walk to midcell and positively regulates cell division there. Deletion experiments show that PomZ, an ATPase, is necessary for this cluster movement. To investigate how the cluster is positioned at midcell, we introduce a mathematical model: ATP-bound PomZ dimers can attach to and quickly diffuse on the nucleoid. At the cluster, they can hydrolyze ATP and subsequently detach into the cytosol as ADP-bound monomers. It is known that this type of particle dynamics leads to different fluxes of PomZ into the cluster from both sides along the long cell axis, if the cluster is at an off-center position. We investigate this model both numerically, using stochastic simulations, and analytically, using reaction-diffusion equations. With our model, we are able to reproduce the movement of the cluster towards midcell. We perform parameter sweeps to test the robustness of the mechanism. Furthermore, we investigate the reaction-diffusion equations in a three-dimensional geometry mimicking the cell to study geometric effects. In summary, our study provides new mechanistic insights into self-organized intracellular positioning of protein clusters.

BP 9.7 Mon 17:30 P3

The mechanical framework of cells: Modeling eukaryotic cells as thick-shell multilayer elastic materials — •CONSTANTIN D. C.

KOHL and CHRISTOPH F. SCHMIDT — 1Drittes Physikalisches Institut, Fakultät für Physik, Georg-August-Universität, Göttingen

Cells are complex mechanical entities. They respond passively and actively to forces exerted by their environment, and, as active materials, they probe their surroundings by exerting forces. To understand such processes, one needs a detailed quantitative model describing the mechanical properties of a cell. Components of such a model will be the external lipid bilayer, the polymeric actin cortex, and the inner cytoplasmic structures, including the microtubule network, intermediate filaments, membranous compartments and the nucleus. An important quantity controlling cell volume is the osmotic pressure. Internal osmolyte concentration and its regulation by transport processes plays a crucial role for the mechanical properties of the cell. Most existing cell models do not consider the osmotic pressure in cells that are exposed to mechanical forces. We present finite element simulations where we model the cell as a thick-shell multiple layer object with spherical symmetry. In our model, we vary the elastic properties and the thickness of the different shell compartments and include osmotic pressure. We indent the cell by beads and investigate the resulting force curves.

BP 9.8 Mon 17:30 P3

Effect of the flexural rigidity of type IV pili on the motility of *N. gonorrhoeae* bacteria. — ●MAXIM A. BELIAEV¹, WOLFRAM PÖNISCH¹, NICOLAS BIAIS², and VASILY ZABURDAEV¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Brooklyn College, New York, USA

Gonorrhea is the second most common sexually transmitted disease in the world. *Neisseria gonorrhoeae* bacteria, the causative agent of the gonorrhea infection, use multiple long and semiflexible filaments, called type IV pili to move, attach to the epithelium and form colonies. These filaments assemble and elongate from the cell membrane towards its environment where they can attach to various substrates and pili of other cells. The retraction of pili can generate significant pulling forces of up to 180 pN. Although currently there exist several models of pili driven motility, they do not consider the semiflexible nature of pili filaments. In this work we explicitly analyze the effect of pili flexural rigidity on the motility of *N. gonorrhoeae* bacteria. We use two approaches to model pili. In the first one, a pilus is modelled as an Euler-Bernoulli cantilever beam with a point load at the tip whereas in the second approach, a pilus is modelled as a stiff rod connected to the cell membrane by a pivotal spring. For both models we compare the results of the numerical simulations of the moving cell to the experimental data and analyze how the flexibility of pili affects the cell persistence and orientation during motility.

BP 9.9 Mon 17:30 P3

passive and active response of bacteria under mechanical compression — ●RENATA GARCES¹, SAMANTHA MILLER², and CHRISTOPH F. SCHMIDT¹ — ¹Georg-August-Universität Göttingen, Göttingen, Germany — ²The University of Aberdeen, Aberdeen, United Kingdom

Bacteria display simple but fascinating cellular structures and geometries. Their shapes are the result of the interplay between osmotic pressure and cell wall construction. Typically, bacteria maintain a high difference of osmotic pressure (on the order of 1 atm) to the environment. This pressure difference (turgor pressure) is supported by the cell envelope, a composite of lipid membranes and a rigid cell wall. The response of the cell envelope to mechanical perturbations such as geometrical confinements is important for the cells survival. Another key property of bacteria is the ability to regulate turgor pressure after abrupt changes of external osmotic conditions. This response relies on the activity of mechanosensitive (MS) channels: membrane proteins that release solutes in response to excessive stress in the cell envelope. We here present experimental data on the mechanical response of the cell envelope and on turgor regulation of bacteria subjected to compressive forces. We indent living cells with micron-sized beads attached to the cantilever of an atomic force microscope (AFM). This approach ensures global deformation of the cell. We show that such mechanical loading is sufficient to gate mechanosensitive channels in isosmotic conditions.

BP 9.10 Mon 17:30 P3

Regulation of muscle contraction by Drebrin-like protein 1 probed by atomic force microscopy — ●PETER WEIST, EUGENIA BUTKEVICH, DIETER R. KLOPFENSTEIN, RENATA GARCES, and CHRISTOPH F. SCHMIDT — Drittes Physikalisches Institut-Biophysik, Georg-August-Universität Göttingen, Germany

Sarcomeres are the fundamental contractile units of striated muscle cells. They are composed of a variety of structural and regulatory proteins functioning in a precisely orchestrated fashion to enable co-ordinated force generation in muscles. Recently, we have identified a drebrin-like protein 1 (DBN-1) as a novel sarcomere component in the nematode *C. elegans*. DBN-1 stabilizes actin filaments during muscle contraction. Absence of DBN-1 results in a unique worm movement phenotype, characterized by hyper-bending. The origin of the hyper-bending is not clear yet. DBN-1 could have a regulatory role in proper muscle contraction. The phenotype of the knockout of DBN-1 protein could be caused by either enhanced contraction or enhanced relaxation of the muscles. We present here an experimental study on *C. elegans* muscle mechanics by atomic force microscopy. We measured the stiffness of the whole worm by gently indenting living *C. elegans* with a micron-sized sphere adhered to the cantilever of an atomic force microscope (AFM). Using chemical treatments in wild-type worms we probed that the degree of contraction of the muscle is directly related to the measured elastic compliance of the worm. We compared responses of wild-type and mutant *C. elegans* in which DBN-1 is not expressed.

BP 9.11 Mon 17:30 P3

Rheology of the active cell cortex in mitosis — ●ELISABETH FISCHER-FRIEDRICH^{1,2}, YUSUKE TOYODA^{2,3}, CEDRIC CATTIN⁴, DANIEL MÜLLER⁴, ANTHONY HYMAN², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — ²Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — ³Institute of Life Science, Kurume University, Kurume, Japan — ⁴D-BSE, Eidgenössische Technische Hochschule Zürich, Mattenstr. 26, 4058 Basel, Switzerland

The cell cortex is a key structure for the regulation of cell shape and tissue organization. To reach a better understanding of the mechanics and dynamics of the cortex, we study here HeLa cells in mitotic arrest dynamically compressed between two parallel plates. We investigate the dependence of this mechanical response on the geometry of the cell and find strong indications, that the cortical layer is the dominant mechanical element. To characterize the time-dependent rheological response, we perform step strain experiments and oscillatory cell compressions. We extract a complex elastic modulus which characterizes the resistance of the cortex against area dilation. In this way, we present a rheological characterization of the cortical actomyosin network in cells. Furthermore, we investigate the influence of actin cross-linkers and the impact of active prestress on rheological behavior. Intriguingly, we find that cell mechanics in mitosis is captured by a simple rheological model characterized by a single time scale on the order of 10 s which marks the onset of fluidization in the system.

BP 9.12 Mon 17:30 P3

Force fluctuations of suspended cells- effects of osmotic pressure and motor inhibition — ●SAMANEH REZVANI¹, TODD M. SQUIRES², and CHRISTOPH F. SCHMIDT¹ — ¹Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Germany — ²Department of Chemical Engineering, University of California, Santa Barbara, USA

Cells communicate with their environment through biochemical and mechanical interactions. They can respond to stimuli by undergoing shape- and, in some situations, volume changes. Key determinants of the mechanical response of a cell are the viscoelastic properties of the actomyosin cortex, effective surface tension, and osmotic pressure. We use a custom-designed microfluidic device with integrated hydrogel micro-windows to rapidly change solution conditions for cells suspended by optical traps without direct fluid flow. We use biochemical inhibitors and different osmolytes and investigate the time-dependent response of individual cells. Using a dual optical trap makes it possible to probe the viscoelasticity of suspended cells by active and passive microrheology to quantify the mechanical response of the cells under the various conditions.

BP 9.13 Mon 17:30 P3

Local tubulin concentrations in the *C. elegans* metaphase spindle — ●JOHANNES BAUMGART¹, MARCEL KIRCHNER², STEFANIE REDEMANN², JEFFREY WOODRUFF³, JEAN-MARC VERBAVATZ³, ANTHONY HYMAN³, THOMAS MÜLLER-REICHERT², JAN BRUGUÉS¹, and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, Dresden — ²Experimental Centre, Medical Faculty Carl Gustav Carus, Technische Universität Dresden — ³Max Planck Institute of Molecular Cell Biology and Genetics, Dresden

During cell division, the mitotic spindle physically separates the duplicated chromosomes. The spindle is formed by many highly dynamic microtubules. Microtubules are stiff filaments that form by polymerization of tubulin dimers. Here we determine the concentration profile of tubulin dimers by combining electron with light microscopy data.

Tomographic electron microscopy is able to identify microtubules in the spindle, but cannot resolve the tubulin dimers. Therefore it provides a quantitative measure of the local concentration of tubulin within microtubules. Light microscopy data with a GFP staining of tubulin provide a relative measure of the total tubulin concentration, since both polymerized and dimeric tubulin, are stained. We calibrate the light microscopy signal using the electron microscopy data. From this quantitative analysis we determine a local enrichment of the dimeric tubulin at the centrosome. Our results suggest that the centrosome accumulates tubulin dimers which have a high affinity to the pericentriolar material and thereby facilitate localized microtubule nucleation.

BP 9.14 Mon 17:30 P3

Dynamics of single human cardiomyocytes tracked by endogenous labeling of z-lines using CRISPR/Cas9 — •DANIEL HÄRTTER¹, TIL DRIEHORST^{1,2}, MALTE TIBURCY², KENGO NISHI¹, WOLFRAM-H. ZIMMERMANN², and CHRISTOPH F. SCHMIDT¹ — ¹Georg-August Universität Göttingen, Germany — ²University Medical Center Göttingen, Germany

The dynamics of single cardiomyocytes (CM) may provide insight into cardiac function and dysfunction. The CMs' regulated and coordinated sarcomeric contractility is, however, not fully understood.

We here present a new method using endogenous labeling of the z-lines in living human stem cell-derived CMs using CRISPR/Cas9. We applied methods of micro-contact printing to shape the cells to physiological aspect ratios. Using high-speed confocal microscopy, we imaged the contractile dynamics of individual sarcomeres with high spatial and temporal resolution. We developed a method to track z-lines over time and to analyze their dynamics. We utilize approaches from nonlinear dynamic systems theory to study phase-coherence and synchronization. We could show that the phase coherence of sarcomeres strongly depends on the elastic properties of the underlying substrate. We further investigated the effects of drug interference on the sarcomeric level.

BP 9.15 Mon 17:30 P3

E-Cadherin Expression and Localization is Correlated to Cellular Softness in Cancer Development — •ERIK MORAWETZ¹, LARS-CHRISTIAN HORN², SUSANNE BRIEST³, MICHAEL HÖCKEL³, and

JOSEF KÄS¹ — ¹Physik der weichen Materie, University of Leipzig, Leipzig, Germany — ²Institut für Pathologie, Universitätsklinikum Leipzig, Leipzig, Germany — ³Klinik und Poliklinik für Frauenheilkunde, Universitätsklinikum Leipzig, Leipzig, Germany

The concept of the epithelial to mesenchymal transition is believed to play a crucial role in cancer development. One of its main markers is the loss of epithelial cadherin (E-Cad). The malignant transformation of cells is also linked to increased softness of the cell body. To investigate correlations between this two fundamental cellular changes, we use cell lines, as well as primary human tumor samples. In the Optical Stretcher (OS), the softness of a single cell, its reaction to the deformation, as well as the corresponding distribution of E-Cad on the cell surface can be measured simultaneously. In the cell line model we show, that the loss of E-Cad expression is linked to softer cell bodies (MDA-MB 231, MDA-M 436, MCF-10A). In addition, EMT has been induced in MCF-10A cells by cultivation under the influence of epithelial growth factor. A significant drop in the elastic modulus as well in the reaction to external forces can be observed. Primary human mamma and cervix carcinoma samples are provided by the Universitätsklinik Leipzig. The tumor samples are processed into a single cell suspension and measured in the OS. We show that a primary tumor sample can be sorted into two sub-populations of soft and stiff cells by their E-Cad level.

BP 9.16 Mon 17:30 P3

Myosin Activity in Epithelial and Mesenchymal Cells — •ENRICO WARMT, ERIK MORAWETZ, STEFFEN GROSSER, and JOSEF KÄS — Uni Leipzig, Soft Matter Physics, Linnéstr. 5, 04103 Leipzig

Epithelial-Mesenchymal-Transition is a critical process during cancer development. Epithelial cells are tightly junked by a complex of interlinked actin, E-cadherin and other cytoskeletal proteins. During EMT, cells decrease their E-Cadherin expression. Additionally a pre-stressed acto-myosin cortex is also hindering cells to migrate freely. Thus, during EMT cells might further form back their acto-myosin cortex. In Optical Stretcher experiments, we observe an active contraction of epithelial cells. That means, despite optical pulling forces cells counteract these forces, leading to cell shrinkage. These internal forces might be closely related to actin-myosin contraction, since we observe a clear loss of this contractility by inhibiting myosin activity for instance by Blebbistatin. By adding epidermal growth factor, we could induce EMT for MCF10A cells. An E-Cadherin stain was further used to determine whether cells are more epithelial- or mesenchymal like. We could directly correlate a higher contractility for cell which have more E-Cadherins expressed. These findings support strongly a down regulation of actin-myosin activity during EMT.

BP 10: Posters - Single Molecule Biophysics

Time: Monday 17:30–19:30

Location: P3

BP 10.1 Mon 17:30 P3

Single molecule detection in microflow — •ELEONORA PEREGO, VIKTOR SCHROEDER, and SARAH KÖSTER — Institute for X-Ray Physics, Georg-August-Universität Göttingen, Germany

In recent years single molecule fluorescence methods have emerged as powerful method to study assembly, aggregation and diffusion of biomolecules. We use techniques like fluorescence correlation spectroscopy (FCS) or photon counting histogram (PCH) to study these process with high spatial resolution. However these techniques are inherently "slow". Thus in order to overcome this limitation, we combine these methods with microfluidics. This allow us to study the assembly and the diffusion of biomolecules in a time-resolves manner. One application is the study of early time points of protein assembly, like intermediate filaments, that are usually difficult to measure with more classical bulk experiments. Moreover, by employing our setup, it is possible to identify the passage of a single molecule through the excitation volume by tuning the concentration and the flow conditions of the sample stream. Our results show that the combination of microfluidic and single molecule fluorescence methods provides a very suitable approach for studying the aggregation of biomolecules in real time, which is important for understanding cellular behavior.

BP 10.2 Mon 17:30 P3

Plasmonics and Nanofluidics for DNA-Single Molecule De-

tection — •PARISA BAYAT, IRENE FERNANDEZ-CUESTA, FRANZISKA ESMEK, THOMAS KLING, and ROBERT H. BLICK — Center for Hybrid Nanostructures & Institute of Nanostructure- and Solid State Physics, University of Hamburg, Germany

Plasmonic antenna nano-focus the light beyond diffraction. These hot spots are ultra-sensitive, what can be exploited for single molecule (bio) sensing. But there is a major challenge: placing the target element at the sensitive area. Here, we have integrated a sub-100nm nanochannel crossing the antenna gap, what allows the in-line detection of single molecules of DNA in real-time as they pass through the light "hot-spot". In this configuration, the molecules are detected as peaks in the fluorescent signal in time scans. This allows real time read-out of the molecules with no limitation in the length and without an expensive camera. For total liquid control, the nanochannel is connected to a complete fluidic system. This represents a new type of super-sensitive (bio) sensor, with single- molecule real time detection capabilities. We have developed a wafer-scale fabrication process, based on nanoimprint lithography [1], to make the complete fluidic devices in one single step, only 120 seconds. Discrete DNA molecules have been detected and counted by in-line detection in real time. Different types of viral DNA molecules (λ -Bacteriophage and Kaposi's sarcoma herpesvirus) were stained with intercalating dyes and stretched in the nanochannels.

[1] I. Fernandez-Cuesta et al., J. Vac. Sci. Technol. B29, 06F801 (2011)

BP 10.3 Mon 17:30 P3

Label-free iSCAT detection of secretory proteins from single living cells — ●ANDRE GEMEINHARDT¹, MATTHEW McDONALD¹, KATHARINA KÖNIG¹, STEFANIE SCHALLER², MICHAEL AIGNER², ANDREAS MACKENSEN², and VAHID SANDOGHDAR¹ — ¹Max Planck Institute for the Science of Light, Erlangen, Germany — ²Department of Haematology and Oncology, Universitätsklinikum Erlangen, Germany

Interaction and communication between cells is partly guided via an exchange of different proteins. Here, we report the detection of single unlabeled proteins secreted by individual living cells. This is realized via an interferometric scattering technique (iSCAT) developed in our laboratory that circumvents the need to fluorescently label the biomolecules under study. The technique's use of interference between a small scattering signal and a larger reference wave paves the way to detect even the smallest particles. We apply this method to analyze the secretomics of single cytotoxic T-cells under external stimulation. By varying the system between body temperature and fever-like conditions, we observe a clear trend towards shorter reaction times after triggering cytokine secretion. The developed method is a promising way to elucidate the complicated nature of immune response through the basic principles of membrane-mediated protein release and cellular exchange.

BP 10.4 Mon 17:30 P3

Mechanical Properties of Leishmania Myosin XXI determined with an Optical Tweezers based Force Transducer —

●ANDREAS GRAW, CHRISTOPHER BATTERS, and CLAUDIA VEIGEL — Department of Cellular Physiology (LMU) and Center for Nanoscience (CeNS), München, Germany

Myosins form a large family of actin-based motor proteins that are involved in different forms of cellular motility. Force and movement are generated by changes in conformation of the actomyosin complex. Myosin XXI is the only myosin shown to be expressed in *Leishmania* parasites and is involved in a variety of motile functions. Previous studies indicated that members of the calmodulin family regulate dimerization, motility, and lipid binding of this molecular motor.

Here we present the first mechanical measurements to determine the stiffness and working stroke of a single myosin XXI motor molecule using optical tweezers. These measurements are performed using the "three bead" geometry in which an actin filament is stretched out via two optically trapped handle beads attached to either end of the filament to form a dumbbell. The dumbbell is positioned in the vicinity of a third bead carrying the myosin motor². The movements and forces produced by the actomyosin interactions are observed by detecting the position of both trapped beads with four-quadrant-photodiodes. In order to characterize the effect of the C-terminal tail on the mechanical performance of the motor we immobilized the motor using different attachment modes including physiological phospholipids.

BP 10.5 Mon 17:30 P3

Universal bound on the efficiency of molecular motors —

●PATRICK PIETZONKA¹, ANDRE C. BARATO², and UDO SEIFERT¹ — ¹II. Institut für theoretische Physik, Universität Stuttgart — ²Max Planck Institute for the Physics of Complex Systems, Dresden

The thermodynamic uncertainty relation provides an inequality relating any mean current, the associated dispersion and the entropy production rate for arbitrary non-equilibrium steady states. Applying it here to a general model of a molecular motor running against an external force or torque, we show that the thermodynamic efficiency of such motors is universally bounded by an expression involving only experimentally accessible quantities [1]. For motors pulling cargo through a viscous fluid, a universal bound for the corresponding Stokes efficiency follows as a variant. A similar result holds if mechanical force is used to synthesize molecules of high chemical potential. Crucially, no knowledge of the detailed underlying mechano-chemical mechanism is required for applying these bounds.

[1] P. Pietzonka, A. C. Barato, U. Seifert, J. Stat. Mech. *in press*, arXiv:1609.08046

BP 10.6 Mon 17:30 P3

Catch bond interaction between cell surface sulfatase Sulf2 and glycosaminoglycans — AHMET EROL¹, ●SÖREN GRANNEMANN¹, CHRISTIAN BARTZ², VOLKER WALHORN¹, THOMAS DIERKS², and DARIO ANSELMETTI¹ — ¹Experimental Biophysics & Applied Nanoscience, Bielefeld University, Germany — ²Biochemistry I, Bielefeld University, Germany

In biological adhesion, the biophysical mechanism of specific non-covalent biomolecular interaction can be divided in slip- and catch-bonds, respectively. Conceptually, slip bonds exhibit a reduced bond lifetime under increased external force and catch-bonds, in contrast, an increased lifetime for a certain force interval. Catch bonds therefore act in a counter intuitive manner.

Upon investigating the specific interaction between the unique hydrophilic domain (HD) of the human cell-surface sulfatase Sulf2 against its native glycosaminoglycan (GAG) target substrate heparan sulfate (HS) by single-molecule force spectroscopy (SMFS), we found clear evidence of catch-bond behavior which, by means of control experiments, could be specifically related to the GAG 6-O-sulfation site. Alongside to our previous work on the catch bond behavior of HDSulf1 [1], we analyzed the data within the theoretical framework of a force mediated transition between two coupled slip bond regimes.

[1] A. Harder et al., Biophysical Journal 108(7), p1709-1717 (2015)

BP 10.7 Mon 17:30 P3

Investigation of cardiomyopathy-related desmoglein-2 variants — ●MAREIKE DIEDING¹, RAIMUND KERKHOFF¹, JANA DEBUS², ANNA GÄRTNER-ROMMEL², VOLKER WALHORN¹, HENDRIK MILTING², and DARIO ANSELMETTI¹ — ¹Experimental Biophysics & Applied Nanoscience, Bielefeld University, Germany — ²Erich und Hanna Klessmann-Institut, Herz- und Diabeteszentrum Bad Oeynhausen, Germany

Desmoglein-2 (DSG2) is a desmosomal transmembrane glycoprotein in heart muscle cells. The homophilic interaction of its extracellular domains provide the intracellular mechanical contract between the desmosomes of adjacent cells. Variants of DSG2 are associated with arrhythmogenic right ventricular cardiomyopathy (ARVC) a rare but severe heart muscle disease. DSG2 wildtype (WT) and several variants were investigated on the cellular and the single molecule level, respectively. The adhesion of single DSG2 homo-complexes was analyzed by means of atomic force microscopy based single-molecule force spectroscopy (AFM-SMFS). Moreover, using Jarzynski's equation we estimated the difference of free energy in order to fully characterize the kinetics and thermodynamics of the homophilic DSG2 binding. Furthermore, cell-cell adhesion was analyzed using confluent monolayers of stable transfected full-length-DSG2 WT and DSG2 variant HT1080 cultures that were subjected to mechanical stress.

The results of the dissociation assay and AFM experiments consistently revealed that DSG2 variants tend to an increased cell-cell adhesion and a prolonged DSG2 bond life-time, respectively.

BP 10.8 Mon 17:30 P3

Biophysical investigation of the association of histones with double- and single-stranded DNA — YING WANG¹,

●DENNIS KREFT¹, LUIS VAN MERWYK¹, KATJA TÖNSING¹, VOLKER WALHORN¹, XAVIER FERNÁNDEZ-BUSQUETS², and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University, Bielefeld, Germany — ²Institute for Bioengineering of Catalonia and Barcelona Institute for Global Health, Barcelona, Spain

Nucleosome formation is the process of how nucleic dsDNA is packed in eukaryotes. Nucleosome core particles consist of 147 bp of dsDNA, which wrapped in 1.67 left-handed superhelical turns around a histone octamer, consisting of 2 copies each of the core histones (H2A, H2B, H3, H4) and stabilized by the linker histone H1, forming the well-known "beads on a string" chromatin structure. Despite many studies of histones associating with dsDNA, little is known about the structures generated by the interaction of histones with ssDNA. In this work, we employed magnetic tweezers (MT) and atomic force microscopy (AFM) to investigate the association of histones with dsDNA and ssDNA. For ssDNA in the presence of histones, the results of MT assays indicate a shortening of ssDNA upon its interaction with histones as well as AFM imaging exhibits a compacted ssDNA structure. Compared with the characteristics of histones-dsDNA binding, these data suggest that histones and ssDNA associate into some type of nucleosome-like assembly that may facilitate the participation of histones in the replication and transcription of chromatin.

BP 10.9 Mon 17:30 P3

Recombinant mammalian kinesin-3, KIF16B, is not autoinhibited and moderately processive by itself — ●RAHUL GROVER^{1,2}, RALUCA GROZA¹, TIM REHFELDT¹, and STEFAN DIEZ^{1,2} — ¹B CUBE & cfaed, TU Dresden, Germany — ²MPI-CBG, Dresden, Germany

KIF16B, a kinesin-3 family motor, is involved in the transport and localization of early endosomes. It exhibits a lipid-binding PX-domain, through which it directly binds to PI(3)P-containing vesicles. Recent in-vivo studies on KIF16B have proposed contradictory mechanisms for its activity and transport properties. One study proposed that KIF16B is a monomer and dimerizes only when bound to a membranous cargo, upon which it becomes activated and super-processive (run length > 10 μm). In contrast, another study proposed that KIF16B is autoinhibited by its stalk domain in an ATP-dependent manner without any influence of the presence of membranous cargo or PX-domains. Thus, studying single KIF16B motors in the complex environment of a cell appears to be difficult, resulting in inconsistent postulations about its functional principles. To understand the molecular mechanism of KIF16B we carried out in-vitro assays with purified components. We expressed full-length KIF16B motors labeled with GFP and performed stepping motility assays as well as photobleaching analysis. We found that single molecules of KIF16B are active, dimeric and moderately processive (run length < 2 μm). Our results suggest that other auxiliary proteins (e.g. Rab-family proteins) can be involved in regulating the activity of KIF16B in cells.

BP 10.10 Mon 17:30 P3

Ribonucleic acid induced fluorescence enhancement (RIFE) - Carbocyanines in the realm of RNA — FABIO STEFFEN,

ROLAND K.O. SIGEL, and •RICHARD BÖRNER — Department of Chemistry, University Zürich, Zürich, Switzerland

The popularity of carbocyanine dyes in single molecule spectroscopy of nucleic acids is unbroken (1,2). Studying the dynamics of large RNA constructs such as the group II intron in *S. Cerevisiae* on the single molecule level by means of FRET (3) have motivated a thorough photophysical characterization of the FRET pair Cy3/Cy5 in context of nucleic acids and RNA in particular (4). We observe that, apart from strand composition, structural features of the biomolecule play a fundamental role in RNA-dye recognition. In this respect, secondary structure motifs and its intrinsic flexibility sets RNA well apart from DNA and justifies the introduction of RNA-induced fluorescence enhancement (RIFE) (4) as a phenomenon akin to proteins (PIFE) (5) to describe a series of photophysical effects caused by structural motifs of RNA in vicinity of an isomerizable cyanine fluorophore. Besides quantitative studies of RIFE, we outline possible applications of ALEX-based RIFE-FRET studies with immobilized RNA molecules.

(1) Börner R, Kowanko D, Guisett-Miserach H, Schaffer MF, Sigel RKO. (2016) Coord. Chem. Rev. 327-328:123. (2) Levitus M, Ranjit S. (2011) Q. Rev. Biophys. 44:123. (3) Fiorini E, Börner R, Sigel RKO. (2015) Chimia. 69(4):207. (4) Steffen F, Sigel RKO, Börner R. (2016) Phys. Chem. Chem. Phys. 18(42):29045. (5) Lerner E, Ploetz E, Hohlbein J, Cordes T, Weiss S. (2016) J. Phys. Chem. B. 120(26):6401.

BP 11: Bioinspired Functional Materials: From Nature's Nanoarchitectures to Nanofabricated Designs (Joint Symposium CPP/BP/MM/DF/DY/MI)

Time: Tuesday 9:30–12:15

Location: HSZ 02

Invited Talk

BP 11.1 Tue 9:30 HSZ 02

New twists in biological photonics: circular polarisation and beyond. — •PETE VUKUSIC, LUKE McDONALD, and EWAN FINLAYSON — University of Exeter, Exeter, UK.

The evolution of structural colour mechanisms in many biological systems has given rise to many specialised and often highly functional optical effects both in animals and in plants. Recent scientific works yielded several examples that are being developed for use across technology. Among many thousands of biological systems, a distinctive example involving circular polarisation (CP) was described by Michelson himself: the scarab beetle *Chrysina resplendens*. Its exoskeleton has a bright, golden appearance that reflects both right-handed and left-handed CP light. The chiral nanostructure responsible for this is a helicoid comprising twisted birefringent dielectric planes. This presentation revisits the *C. resplendens* beetle, correlating details of its CP reflectance spectra directly with detailed analysis of its morphology that includes a chiral multilayer configuration comprising two chirped, left-handed, helicoids separated by a birefringent retarder. The system's optical behaviour is modelled using a scattering matrix simulation, where the optical roles of each component of the morphological substructure are elucidated. The *C. resplendens*' model is presented here, alongside summaries of other inspirational biological structural colour generation strategies, as a key example of highly adapted optical design.

Invited Talk

BP 11.2 Tue 10:00 HSZ 02

Bio-inspired materials and structures for technology and architecture — •THOMAS SPECK — Plant Biomechanics Group & Botanic Garden, University of Freiburg

Biological structures and materials are typically multi-layered, hierarchically structured, finely tuned and highly differentiated based on the combination of a few basic molecular components. This leads to materials and structures that are characterized by multiple networked functions and (often) possess excellent mechanical properties, a pronounced adaptability to changing environmental conditions and many-fold self-x-properties.

During the last decades biomimetics, i.e. using living organisms as inspiration for technical developments products, has attracted increasing attention as well from basic and applied research as from various fields of industry. Biomimetics has a high innovation potential and offers the possibility for the development of sustainable technical products and production chains. On the one hand, novel sophisticated methods for quantitatively analyzing and simulating the form-structure-function-relationship on various hierarchical levels allow new

fascination insights in multi-scale mechanics and other functions of biological structures, materials and surfaces. On the other hand, recent developments in computational design and simulation together with new production methods enable for the first time the transfer of many outstanding properties of the biological role models into innovative biomimetic products for reasonable costs which makes them interesting for applications in many fields of technology and building construction.

Invited Talk

BP 11.3 Tue 10:30 HSZ 02

Cellulose bio-inspired hierarchical structures — •SILVIA VIGNOLINI — Lensfield Road Cambridge CB2 1EW UK

Nature's most vivid colours rely on the ability to produce complex and hierarchical photonic structures with lattice constants on the order of the wavelength of visible radiation. A recurring strategy design that is found both in the animal and plant kingdoms for producing such effects is the helicoidal multilayers. In such structures, a series of individual nano-fibers (made of natural polymers as cellulose and chitin) are arranged parallel to each other in stacked planes. When distance between such planes is comparable to the wavelength of light, a strong polarised, colour selective response can be obtained. These helicoidal multilayers are generally structured on the micro-scale and macroscopic scale giving rise to complex hierarchical structures.

Biomimetic with cellulose-based architectures enables us to fabricate novel photonic structures using low cost materials in ambient conditions. Importantly, it also allows us to understand the biological processes at work during the growth of these structures in plants. In this talk the route for the fabrication of complex bio-mimetic cellulose-based photonic structures will be presented and the optical properties of artificial structures will be analyzed and compared with the natural ones.

15 min break

Invited Talk

BP 11.4 Tue 11:15 HSZ 02

Strong Flexible Bioenabled Nanocomposites for Sustainable Sensing — •VLADIMIR TSUKURUK — School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, USA

I discuss recent results from our research group on designing flexible and strong responsive polymer and biopolymer nanocomposite materials and structures for advanced flexible sensing and electronic applications. Ultrathin silk fibroin proteins and chemically modified cellulose nanocrystals were assembled in order to control intimate assembly with graphene oxide sheets with controlled surface chemical composition on

planar and curved substrates. We demonstrated flexible laminated bionanocomposites with developed biointerphases that facilitate extremely high elastic modulus, bending flexibility, and toughness. Both experimental and computational methods were undertaken to address silk fibroin adsorption at heterogeneous surfaces of graphene oxide with different degrees of oxidation. Graphene oxide and reduced graphene oxide sheets at various levels of oxidation were compared with silicon dioxide (SiO₂) as a benchmark substrate. We concluded that silk fibroin readily forms single molecule proto-nanofibrils with β -sheet structures on oxidized graphene oxide surfaces but aggregated globular structures on the hydrophobic surfaces. Finally, electrochemical-assisted photolithography has been utilized for high spatial resolution conductive patterning of these nanocomposites with high local electrical conductivity, sharp boundaries, and optical transparency. Some peculiar features of these flexible bionanocomposites can be explored for tactile recognition, remote sensing, and low-noise SERS substrates.

BP 12: Microswimmers I (Joint Session DY/BP)

Time: Tuesday 9:30–13:00

Location: HÜL 186

Invited Talk

BP 12.1 Tue 9:30 HÜL 186

Tactic Response of Synthetic Microswimmers in Gravitational and Optical Fields — ●CLEMENS BECHINGER — 2. Physikalisches Institut, Universität Stuttgart

Numerous motile organisms have developed intriguing steering mechanisms allowing them to orientate and navigate within gravitational, chemical or light fields. Such tactic response strongly promotes e.g., the search for food, reproduction and/or escape from unfavorable ambient conditions and is therefore an essential aspect of life. Unlike living systems, where tactic behavior is typically achieved by complex internal signal pathways, it is not obvious how this can be imposed on synthetic microswimmers which are distinguished by rather simple internal structures. Using light-activated self-propelled particles, we demonstrate that autonomous steering in gravitational fields and light gradients can be achieved without invoking a complex internal machinery but simply by the combination of viscous forces and torques which naturally arise during self-propulsion in liquids. These findings, which are confirmed by theory and simulations, make the use of artificial swimmers as micro-shuttles for targeted drug delivery to appear promising.

1. Lozano, Hagen, Löwen, Bechinger, Nat. Comm. 7, 12828 (2016).
2. Hagen, Kümmel, Wittkowski, Takagi, Löwen, Bechinger, Nat. Comm. 5, 4829 (2014).

BP 12.2 Tue 10:00 HÜL 186

Fission and fusion of microswimmer clusters — ●ANDREAS KAISER¹, FRANCISCA GUZMÁN-LASTRA², and HARTMUT LÖWEN² — ¹Materials Science Division, Argonne National Laboratory, 9700 South Cass Ave, Argonne, Illinois 60439, USA — ²Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

Fission and fusion processes of particles clusters occur in many areas of physics and chemistry from subnuclear to astronomic length scales. Here we study fission and fusion of magnetic microswimmer clusters [1] as governed by their hydrodynamic and dipolar interactions. Rich scenarios are found which depend crucially on whether the swimmer is a pusher or a puller.

A linear magnetic chain of pullers is stable while a pusher chain shows a cascade of fission processes as the self-propulsion velocity is increased. Contrarily, magnetic ring clusters show fission for any type of swimmer. Moreover, we find a plethora of possible fusion scenarios if a single swimmer collides with a ringlike cluster and two rings spontaneously collide [2].

[1] A. Kaiser, K. Popowa, and H. Löwen, Phys. Rev. E 92, 012301 (2015)

[2] F. Guzmán-Lastra, A. Kaiser, and H. Löwen, Nature Commun. 7, 13519 (2016)

BP 12.3 Tue 10:15 HÜL 186

Optimal decision making in sperm chemotaxis — ●JUSTUS A. KROMER and BENJAMIN M. FRIEDRICH — cfaed, TU Dresden

Sperm cells follow dilute chemical gradients to find the egg in a process termed chemotaxis. To evaluate local concentrations of chemoattractant,

Invited Talk

BP 11.5 Tue 11:45 HSZ 02

3D laser nano-printing of rationally designed materials — ●MARTIN WEGENER — Karlsruhe Institute of Technology, Karlsruhe, Germany

Broadly speaking, 3D structures and materials can be designed by using the human brain, computer-based (topology) optimization, or inspiration from nature. Regardless of how a 3D blueprint has been obtained, it eventually needs to be manufactured. 3D laser printing on the micro- and nanometer scale has become a versatile and reliable workhorse for accomplishing this task. Here, we review recent examples from our group. This includes micropolar metamaterials with behavior beyond ordinary continuum mechanics, metamaterials with effectively negative thermal expansion from positive constituents, and electrical metamaterials with unusual direction and sign of the Hall voltage.

tant, sperm detect single attractant molecules, while moving along helical paths. This noisy chemical input signal regulates the flagellar beat to steer the cell up-gradient. Recent experiments showed that sperm cells can switch between two distinct steering modes in a situation-specific manner [1]. While swimming up-gradient, cells employ a mode of conservative steering, characterized by slow bending of the helical swimming path towards the direction of the concentration gradient. In contrast, if a cell accidentally swims down-gradient, it responds with a vigorous steering maneuver, characterized by fast helix bending.

Here, we present a theoretical description of this cellular decision making, formulated as a Markov decision process in the framework of a stochastic single-player game. We predict that decision making would provide no benefit in a hypothetical noise-free world, but substantially increases the chances to find the egg at physiological levels of sensing noise. Our work exemplifies the fundamental trade-off choice between responding accurately or responding fast for navigating cells.

[1] J.F. Jikeli et al. Nature Communications 6, 7985 (2015)

BP 12.4 Tue 10:30 HÜL 186

Lattice Boltzmann study of magnetocapillary microswimmers — ●ALEXANDER SUKHOV¹, QINGGUANG XIE², and JENS HARTING^{1,2} — ¹Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Forschungszentrum Jülich GmbH, Fürther Straße 248, 90429 Nürnberg, Germany — ²Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, NL-5600MB Eindhoven, The Netherlands

Magnetocapillary swimmers - a system of three or more paramagnetic beads trapped at a fluid-gas interface - attracted recently considerable theoretical [1] and experimental attention [2]. Due to an interplay of attractive capillary and repulsive magnetic dipole-dipole interactions the swimmer can be stabilized. By applying a set of a static and a time-dependent magnetic field its position and the velocity direction can also be well manipulated. The last makes the swimmers potentially interesting for multiple applications ranging from a controlled cleaning of liquid interfaces to even a drug delivery or other medical applications *in vivo*.

Using a hybrid lattice Boltzmann and discrete element method we show a sharp dependence of the average speed of the swimmer on the frequency of the time-dependent magnetic field, demonstrate the control of the direction of the swimmer motion using B-fields and also analyze the obtained results analytically. [1] R. Chinomona, J. Lajeunesse, W.H. Mitchell, Y. Yao and S.E. Spagnolie, Soft Matter 11, 1828 (2015). [2] G. Grosjean, G. Lagubeau, A. Darras, M. Hubert, G. Lumay and N. Vanderwalle, Sci. Rep. 5, 16035 (2015).

BP 12.5 Tue 10:45 HÜL 186

Swimming *Bacillus subtilis* with different number of flagella — ●JAVAD NAJAFI¹, FLORIAN ALTEGOER², THOMAS JOHN¹, GERT BANGE², and CHRISTIAN WAGNER¹ — ¹Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — ²LOEWE Center for Synthetic Microbiology (Synmikro), Philipps-University Marburg, Marburg, Germany

Microorganisms generally use so called flexible appendages known as

flagella to swim in aqueous media. Different species have various flagellar number and while single flagellum is enough for swimming, it is not understood well why some bacteria synthesize several flagella. We statistically investigate the swimming of multi-flagellated bacteria by characterizing the influence of flagellar number of genetically manipulated strains of *Bacillus subtilis* on diverse swimming parameters. We find that while numerous flagella are not significantly advantageous in terms of propulsion speed, it slightly changes running time and angular quantities. In a homogeneous medium, the strain with more flagella has an increased rotational diffusion and turning angle after tumbling. Consequently, the cells with more flagella tend to turn in larger angles that causes smaller translational diffusion coefficient and localized motion. We use Langevin simulation based on experimental parameters which enables us to disentangle the effect of turning angle and rotational diffusion on translational diffusion.

BP 12.6 Tue 11:00 HÜL 186

Intermediate scattering function of an anisotropic circle swimmer — ●CHRISTINA KURZTHALER and THOMAS FRANOSCH — Institut für theoretische Physik, Universität Innsbruck, Technikerstraße 21A, 6020 Innsbruck, Austria

A plethora of active agents ranging from biological microswimmers to artificially synthesized self-propelled particles exhibit peculiar dynamical behavior while moving in aqueous media at low Reynolds number. These active particles are intrinsically out of equilibrium and their transport properties are highly sensitive to their body shape, the symmetry of the propulsion mechanism, and also interactions with interfaces, which all have shown to induce a chiral swimming pattern. Here, we theoretically characterize the oscillatory dynamics of these Brownian circle swimmers in terms of the directly measurable intermediate scattering function (ISF), i.e. the characteristic function of the random displacements [1]. We identify different spatiotemporal regimes reflecting the bare translational diffusion at large wavenumbers, the persistent circular motion at intermediate wavenumbers and an enhanced effective diffusion at small wavenumbers. In particular, the circular motion of the particle manifests in characteristic oscillations of the ISF away from zero in contrast to oscillations around zero that can be traced back to the persistent swimming motion only. Furthermore, we obtain an exact expression for the non-Gaussian parameter, which displays oscillations at intermediate times mirroring the chiral swimming pattern of these active agents. [1] C. Kurzthaler, S. Leitmann, T. Franosch, Scientific Reports 6, 36702 (2016).

15min. break

Invited Talk

BP 12.7 Tue 11:30 HÜL 186

Emergent structures in actuated magnetic and active colloidal suspensions — ●IGNACIO PAGONABARRAGA — University of Barcelona, Barcelona, Spain

Actuated and autocatalytic colloids constitute systems that are intrinsically out of equilibrium. As a result of their dynamic interactions, they can show a rich variety of self-assembly scenarios. The observed self-assembled structures make these systems very sensitive to external forcing, hence making actuated and active matter a fertile ground to explore and develop mechanically tunable materials.

I will analyze the basic physical mechanisms that control the collective behavior of two kinds of colloidal particles that move in a liquid medium. Confined magnetic colloids can rectify their motion when actuated with a rotating magnetic field, acting as a hydrodynamic conveyor belt. Self-assembled chains of rotors propel faster than individual ones, reaching a saturation speed at distances where induced-flow additivity vanishes. The development of Janus colloids has opened the possibility to create synthetic microrobots that can move due to the chemical reactions they catalyze on their heterogeneous surfaces. The motion of chemically powered colloids is intricate because of the interplay between chemical and hydrodynamic interactions. These dynamic interactions have a strong impact in the collective behavior of these suspensions. I will describe the analogies and specificities in the hydrodynamic coupling that characterize these two types of systems.

BP 12.8 Tue 12:00 HÜL 186

Phase diagram of microswimmers in bulk — ●FABIAN JAN

SCHWARZENDAHL, STEPHAN HERMINGHAUS, and MARCO G. MAZZA — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany

The hydrodynamic flow field of microswimmers such as bacteria or algae can be classified into two categories: pushers and pullers. Bacteria like *E. coli* create a force dipole pushing the fluid away at their front and rear. On the other hand algae like *Chlamydomonas reinhardtii* create a force dipole that pulls the fluid towards them at the front and rear. We study the bulk behaviour of both types using a combination of molecular dynamic (MD) and stochastic rotational dynamic (SRD) simulations. Here, we use a minimal model for the swimmers accounting for hydrodynamic (SRD) as well as steric (MD) interactions. We find a rich phase diagram showing clustering as well as nematic states.

BP 12.9 Tue 12:15 HÜL 186

Collective migration under hydrodynamic interactions - a computational approach — ●AXEL VOIGT and WIELAND MARTH — Institut für Wissenschaftliches Rechnen, TU Dresden, Germany

Substrate-based cell motility is essential for fundamental biological processes, such as tissue growth, wound healing and immune response. Even if a comprehensive understanding of this motility mode remains elusive, progress has been achieved in its modeling using a whole cell physical model. The model takes into account the main mechanisms of cell motility - actin polymerization, substrate mediated adhesion and actin-myosin dynamics and combines it with steric cell-cell and hydrodynamic interactions. The model predicts the onset of collective cell migration, which emerges spontaneously as a result of inelastic collisions of neighboring cells. Each cell here modeled as an active polar gel, is accomplished with two vortices if it moves. Open collision of two cells the two vortices which come close to each other annihilate. This leads to a rotation of the cells and together with the deformation and the reorientation of the actin filaments in each cell induces alignment of these cells and leads to persistent translational collective migration. The effect for low Reynolds numbers is as strong as in the non-hydrodynamic model, but it decreases with increasing Reynolds number.

BP 12.10 Tue 12:30 HÜL 186

Swimming by buckling: low Reynolds number swimming by shape hysteresis — ●HORST-HOLGER BOLTZ^{1,2} and JAN KIERFELD² — ¹Institut für nichtlineare Dynamik, Fakultät Physik, Georg-August-Universität Göttingen, Göttingen, Deutschland — ²Fakultät Physik, Technische Universität Dortmund, Dortmund, Deutschland

We present a low Reynolds number swimming concept based on an oscillatory change in a parameter controlling a hysteretic shape transition, which converts the time-reversible parameter changes into non-time-reversible shape changes leading to a net swimming motion. As realization of this general concept we propose and investigate the swimming locomotion of a spherical elastic capsule that undergoes repeated hysteretic buckling under a time-reversible periodic volume change. We show analytically and by numerical simulation based on the boundary integral method that the hysteretic switching gives rise to net locomotion at low Reynolds numbers. We characterize the swimming mechanism and its efficiency in dependence on the elastic properties capsule and derive the characteristic behaviour of the net swimming velocity.

BP 12.11 Tue 12:45 HÜL 186

A kinetic theory for dynamics of self-propelled magnetic suspensions — ●FABIAN ROUVEN KÖSSEL and SARA JABBARI-FAROUI — Johannes Gutenberg-Universität - Institut für Physik

Inspired by novel dynamical behaviour of magnetotactic bacteria, we present a minimal kinetic model for dilute suspensions of magnetic self-propelled particles. Our kinetic theory couples a Fokker-Planck equation of active particles in an external magnetic field to a Stokes-flow equation. Including the hydrodynamic stress contributions due to self-propulsion and magnetic torque in the Stokes flow we investigate the interplay between internal and external drives on the dynamics and effective viscosity of active suspensions. Through the linear stability analysis and full numerical simulations of our model, we examine the role of the external magnetic field on stability of aligned suspensions and their complex flow patterns.

BP 13: Bioimaging and Spectroscopy II

Time: Tuesday 9:30–11:00

Location: HÜL 386

Invited Talk

BP 13.1 Tue 9:30 HÜL 386

X-ray imaging of Cells and Tissues — •TIM SALDITT — Georg-August-Universität Göttingen, Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

X-rays can provide information about the functional (interior) architecture of unstained biological cells and tissues. However, this potential of hard x-rays in view of penetration power, high spatial resolution, quantitative contrast, and compatibility with environmental conditions has to date not been fully developed, mainly due to significant challenges in x-ray optics. With the advent of highly brilliant radiation, coherent focusing, and lens-less diffractive imaging this situation has changed. We show how nano-focused coherent x-ray synchrotron beams can be used for scanning as well as for full field holographic x-ray imaging.

Following an introduction to the basic concepts of lensless x-ray imaging, different recent examples of biological imaging are presented, ranging from bacterial and eukaryotic cells, to the level of tissue and organs.

BP 13.2 Tue 10:00 HÜL 386

(Nanoscale) 3D virtual histology of neuronal tissues — •MAREIKE TÖPPERWIEN¹, MARTIN KRENKEL¹, KRISTIN MÜLLER¹, BENJAMIN COOPER², JÜRGEN GOLDSCHMIDT³, and TIM SALDITT¹ — ¹Institute for X-Ray Physics, Göttingen, Germany — ²Max Planck Institute for Experimental Medicine, Göttingen, Germany — ³Leibniz Institute for Neurobiology, Magdeburg, Germany

Studies of the brain cytoarchitecture in mammals are routinely performed by classical histology, i.e. by examining the tissue under a light microscope after serial sectioning and subsequent staining of the sections. The procedure is labor-intensive and the three-dimensional (3d) anatomy can only be determined after aligning the individual sections. Hard x-ray computed tomography (CT) is a promising alternative due to the potential resolution and high penetration depth, allowing for non-destructive imaging of the sample. However, in classical CT contrast formation is based on absorption of the x-rays, leading to a weak contrast for soft tissue like the brain and therefore diminishing the resolution. In order to visualize also weakly absorbing samples, the phase shift induced by the sample in the (partially) coherent beam can be used instead. As the optical constants leading to this shifted phase are up to 1000 times larger for soft tissues, contrast is increased. We use free-space propagation behind the object to convert this phase shift to a measurable intensity image. As contrast formation is based on interference of the disturbed wave fronts, the original phase distribution has to be reconstructed from the intensity images using suitable phase retrieval algorithms. In this work, we present x-ray phase-contrast tomography of neuronal tissues at our recently upgraded waveguide-based holo-tomography instrument GINIX at DESY. This setup allows for high resolution recordings with adjustable field of view and resolution, down to voxel sizes in the range of a few ten nanometers. We optimize for contrast and resolution by comparing different preparation techniques and recording strategies, reaching sub-cellular resolution in mm-sized tissue. Further, we show that even compact laboratory CT at an optimized liquid-metal jet microfocus source combined with suitable phase retrieval algorithms and preparation protocols enables single cell sensitivity in large reconstruction volumes of mouse brain which are consistent with classical histology results.

BP 13.3 Tue 10:15 HÜL 386

Brillouin Microscopy: A non-invasive way of studying elasticity in biological tissue — •DMITRY RICHTER^{1,2}, ALBA DIZ-MUÑOZ¹, and ROBERT PREVEDEL¹ — ¹European Molecular Biology Laboratory, Heidelberg, Germany — ²Heidelberg University, Heidelberg, Germany

In order to map the elastic properties of cells and tissues, a spatial resolution in the order of the diffraction limit and access to internal

structures is required. Up until now elastography has employed insufficient methods; techniques such as atomic-force microscopy require mechanical contact or invasion, giving no information about the internal structure. On the other hand, macroscopic methods like ultrasound imaging are unable to resolve cellular/subcellular components.

A possible alternative is Brillouin spectroscopy. It is based on the inelastic scattering of light on thermally induced, low frequency phonons, enabling a non-contact, high resolution study of elastic properties [1, 2]. Here, we discuss Brillouin microscopy as an imaging tool, highlighting its potential applications in biology as well as its inherent challenges and limitations. Moreover we show preliminary experimental results on single cells and multicellular organisms.

[1] G. Scarcelli, S. H. Yun, *Nature photonics* (2008)

[2] F. Palombo et al, *Analyst* (2014)

BP 13.4 Tue 10:30 HÜL 386

Three-dimensional surface reconstruction and panoramic optical action potential mapping of mammalian hearts — •JOHANNES SCHRÖDER-SCHETELIG¹, TARIQ BAIG-MEININGHAUS¹, DANIEL HORNING¹, and STEFAN LUTHER^{1,2,3} — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Germany — ³Department of Pharmacology, University Medical Center, Göttingen, Germany

We describe experimental setup and methods for 3D panoramic optical mapping of small to big mammalian hearts to study various dynamic electro-physiological properties of the healthy and diseased heart. Whole hearts of rabbits and pigs were excised and kept alive in a Langendorff-perfusion system, immobilized by excitation-contraction decoupler and stained with voltage-sensitive dye. Four high-speed cameras were positioned around the perfusion bath and their optical mapping calibrated. The 3D epicardium was reconstructed as a triangular mesh. Images from all cameras were projected onto the mesh and combined into a 2D texture image, for which a suitable mapping to the unit sphere was established. The system facilitates accurate measurement and analysis of the dynamic excitation wave propagation on the 3D heart surface during regular and irregular activity. Knowledge of the coordinate mapping between 2D texture images and 3D curved surface allows for computation of properties like curvature-corrected conduction velocity. Alignment with CT-scan of the heart is used for analyzing the correlation between surficial activity and underlying structure.

BP 13.5 Tue 10:45 HÜL 386

Investigations of squamous cell carcinoma cells and dysplastic oral keratinocytes — •MAJA STRUGAČEVAC¹, SUSANNE STEEGER¹, JAN LIETZ¹, JULIA KRISTIN², MARCEL GLAAS², JÖRG SCHIPPER², and MATHIAS GETZLAFF¹ — ¹Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf — ²Hals-Nasen-Ohrenklinik, Universitätsklinikum Düsseldorf

The aim of this study is to develop new, alternative, cell-selective treatment strategies for squamous cell carcinoma of the head-neck area. As one of first steps mechano-elastic properties of oral carcinoma cells (HNSCC) were examined using Atomic Force Microscopy (AFM). The Young's Modulus calculated by the Hertzian Model was determined in order to quantify the elasticity of the cells. As known the differences between elasticities of carcinoma and benign cells can - in part - be attributed to the modified cytoskeleton of cancer cells.

Squamous cell carcinoma cells as well as oral keratinocytes are examined by confocal fluorescence microscopy in order to obtain more information about physical cell properties. Different markers allow us to highlight specific cell organelles including cell membranes and cytoskeleton. This contribution focuses on staining optimization and investigation of differences between both cell lines.

BP 14: Physics of *Physarum polycephalum* and Other Slime Molds - Joint Focus Session (BP/DY) organized by Hans-Günther Döbereiner

Time: Tuesday 9:30–13:00

Location: SCH A251

Invited Talk

BP 14.1 Tue 9:30 SCH A251

Laminar mixing in tubular networks of plasmodial slime moulds — ●MARCUS HAUSER — Otto-von-Guericke-Universität Magdeburg, Institut für Biometrie und Medizinische Informatik, Magdeburg, Germany

The plasmodium of the unicellular slime mould *Physarum polycephalum* forms an extended, at times giant, vascular network which is used for transportation of protoplasm through the cell. The transport is driven by pressure gradients generated by peristaltic pumping, leading to a flow that reverses its direction periodically. Although the flow in the veins of *P. polycephalum* is always parabolic, protoplasm and particles suspended in it are effectively and rapidly distributed within the cell. To elucidate how an effective mixing is achieved in such a microfluidic system with Womersley flow (at low Womersley and Reynolds numbers), we performed micro-PIV experiments and advect virtual tracers in the determined time-dependent flow fields. Flow splitting and flow reversals at branchings of veins, as well as small fluctuations in the flow patterns at the branchings of veins play key roles in providing for an efficient mixing of protoplasm in the cell.

BP 14.2 Tue 10:00 SCH A251

Calcium dynamics in *Physarum polycephalum* — ●MIRNA KRAMAR and KAREN ALIM — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Calcium is a known regulator of myosin across all living organisms, as well as a key player in cell signalling. We study the effects of calcium on morphogenesis, locomotion and healing in the plasmodium of *Physarum polycephalum*. *Physarum* is a giant multinucleate and unicellular organism. The organism uses peristaltic contractions of the actomyosin layer to create shuttle streaming of the cytoplasm throughout its network of tubes. Upon a change of environmental conditions, the contractions change and cause a reorganization of the network. The mechanism that propagates information within the body and results in the network reorganization is not yet clear. We hypothesise that calcium plays the key role in this process by directly influencing the myosin and thus causing a local change in the contractions. Using an approach with two fluorescent dyes, we label free calcium ions and show the response of calcium upon the application of various stimuli to the plasmodium.

BP 14.3 Tue 10:15 SCH A251

Light stimuli trigger local and global cellular response in *Physarum polycephalum* — ●FELIX BÄUERLE and KAREN ALIM — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The slime mold *Physarum polycephalum* excels in adapting its network-like morphology to its environment. As a giant, single cell it is able to collect localised cues and form a complex organism-wide response. For example, *Physarum* can find the shortest path in a maze and connect sparse food sources to choose a balanced diet. How are localised cues collected, integrated and mediated over the whole organism to perform these complex tasks? To tackle these questions we study *Physarum*'s pruning reaction to light stimuli. *Physarum*'s body consists of protoplasmic tubes which contract rhythmically. These contractions show distinct temporal patterns until pruning is completed. We found that *Physarum* shows a whole-cell response shortly after light application and then gradually transforms the illuminated region into an autonomous domain. Identifying the interplay between such global and local reactions may advance our understanding of more general processes like wound healing or cell signalling.

BP 14.4 Tue 10:30 SCH A251

Scaling of foraging patterns under starvation in *Physarum polycephalum* — ●JONGHYUN LEE, CHRISTINA OETTMEIER, and HANS-GÜNTHER DÖBEREINER — Institut für Biophysik, Universität Bremen

Physarum polycephalum is garnering attention as a model organism for primitive intelligence and decision-making. We utilize microplasmodia, quasi-spherical fragments on the micrometer range, to investigate the reconstitution of the macroplasmodium from smaller components.

Generally, *Physarum* grows as an extended network, of which the transition from micro- to macroplasmodia occurs via percolation [1]. However, under starvation conditions, this transition does not occur. Instead, several bodies on the millimeter scale form and migrate radially away from the site of inoculation. We term these motile mesoplasmodia *satellites*. Satellite growth mode has defined phases of motility and rest, and their behaviour is spatio-temporally correlated. Satellites also have a stable and defined morphology, as well as a constant direction of movement.

Here, we present a description of this growth mode with simplified geometrical shapes. We describe scaling relationships of the number of satellites produced and their size based on initial conditions. The model predicts the size to increase and the number to decrease as the initial biomass increases, which fits well with the data. We discuss implications of assumptions and limitations of our scaling model.

[1] Fessel, A. et al. (2012), *Physical Review Letters* 109, 078103.

BP 14.5 Tue 10:45 SCH A251

Hydrodynamic Mechanism of Information Processing in *Physarum polycephalum* — ●CHRISTINA OETTMEIER, JONGHYUN LEE, and HANS-GÜNTHER DÖBEREINER — Institut für Biophysik, Universität Bremen

P. polycephalum exhibits rich spatiotemporal oscillatory behaviour. The organism's size spans orders of magnitude, from meter-sized networks to micrometer-sized amoebae. All morphotypes show actomyosin-based contraction-relaxation cycles resulting in protoplasmic streaming. When a food source is encountered, oscillations at the stimulated site increase in frequency. If repellents are encountered, the local oscillation frequency decreases [1]. This either leads to movement towards the attractant or away from the repellent. We study hydrodynamic information processing in amoeboid locomotion. Autonomous foraging units (mesoplasmodia) maintain their shape over hours while moving in straight trajectories at constant mean speed. Oscillations in the back of the mesoplasmodium cause endoplasm flows through the internal vein system and expand the frontal membrane. Frequencies at the back are higher than those at the front due to filtering. We use the electronic-hydraulic analogy to investigate this case of information processing. A vein segment can be described as a flexible tube, possessing a fluidic resistance (R) and fluidic capacitance (C). The electronic equivalent is a passive RC low pass filter. We use SPICE to simulate vein behaviour. Light- and EM data of mesoplasmodia and other morphotypes provide geometrical and elastic parameters.

[1] Durham, A.C.H. & Ridgway, E.B. (1976), *J. Cell Biol.* 69, 218-223

15 min break

BP 14.6 Tue 11:15 SCH A251

Control of Pattern Formation in *Dictyostelium discoideum* — ●TORSTEN ECKSTEIN, ALBERT BAE, VLADIMIR ZYKOV, EBERHARD BODENSCHATZ, and AZAM GHOLAMI — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We performed experiments to study pattern formation in colonies of *Dictyostelium discoideum* cells under the influence of a regular array of pillars in a petri dish.

We observed a new phenomenon: In the presence of caffeine, synchronized circular waves center on the pillars and dominate the wave dynamics. In a periodic arrangement of pillars, this results in regular macroscopic streaming patterns reminiscent of Voronoi domains centered around the pillars. The shape of these Voronoi domains is based on the underlying shape of the array of pillars. Thus, the macroscopic pattern can be tuned by changing the geometry of the array. We have shown that this phenomenon is found for different geometries, like a rectangular grid of pillars, a hexagonal grid of pillars and long walls as obstacles. It seems the defining characteristic in the system is the presence of a wall. Indeed, the phenomenon persists for pillars of a small height and shallow holes. Additionally, we varied the initial starvation times of the cells, finding that cells stream to the pillars for starvation times from 40 minutes to 7 hours. However, for starvation times of at least 5 hours the macroscopic pattern was lost.

BP 14.7 Tue 11:30 SCH A251

***Physarum polycephalum* single cells proceed through variable trajectories of gene expression to commitment and differentiation** — ●WOLFGANG MARWAN — Magdeburg Centre for Systems Biology, Otto-von-Guericke University, Magdeburg

Physarum polycephalum multinucleate giant plasmodial cells with their naturally synchronous population of nuclei provide ample homogeneous biological material for the analysis of signaling and gene expression dynamics at the single cell level. The developmental program of sporulation was triggered by a brief pulse of far-red light. By taking samples at different time points after the stimulus pulse, we followed how the gene expression pattern changes during commitment and differentiation. Time-dependent patterns of differential gene regulation showed that developmental trajectories were highly variable between individual cells. Differentiation control mutants that are locked in the proliferative state responded to the stimulus pulse by taking altered trajectories of gene expression that did not lead to sporulation. The results are discussed in the context of a Waddington-type quasipotential landscape of cell differentiation and the impact of mutations on its topology. We further discuss how *Physarum polycephalum* can contribute to a data-driven theoretically sound dynamic systems approach to the regulatory control of eukaryotic cell differentiation at genome-wide scale.

BP 14.8 Tue 11:55 SCH A251

Evolutionary experiments with slime molds — ●MARTIN GRUBE — Institute of Plant Science, University Graz, 8010 Graz, Austria

Acclimatisation describes adaptive physiological or behavioural changes of an organism, whereas adaptation is a process that involves heredity of selected traits. Slime molds seem to use information about past experiences for optimal decision-making, which is a simple form of learning. Yet it is still unclear to what extent this type of learning is mediated by acclimatization, habituation, or by hereditary adaptation. If slime molds can adapt by hereditary mechanisms to a wider range of growth conditions, and modify their growth features and foraging patterns accordingly, the diverged strains should then consistently differ by these properties, even when grown under the same conditions. We use serial transfers of plasmodia to select the best performing plasmodium after each transfer. By using micropasmodia initially we generate a genetic bottleneck to increase genetic drift. In our work we encountered several challenges, including the size variation of micropasmodia, which may cause a bias in the selection procedure, and which need to be addressed.

BP 14.9 Tue 12:20 SCH A251

Mechanochemical pattern formation in simple models of active viscoelastic fluids and solids with application to *Physarum polycephalum* — SERGIO ALONSO¹, MARKUS RADSZUWEIT², HARALD ENGEL³, and ●MARKUS BÄR⁴ — ¹Department of Physics, UPC Barcelona, Spain — ²Weierstrass Institute Berlin, Germany — ³Theoretische Physik, Technische Universität Berlin, Germany — ⁴Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, 10587 Berlin, Germany

A simple description for active stress generation is coupled to different model of passive viscoelasticity. Specifically, two models for viscoelastic fluids (Maxwell and Jeffrey model) and two models for viscoelastic solids (Kelvin-Voigt and Standard model) are investigated. Our focus is on the onset of mechano-chemical waves and patterns. We carry out linear stability analysis and numerical simulations in one spatial dimension. The primary instability is stationary for all active fluids considered, whereas all active solids exhibit an oscillatory instability. All instabilities found are of long-wavelength nature. The special case of a poroelastic two-phase model, where the active solid represents the cytoskeleton and is described by a Kelvin-Voigt model is coupled to a viscous fluid (cytosol) in which the free calcium concentrations obeys a potentially oscillatory reaction-diffusion dynamics. M. Radszuweit, H. Engel, M. Bär, PLoS One 2014; S. Alonso et al. Physica D 2016.

BP 14.10 Tue 12:45 SCH A251

Poroelastic two-phase model for droplets of *Physarum polycephalum* with free boundaries — ●DIRK ALEXANDER KULAWIAK¹, JAKOB LÖBER¹, MARKUS BÄR², and HARALD ENGEL¹ — ¹Institut für Theoretische Physik, TU Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — ²Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, 10587 Berlin, Germany

The model describes the cytoskeleton as an active viscoelastic solid phase coupled to a passive viscous fluid representing the cytosol. The active tension in the solid phase depends on the concentration of a regulating agent that is advected by the fluid phase. In [1] it was shown that under rigid boundary conditions that impose a fixed shape, this model reproduces a large variety of mechano-chemical patterns; these include traveling and standing waves, turbulent patterns, rotating spirals and antiphase oscillations in line with experimental observations of contraction patterns in protoplasmic droplets of *Physarum polycephalum*. Here we present a free-boundary approach to the model of the moving droplet. We find deformations of the droplet boundary as well as oscillatory and chaotic changes in the droplets position.

BP 15: Colloids and Complex Fluids I (Joint Session CPP/BP/DY)

Time: Tuesday 11:30–13:00

Location: ZEU 255

BP 15.1 Tue 11:30 ZEU 255

Small activity differences drive phase separation in polymers — ●JAN SMREK and KURT KREMER — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Recent theoretical studies found that mixtures of active and passive colloidal particles phase separate but only at very high activity ratio. The high value poses serious obstacles for experimental exploration of this phenomenon. Here we show using simulations that when the active and passive particles are *polymers*, the critical activity ratio decreases with the polymer length. This not only facilitates the experiments but also has implications on the DNA organization in living cell nuclei. Entropy production can be used as an accurate indicator of this non-equilibrium phase transition.

BP 15.2 Tue 11:45 ZEU 255

Corresponding States Law For Protein Solutions — ●FLORIAN PLATTEN and STEFAN U. EGELHAAF — Heinrich Heine University, Condensed Matter Physics Laboratory, Duesseldorf, Germany

The extended law of corresponding states, as proposed by Noro and Frenkel, involves a mapping of the phase behavior of systems with short-ranged attractions. We test its applicability to protein solutions with their complex interactions. We successfully map the experimentally determined metastable gas-liquid binodals to the binodals of short-ranged square-well fluids. This is achieved by representing the binodals as a function of the temperature scaled with the critical temperature (or as a function of the reduced second virial coefficient) and

the concentration scaled by the cube of an effective particle diameter, where the scalings take into account the attractive and repulsive contributions to the interaction potential, respectively. The scaled binodals of the protein solutions coincide with simulation data of the adhesive hard-sphere fluid. Furthermore, once the repulsive contributions are taken into account by the effective particle diameter, the temperature dependence of the reduced second virial coefficients follows a master curve that corresponds to a linear temperature dependence of the depth of the square-well potential. We moreover demonstrate that, based on this approach and cloud-point measurements only, second virial coefficients can be estimated, which we show to agree with values determined by light scattering or by Derjaguin-Landau-Verwey-Overbeek (DLVO)-based calculations.

Platten et al., J. Chem. Phys. 142, 174905 (2015).

BP 15.3 Tue 12:00 ZEU 255

Critical Casimir interactions between Janus particles — ●MARCEL LABBÉ-LAURENT and SIEGFRIED DIETRICH — Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Critical fluctuations in binary liquid mixtures give rise to forces acting on immersed colloidal particles. Experiments have demonstrated a remarkable agreement with theoretical predictions for spherical colloids close to a (chemically patterned) substrate [1,2]. At the same time, there has been strong experimental and theoretical interest in studying the self-assembly and the phase behavior of patchy and Janus particles. Although a variety of effective interactions have been proposed to

drive the self-assembly, the critical Casimir effect stands out as being particularly suitable because it provides both attractive and repulsive interactions depending on the chemical surface properties, as well as a sensitive control of their strength via minute temperature changes. We present theoretical calculations for the interaction between a single Janus particle and a chemically structured substrate and the effective pair potential between two Janus cylinders as well as between two Janus spheres [3].

[1] C. Hertlein, L. Helden, A. Gambassi, S. Dietrich, and C. Bechinger, *Nature* **451**, 172 (2008).

[2] M. Tröndle, O. Zvyagolskaya, A. Gambassi, D. Vogt, L. Harnau, C. Bechinger, and S. Dietrich, *Mol. Phys.* **109**, 1169 (2011).

[3] M. Labbé-Laurent, and S. Dietrich, *Soft Matter* **12**, 6621 (2016).

BP 15.4 Tue 12:15 ZEU 255

From criticality to gelation in sticky spheres — DAVID RICHARD^{1,2}, THOMAS SPECK¹, and •CRISTOPHER PATRICK ROYALL² — ¹Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — ²HH Wills Physics Laboratory, Tyndall Avenue, Bristol, United Kingdom

Understanding the mechanism of dynamical arrest in liquids is a long standing challenge. Even for simple fluids, such as sticky spheres, an arrested gel can occur when the system is quenched sufficiently fast such that it cannot relax to equilibrium. For many systems the gelation arises at the gas-liquid phase boundary, forming a rigid but dilute network of bonded particles. In this study, we look at the critical behavior of sticky spheres combining confocal microscopy of colloid-polymer mixtures and Monte Carlo simulations of the square-well model. The mapping between those two is achieved via tracking colloids at the single-particle level and fitting pair distribution functions to the simulation data. We then compare the local structure via the topological cluster classification (TCC) method to identify locally favored structures (LFSs) along the critical path. We observe a very good agreement between experiments and simulations, where the growth of highly ordered structures are triggered even far away from the phase boundary. We discuss the link of those LFSs to the global percolating bond network.

BP 15.5 Tue 12:30 ZEU 255

Determination of crystal nucleation barriers for colloidal crystals from computer simulations — •PETER KOSS^{1,2}, ANTONIA STATT³, PETER VIRNAU¹, and KURT BINDER¹ — ¹Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg

9, 55128 Mainz, Germany — ²Graduate School of Excellence Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — ³Princeton University, Princeton, NJ 08544, USA

A fluid in equilibrium, confined in a finite volume, with a density exceeding the onset of freezing, may exhibit phase coexistence with a crystal nucleus surrounded by liquid or a gas. Classical nucleation theory predicts that the barrier of homogeneous nucleation is given by two contributions, the free energy gained by the creation of a crystal droplet and the free energy loss due to surface tension of the newly created interface. We obtain the excess free energy due to the surface of the crystalline nucleus by using a computational method suitable for the estimation of the chemical potential of dense fluids. Our analysis method is appropriate for crystal nuclei of all shapes, without suffering from ambiguities occurring when one needs a microscopic identification of the crystalline droplet. We present a novel analysis method to determine the coexistence pressure between fluid and crystal, and report that the nucleation barrier for a soft version of the effective Asakura-Oosawa model is compatible with a spherical shape, and consistent with classical nucleation theory [1].

[1] A. Statt, P. Virnau, and K. Binder, *Phys. Rev. Lett.* **114**, 026101 (2015).

BP 15.6 Tue 12:45 ZEU 255

Phonons and Elasticity in Disordered binary Crystals — •TADEUS RAS and MATTHIAS FUCHS — FB Physik, Univ. Konstanz

The “method of long waves” is a well-established tool for the study of elastic constants [1]. However, until recently, it had been lacking in crystals with point defects due to an unclear definition of the displacement field.

We present a generalization of the projection-operator approach employed in [2]. It yields expressions for the elastic constants valid in binary crystals with arbitrary amounts of point defects and up to the melting temperature. Further, both acoustic and optical phonon eigenfrequencies can be computed in linear response.

While density functionals from classical DFT serve as an input parameter to the approach it can also be employed experimentally to process measurement data. For demonstration, dispersion relations will be shown as obtained from molecular dynamics data of a hard sphere model crystal [3].

[1] D. C. Wallace, *Thermodynamics of Crystals* (Wiley, NY 1972).

[2] C. Walz and M. Fuchs, *Phys. Rev. B* **81**, 134110 (2010).

[3] L. Filion et. al., *Phys. Rev. Lett.* **107**, 168302 (2011).

BP 16: Biotechnology and Bioengineering

Time: Tuesday 11:30–12:30

Location: HÜL 386

Invited Talk BP 16.1 Tue 11:30 HÜL 386
Control on the nanoscale with DNA origami — •TIM LIEDL — Ludwig-Maximilians-Universität München

I will discuss two recent applications of DNA origami that illustrate the exceptional control that this technique provides on the nanoscale. Despite enormous efforts, placing guest molecules in designed DNA crystals remains a challenging goal. Ned Seeman and Chengde Mao reported a 3D DNA crystal based on the “tensegrity triangle”, where three DNA duplexes are interconnected in a self-restricting over-under, over-under, over-under fashion. By adopting their design principle, we present a tensegrity triangle design based on DNA origami that crystallizes into three-dimensional, micrometer-scale assemblies that can host gold nanoparticles at designated sites. Then I will present a DNA origami-based method of force spectroscopy that uses self-assembled nanoscopic power gauges, requires no macroscopic tools (magnetic tweezer, AFM tip or alike) to connect to the macroscopic world and can analyze large numbers of molecules in parallel. To exert the force, a single-stranded DNA that contains a specific sequence capable of recruiting a molecule of interest, spans from one arm of the DNA origami force clamp to the other. The force applied to the system can then be tuned by changing the length of the single strand in different variants of the force clamp. Note that the ssDNA here acts as an entropic spring element, whose spring constant is dependent on the number of bases per unit length. In our experiments we first studied a well-known Holliday junction sequence as a benchmark and then determined above which forces TBP fails to bind the TATA box.

BP 16.2 Tue 12:00 HÜL 386

Micropatterning of reagent-free, high energy crosslinked gelatin hydrogels for bioapplications — •ASTRID WEIDT¹, BENEDIKT HEYART², EMILIA WISOTZKI^{1,3}, MAREIKE ZINK¹, and S.G. MAYR^{3,4} — ¹Nachwuchsgruppe Biotechnologie und Biomedizin, Soft Matter Physics Division, Universität Leipzig, Germany — ²Institut für Biochemie und Biotechnologie, Technische Universität Braunschweig, Germany — ³Leibniz Institut für Oberflächenmodifizierung (IOM) e.V., Leipzig, Germany — ⁴Division of Surface Physics, Universität Leipzig, Germany

The development of biocompatible materials that support the regeneration of soft tissues is of high importance for medical applications. Materials such as collagen and gelatin show a great potential as graft materials and cell carriers, since they originate from the extracellular matrix. Adequate structuring of hydrogels as cellular substrates is mandatory for successful cell adhesion. Here, a reagent-free method for crosslinking and subsequent micropatterning of gelatin hydrogels was demonstrated. The simple and effective method of micromolding was employed to transfer structures in the micrometer range during electron irradiation onto gelatin. Thermally-stable substrates were fabricated, characterized by regular grooves with widths of 3.75 to 170 μm and depths of several hundred nanometers. We show that the microstructured hydrogels promote cell adhesion and contact guidance of NIH 3T3 mouse embryonic fibroblasts. Cells attached and adapted on the surfaces. Changes to the cell morphology were observed within 4 days in culture under physiological conditions.

BP 16.3 Tue 12:15 HÜL 386

Self-assembled hybrid protein nanofibers as basis for novel biomaterials — •CHRISTIAN HELBING¹, TANJA DECKERT-GAUDIG², GANG WEI³, VOLKER DECKERT², and KLAUS D. JANDT¹ — ¹Chair of Materials Science, Department of Materials Science and Technology, Otto-Schott-Institute of Materials Research, Faculty of Physics and Astronomy, Friedrich Schiller University Jena, Jena, Germany — ²Institute for Photonic Technology, Jena, Germany — ³Hybrid Materials Interfaces Group, Faculty of Production Engineering, University of Bremen, Bremen, Germany

Over the last years, the interest in materials consisting of biomolecules arranged in nanofibers increased. There is a special focus on plasma proteins for applications in nanofiber materials because of their high

biocompatibility. An easy feasible strategy to create these nanofibers is the self-assembly mechanism of protein molecules. Here we test the hypothesis that novel self-assembled hybrid protein nanofibers (PNNF) can consist of two different proteins. In this work we present, for the first time, self-assembled plasma hybrid PNNF consisting of two different plasma proteins. Further, long-time CD-measurements provide information about the fiber formation dynamics. Especially, for the PNNF hybrid it confirmed interactions between both molecules. Additionally, the influence of the second protein on the properties of the novel hybrid PNNF is shown. We confirmed the existence of a novel PNNF hybrid by tip enhanced raman spectroscopy and immunolabeling. These results lay the foundation for a novel biomaterial based on these PNNF/PNNF hybrids.

BP 17: Microswimmers II (Joint Session DY/BP)

Time: Tuesday 14:30–15:45

Location: HÜL 186

BP 17.1 Tue 14:30 HÜL 186

Self-propelled Janus Droplets: Properties and Applications — •LEONARD LI¹, MAHMOUD HOSSEINZADEH¹, MARTIN BRINKMANN¹, IGNACIO PAGONABARRAGA², RALF SEEMANN¹, and JEAN-BAPTISTE FLEURY¹ — ¹Saarland University, 66123 Saarbrücken, Germany — ²University of Barcelona, 08028 Barcelona, Spain

We report the existence of a new type of self-propelling Janus droplets in a continuous oil/surfactant solution. At start, the self-propulsion originates from a Marangoni flow generated by the solvent solubilization into the oily phase. During active motion, the droplets absorb a large amount of surfactant, which is preferentially soluble in the solvent phase. This surfactant adsorption into the droplet and the loss of solvent from the droplet lead, after some time, to spontaneous water/solvent phase separation and the formation of Janus droplet. In the Janus state, the solvent-rich droplet acts as a sink for the surfactant molecules, which get transported to and dissolved in the trailing droplet and thus drive the locomotion. Depending on initial solvent concentration the time before phase separation and thus the duration in the different propulsion regimes and with it different delivery modes can be programmed. After describing the properties of these active Janus droplets, we will present their possible applications.

BP 17.2 Tue 14:45 HÜL 186

Collective dynamics of active emulsions under light sheet microscopy — •BABAK VAJDI HOKMABAD, CARSTEN KRÜGER, and CORINNA MAASS — MPI for Dynamics and Self Organization, Göttingen

Liquid crystal droplets exhibit Marangoni-flow-induced self-propulsion in an aqueous surfactant solution well above the critical micelle concentration. We can mass produce identical droplets with biomimetic properties, rendering these artificial swimmers promising experimental models to investigate the collective dynamics of biological microswimmers. We have previously shown that dimensional confinement plays a crucial role in the collective behavior of such active emulsions.

We study the collective dynamics of dense droplets ensembles in various conditions of number density, swimmer speed and buoyancy, resulting in effects like clustering and caging, using a custom built light sheet fluorescence microscope. A macroscopic sample volume, containing several hundred swimmers, is scanned via a system of a synchronized thin laser sheet and selective plane microscope, and individual trajectories for multiple swimmers can be recorded over long time scales.

BP 17.3 Tue 15:00 HÜL 186

Chemotaxis and auto-chemotaxis of self-propelling droplets — CHENYU JIN, CARSTEN KRÜGER, and •CORINNA MAASS — MPI for Dynamics and Self Organization, Göttingen

Chemotaxis and auto-chemotaxis are key mechanisms in the dynamics of micro-organisms. However, chemical signalling and the natural environment of biological swimmers are generally complex, making them hard to access analytically. Simple artificial systems showing biomimetic features can provide vital insights. We present self-propelling droplet swimmers with both chemotactic and autochemo-

tactic properties, as well as microfluidic assays to study them quantitatively and reproducibly.

We demonstrate chemotaxis by guiding droplets through mazes in the presence of a chemical gradient.

To study auto-chemotaxis, we let swimmers pass through bifurcating microfluidic channels and record anticorrelations between the branch choices of consecutive droplets. We present an analytical model balancing a Brownian process versus a diffusion-governed gradient force able to explain our experimental findings.

BP 17.4 Tue 15:15 HÜL 186

Extreme fluctuations of active Brownian motion — •PATRICK PIETZONKA, KEVIN KLEINBECK, and UDO SEIFERT — II. Institut für theoretische Physik, Universität Stuttgart

In active Brownian motion, an internal propulsion mechanism interacts with translational and rotational thermal noise and other internal fluctuations to produce directed motion. We derive the distribution of its extreme fluctuations and identify its universal properties using large deviation theory [1]. The limits of slow and fast internal dynamics give rise to a kink-like and parabolic behavior of the corresponding rate functions, respectively. For dipolar Janus particles in two- and three-dimensions interacting with a field, we predict a novel symmetry akin to, but different from, the one related to entropy production. Measurements of these extreme fluctuations could thus be used to infer properties of the underlying, often hidden, network of states.

[1] P. Pietzonka, K. Kleinbeck, U. Seifert, New. J. Phys. **18**, 052001 (2016)

BP 17.5 Tue 15:30 HÜL 186

Collective Sedimentation of Squirmer under Gravity — •JAN-TIMM KUHR, FELIX RÜHLE, JOHANNES BLASCHKE, and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Biological microswimmers such as algae or plankton experience gravity. Recent theoretical studies on the sedimentation of microswimmers often explore the dilute case, where hydrodynamic and steric interactions between them can be neglected [1,2]. We apply parallelized MPCD simulations to study sedimentation of spherical squirmers under gravity and thereby explicitly include long-ranged hydrodynamic interactions also with bounding surfaces. We measure density profiles for systems of thousands of microswimmers and analyze how the ratio of active velocity to passive sedimentation velocity as well as the swimmer type (neutral, pusher, and puller) affect sedimentation.

Lower regions of the system are dominated by incomplete hexagonal layer formation with distinct orientation, whereas we recover an exponential density profile in the upper, less dense region. The average vertical orientation of the squirmers depends strongly on their vertical position as well as their type. Furthermore, we find that hydrodynamics organizes the microswimmers into convection cells, the strength of which changes with swimmer type and influences the sedimentation length.

[1] M. Enculescu and H. Stark, Phys. Rev. Lett. **107**, 058301 (2011).

[2] K. Wolff, A. Hahn, and H. Stark, Eur. Phys. J. E **36**, 43 (2013).

BP 18: Statistical Physics in Biological Systems II (Joint Session DY/BP)

Time: Tuesday 14:00–16:00

Location: ZEU 118

BP 18.1 Tue 14:00 ZEU 118

Epidemic spread in heterogeneous populations - Propagation of uncertainty and linear-noise approximation — ●FRANCISCO HERRERÍAS-AZCUÉ and TOBIAS GALLA — School of Physics and Astronomy, The University of Manchester, Manchester, UK

The assumption of homogeneity in classic epidemic models is known to be far from realistic; Different susceptibilities may arise from gene expression and strain mutation. We explore the effects of heterogeneity in susceptibility and infectivity on the stochastic susceptible-infective-recovered (SIR) model of epidemic spread. Our focus is on understanding how these heterogeneities and uncertainties propagate to long-term periodic outbreaks. To do so, we study a structured population consisting of sub-classes with different susceptibilities and infectivities. These are assigned at birth, drawn from underlying fixed distributions.

We show how the system can be reduced to a four dimensional set of equations at the fixed point in the deterministic limit, independent of the number of sub-classes, and we derive the Langevin dynamics characterising fluctuations about this fixed point. To characterise the resulting noise-induced cycles we calculate the power spectra of fluctuations, and determine the features of the distributions of susceptibilities and infectivities shaping the quasi-cycles. In particular we explore how the mean or spread of susceptibilities affect the magnitude of the epidemic, and the period of outbreak cycles. We also investigate the dynamic behaviour and relative phase lag of different sub-populations during the outbreaks.

BP 18.2 Tue 14:15 ZEU 118

Impact of stochastic migration on species diversity in meta-foodwebs consisting of several patches — ●TATJANA THIEL and BARBARA DROSSEL — Technische Universität Darmstadt, Germany

The structure of space has an appreciable influence on the diversity of ecosystems. So far, there are only few theoretical studies investigating the population dynamics of foodwebs consisting of many species that can migrate between several patches, and in most of these models migration is a continuous, deterministic process. However, when migration events are rare (for instance because the patches are far apart), migration is a stochastic process and should be modelled accordingly.

For this purpose, we place a foodweb model consisting of many species on a spatial network of several patches and evaluate the stable configurations and long-time patterns that arise due to the population dynamics. This dynamics has a deterministic contribution from the processes within a patch, and a stochastic contribution due to migration events, which are implemented using the Gillespie algorithm.

We will discuss how the frequency of migration events impacts species diversity on local and regional scales. Furthermore, we investigate in particular the adiabatic limit in which population dynamics always reaches an equilibrium before the next migration event and we will discuss which long-term scenarios are possible.

BP 18.3 Tue 14:30 ZEU 118

The Evolution of Network Structure and Species Diversity in an Evolutionary Meta-Foodweb Model — ●TOBIAS ROGGE¹, KORINNA T. ALLHOFF², and BARBARA DROSSEL¹ — ¹Technische Universität Darmstadt, Germany — ²Université Pierre et Marie Curie, Paris, France

Evolutionary foodweb models provide important insights into the stability and the functioning of ecosystems on long time scales, since the network structure is a highly nontrivial outcome of the ongoing processes of species addition and species deletion. Here, we present and investigate an evolutionary food web model that includes no population dynamics but generates nevertheless a large variety of complex, multi-trophic networks. In this model, species are characterized by a few traits that are based on their body mass and that determine the connections to other species in the network. The system evolves due to the addition of new species, which are modifications of existing species. Species survival depends on the predators, the prey, and the competitors of the new species. We investigate this model on one habitat as well as on many habitats coupled by migration. Depending on the parameters, the long-term dynamics of the network can show layered structures, highly dynamical configurations with frequent extinctions, or frozen configurations that allow no mutant to survive. We identify the conditions under which the different types of dynam-

ical and structural patterns emerge. Furthermore, we evaluate local and regional species diversities in the spatial model as well as species lifetime distributions, and we discuss them in an ecological context.

BP 18.4 Tue 14:45 ZEU 118

Mixed Percolation as a Model for Intra-Cellular Transport — ●ANDREAS KOHER¹, PATRICK HU¹, IGOR M. SOKOLOV², and PHILIPP HÖVEL¹ — ¹TU Berlin — ²HU Berlin

Intra-cellular diffusion is driven by a complex interplay between passively moving particles and a highly disordered, time-varying environment. To understand transport properties on a microscopical scale we propose a (mixed) percolation model that allows to reproduce a wide range of experimental observations analytically. The novel approach places a random walker on a lattice with *dynamic and static bonds*, i.e. parts of the lattice fluctuate with a given relaxation rate. Similar to static percolation problems, we find that the mean squared displacement undergoes a phase transition from a locally confined to a globally diffusing phase. However, unlike previous models the relaxation rate allows to fit short- and long-term transport properties to experimental observations. Finally, we validate our analytical results with Monte-Carlo simulations.

BP 18.5 Tue 15:00 ZEU 118

Entanglement of knotted DNA ring and an entwined DNA loop — ●SAEED NAJAFI and RAFFAELLO POTESIO — MPIP, Mainz, Germany

Self-entanglement and knotting can play a crucial role in the mechanical and functional properties of bio-polymers such as DNA and RNA strands and fibers. By means of computer simulations of model DNA systems, we demonstrate that the crossing pattern of a braid of entwined DNA rings has a large impact on its structural and dynamical properties. In particular, we identify under which conditions the braid crossing pattern enforces a positive and stronger correlation between the entangled rings.

BP 18.6 Tue 15:15 ZEU 118

Chirality-mediated interaction between knots on tensioned polymers — ●RAFFAELLO POTESIO — Max Planck Institute for Polymer Research, Mainz, Germany

Knots appear frequently in semiflexible (bio)polymers, including double-stranded DNA, and their presence can affect the polymers' physical and functional properties. It is possible and indeed often the case that multiple knots appear on a single chain, with effects which are under scrutiny since only a few years. In this talk I will discuss the equilibrium properties of two knots on a stretched semiflexible polymer, an idealization of a typical optical tweezer experiment. Specifically, I will focus on how the knots' relative chirality affects their interaction, rationalizing some of their pertinent features by means of simple effective models. The implications of the chirality-dependent knot-knot interaction will be discussed, in particular with respect to their consequences for the characterization and manipulation of these systems -be they artificial or of biological origin- and for their technological application.

BP 18.7 Tue 15:30 ZEU 118

Phenotypic switching as a strategy for persistence in stochastic environments — ●PETER HUFTON, YEN TING LIN, and TOBIAS GALLA — School of Physics and Astronomy, The University of Manchester, Manchester, UK

Bet-hedging constitutes a strategy for life to survive in demanding, fluctuating environments. The ideal example is found in bacterial populations: switching stochastically between phenotypes conveys a fitness advantage when exposed to episodes of antibiotics. But what does the optimum switching strategy look like when, as in nature, the environment is itself unpredictable? Here, we present a theoretical study of the dynamics of growing populations subject to stochastic environmental switching, and provide a general framework for the analytic study of the fitness of such populations. Our original approach utilises the piecewise-deterministic Markov process, a technique which has seen increasing use in modelling biochemical process. Our results reveal significantly different behaviours to those found in periodic environmental conditions. We report that stochastic environments produce globally fitter populations, and that the optimum switching regimes in

each case are markedly different.

BP 18.8 Tue 15:45 ZEU 118

Effect of slow-switching genetic states in gene regulatory network governing stem cell pluripotency — ●YEN TING LIN¹, PETER HUFTON², ESTHER LEE³, and DAVIT POTOYAN⁴ — ¹T-6 and CNLS, Los Alamos National Laboratory, USA — ²School of Physics and Astronomy, The University of Manchester, UK — ³Department of Bioengineering, Rice University, USA — ⁴Center for Theoretical Biological Physics, Rice University, USA

Construction of the gene regulatory network (GRN) from experimental data requires a post-experimental analysis which established the pairwise correlations between the measured dynamical quantities. Then as a coarse description, each gene controls and/or is controlled by an-

other gene(s), forming a network (GRN). From another perspective of a single gene, the expression mechanism is encapsulated by the central dogma: the mRNA transcribes the sequence, and then the mRNA left the chromatin and synthesizes proteins.

We present a detailed model combining these two approaches. Utilizing an analytic approximation we previously proposed, we show that the computational efficiency is dramatically increased on a GRN governing stem-cell differentiation. At different switching rates between the genetic states we inferred a unique parameter space which reproduces experimental results. Moreover, we found a unique space for the switching rates reproducing features from single-molecule experiments. Interestingly, the information entropy was maximized in this space. We argue that the consequence may be utilized to cell differentiations as an maximal information is encoded in the dynamics.

BP 19: Posters - Computational Biophysics

Time: Tuesday 14:00–16:00

Location: P1A

BP 19.1 Tue 14:00 P1A

Morphological properties of the epithelial tissue — ●JAKOV LOVRIĆ^{1,2}, SARA KALIMAN², and ANA-SUNČANA SMITH^{1,2} — ¹Institute Ruđer Bošković, Division of Physical Chemistry, Group for Computational Biosciences, Zagreb, Croatia — ²Institute for Theoretical Physics, PULS Group and Cluster of Excellence: EAM, FAU Erlangen-Nürnberg, Germany

Knowing the morphology of an epithelial tissue is important due to understanding processes like growth and development of the tissue, wound healing and progression of the cancer.

We study the structure of the MDCK II epithelial cells in circular colonies. Cell nuclei can be approximated with ellipses and the Voronoi tessellation generated by those ellipses coincides well with the cell membranes. We compare the tissue cells to the Voronoi cells generated by randomly packed ellipses obtained from the cell nuclei. The comparison is done by studying the probability distributions of chosen morphological measures calculated from the cells. We find that randomly packed ellipses reproduce the morphology of the tissue well at the low cell density. At high cell density we observe more regular structure of the tissue and we see the deviations of the random model from the cell tissue.

BP 19.2 Tue 14:00 P1A

Structure formation of oligopeptides in the PRIME20 model — ●ARNE BÖKER and WOLFGANG PAUL — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

Much effort has recently been put into understanding amyloid formation in polypeptides. The amyloid state is a structure in which polypeptides aggregate as a stack of β -sheets, which is usually not the native state, leading to loss of function. Amyloids can cause a variety of diseases (amyloidoses) such as Huntington's chorea, which is caused by an amyloid state of expanded poly-Glutamine sequences.

The relation between conformations of a polypeptide is governed by local minima in the free energy function. Coarse-grained models tend to simplify the free energy in such a way that these local minima are ignored. To circumvent this problem, the level of coarse graining needs to be chosen appropriately. PRIME20² provides reasonable detail by mapping each amino acid to four beads, but keeps parameter space simple with the set of interactions reduced to 19 energy parameters.

We perform thermodynamic simulations of single PRIME20 chains using the "SAMC"³ variation of Wang-Landau Monte Carlo sampling which provides insight in different statistical ensembles at the expense of dynamic information. The aforementioned poly-Glutamines are compared to poly-Alanines with a lower tendency to form β structure motifs.

²M. Cheon, I. Chang, C. K. Hall, *Proteins* **78**(2010):2950

³B. Werlich, T. Shakirov, M. P. Taylor, W. Paul, *Comp. Phys. Comm.* **186**(2015):65

BP 19.3 Tue 14:00 P1A

Automated tracking of Adelie penguins — ●ALEXANDER WINTERL¹, DANIEL ZITTERBART^{1,2}, SEBASTIAN RICHTER¹, RICHARD GERUM¹, and BEN FABRY¹ — ¹Department of Physics, Biophysics Group, Friedrich-Alexander-University Erlangen-Nuremberg, 91052, Erlangen, Germany — ²Alfred Wegener Institut, Helmholtz Zentrum

für Polar und Meeresforschung, 27568 Bremerhaven, Germany

Decision-making processes of colony-forming birds when they approach or leave their home colony e.g. during foraging are currently poorly understood and remain largely unexplored. To identify rules that govern such processes in Adelie penguins, we recorded high-resolution time-lapse images of a colony near Dumont d'Urville, Antarctica, during January and February 2015. We then developed an automated tracking software to follow the movements of all birds outside the colony within the field of view. To correctly allocate crossing tracks when two penguins pass each other, we model the penguin movements by an auto-regressive random walk that assumes that penguins do not abruptly change their speed and direction. 12 ambiguous tracks were selected and analyzed by human observers who watched the full time-lapse image sequence. Compared to this "ground truth", the assignment quality of the algorithm (25% error) was slightly inferior to human observers (17% error) when only the center of mass positions of the crossing tracks are provided. We conclude that reliable automated tracking of passing and crossing penguins requires the analysis of additional image information such as body posture and head orientation.

BP 19.4 Tue 14:00 P1A

Physical Analysis of One-Component Signaling in Bacteria — ●LINDA MARTINI and ULRICH GERLAND — Physics of Complex Biosystems, Department of Physics, Technical University of Munich

Adaptation to changing environments is of vital importance to bacterial cells and is enabled by sophisticated signal transduction systems. While classical two-component signaling is well studied, the mechanisms of one-component systems, where a single protein implements both sensing and response regulation, are mostly uncharacterized.

One such one-component system is the membrane-integrated protein CadC, which is part of the pH-stress response system in *E. Coli*. As it directly binds to the genomic DNA to regulate transcription, it faces a target search problem the dynamics of which are still to be understood.

Using kinetic Monte Carlo simulations of a lattice model, we focus on a characterization of the coupled stochastic dynamics of the DNA and the proteins, and its dependence on the system parameters. Understanding the kinetics of membrane-localized proteins specifically binding to a dynamic DNA will be important to interpret corresponding *in vitro* experiments and more generally to understand the biophysics of one-component signal transduction.

BP 19.5 Tue 14:00 P1A

Huddle-behavior simulation of emperor penguins — ●FLORIAN MORAWETZ¹, KLAUS MORAWETZ^{2,3,4}, and DANIEL ZITTERBART^{5,6} — ¹University of Rostock, Wismarsche Straße 8,18057 Rostock, Germany — ²Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — ³International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — ⁴Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ⁵Department of Physics, University of Erlangen-Nuremberg, Henkestrasse 91, 91052 Erlangen, Germany — ⁶Alfred Wegener Institut für Polar- und Meeresforschung, Am Handelshafen 12, 27570 Bremerhaven, Germany

Despite the deadly environmental conditions in the Antarctic, emperor

penguins have developed a surviving strategy which allows them to breed the eggs during 4 months of winter time. This is realized by a huddle of huge numbers of tightly grouped penguins. Though no individual has the overview to realize an optimized strategy of the whole huddle, it behaves according to certain rules which are vital for the survive. These rules are found employing a cellular automates model. First, each individual feels attracted by the most nearest *and* next-but-next-nearest neighbors which creates the attraction of the huddle. If a stress situation occurs like created by external enemy, the individuals cease to see the next-but-next-nearest neighbor but see only the next neighbors which leads to an expel of the crowded. Second, there is a pushing of an individual in front if too many sides of the individual are uncovered.

BP 19.6 Tue 14:00 P1A

Adaptive Resolution Simulations of Biomolecular Systems — ●RAFFAELE FIORENTINI, AOIFE FOGARTY, RAFFAELLO POTESTIO, and KURT KREMER — Max-Planck-Institut für Polymerforschung, Mainz, Germany

A fully atomistic modelling of many biophysical and biochemical processes at biologically relevant length- and time-scales is beyond our reach with current computational resources. One approach to overcome this difficulty is the use of multiscale simulation techniques in which different system components are simultaneously modelled at different levels of resolution, these being smoothly coupled together. In the case of biomolecules, functionally relevant parts of the system are modelled at as high a level of detail as necessary, while the remainder of the system is represented using less expensive models. Such a multiscale simulation can employ an adaptive resolution scheme, in which system components change their resolution on the fly during the simulation. Recently, the existing adaptive resolution (AdResS) methodology has been extended to biomolecular systems. We now demonstrate how the AdResS approach applies to the calculation of thermodynamical properties of such biomolecular systems.

BP 19.7 Tue 14:00 P1A

Classificatory Analysis of Biological Autofluorescence Spectra — ●IGNAS CIPLYŠ^{1,2}, VILMANTAS GEGŽNA^{1,2}, DARIUS VARANIUS^{1,2}, AURELIJA VAITKUVIENĖ¹, GUNORAS TERBETAS³, RUTA KURTINAITIENĖ⁴, JURGITA USINSKIENĖ⁵, and JUOZAS VILMANTIS VAITKUS¹ — ¹Institute of Applied Research, Vilnius University, Vilnius, Lithuania — ²Life Sciences Center, Institute of Biosciences, Vilnius University, Vilnius, Lithuania — ³Clinics of Neurology and Neurosurgery, Vilnius University, Vilnius, Lithuania — ⁴Hospital Santariskiu Klinikos, Vilnius University, Vilnius, Lithuania — ⁵National Cancer Institute, Vilnius University, Vilnius, Lithuania

This research deals with auto-fluorescence of biological specimens and its relations to medical diagnostics. The purpose of this study is to collect auto-fluorescence spectra from gynecological and intervertebral disc related specimens in various medical conditions and extract diagnostically relevant information through computational methods. The methods used include non-linear, univariate as well as multivariate statistical techniques focused on performance of classification and identification of the most informative spectral ranges. The main result: the fluorescence spectroscopy analysis might be recommended for medical practice, as well as at a point of care, and the efficiency of diagnostics expressed via balanced accuracy is up to 0.75-0.90. Further results and interpretation of analysis will be demonstrated during conference. The collected data base has to be increased to achieve more precise results.

BP 19.8 Tue 14:00 P1A

Optical-tweezer controlled translocation of DNA-bound proteins in MoS₂ nanopores — ●ANDREAS J MEYER and PETER REIMANN — Universität Bielefeld, Germany

Atomic monolayer MoS₂ membranes promise great sensitivity improvements in nanopore experiments compared to commonly used, much thicker silicon-nitride membranes.

We study the translocation dynamics of DNA and DNA-bound proteins in ultra-thin MoS₂ nanopores. Employing a worm-like chain model and Brownian dynamics we examine effects like two-state hopping and force hystereses, as were previously reported in SiN nanopores [1].

[1] A. Spiering, S. Getfert, A. Sischka, P. Reimann, and D. Anselmetti, Nano Lett., 11, 2978 (2011)

BP 19.9 Tue 14:00 P1A

Lateral trapping of DNA inside voltage gated nanopores —

●THOMAS TÖWS and PETER REIMANN — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

We consider a rigid cylinder, modelling a section of DNA, inside a solid state nanopore which is electrically gated by an all-around electrode integrated into the membrane. We study the interaction of DNA with the pore wall by means of potential energy landscapes. For this purpose we solve the fully 3D Poisson-Nernst-Planck and Stokes equations numerically and complement it by a 2D model and a 1D analytical calculation. We find that the DNA can be efficiently trapped parallel to the wall and off the symmetry axis of the pore by a proper choice of the gate voltage. Due to the hence induced confinement of accessible space lateral fluctuations of the DNA will be reduced. Furthermore we elucidate the dislike charge repulsion behaviour close to the wall which is necessary for such local minima of the potential energy.

BP 19.10 Tue 14:00 P1A

Cycle-based non-equilibrium Markov state modeling for periodic driving — ●FABIAN KNOCH and THOMAS SPECK — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

A major current challenge in statistical mechanics poses the systematic construction of coarse-grained Markov State Models [1] that are dynamically consistent, and, moreover, might be used for systems driven out of thermal equilibrium. We previously introduced a novel prescription that extends the Markov state modeling approach to systems with dynamics breaking detailed-balance [2,3]. Here, we show that our approach also holds for systems driven by a time-dependent periodic protocol. In particular, we apply the methodology to alanine dipeptide exposed to an oscillating electric field. Markov state modeling allows us to examine how the frequency of the external field influences the long term dynamics without conducting new simulations.

[1] Prinz, J.-H., Wu, H., Sarich, M., Keller, B., Senne, M., Held, M., Chodera, J. D., Schütte, C. and Noé, F. Markov models of molecular kinetics: Generation and validation. JCP 134(17), 2011

[2] Knoch, F. and Speck, T. Cycle representatives for the coarse-graining of systems driven into a non-equilibrium steady state. New Journal of Physics 17(11), 2015

[3] Knoch, F. and Speck, T. Non-Equilibrium Markov State Modeling of the Globule-Stretch Transition. arXiv:1611.02990, 2016

BP 19.11 Tue 14:00 P1A

Large Deviation Properties of RNA Neutral Set Size — ●CHARLOTTE J. BEELEN and ALEXANDER K. HARTMANN — Institute of Physics, University of Oldenburg

The functionality of noncoding RNA molecules is mainly determined by their structure. Sequences with the same structure form the *neutral set*. The neutral set may be partitioned into several components, called neutral networks, traversable by structure-preserving point mutations. The neutral network size is biologically relevant: large neutral networks appear to be favourable in terms of mutational robustness and evolvability. We investigate the neutral set and neutral network size using computer simulations.

We apply a dynamic programming approach [1] to obtain the secondary structures of RNA sequences. The neutral set size can be estimated using a *Nested Set Monte Carlo* Simulation [2]. We implemented a combination of the algorithm with the *Ballistic Search* approach to estimate the neutral network size. The distribution of neutral set and network sizes is determined for randomly generated RNA and compared to biological RNA molecules. To improve the accuracy in the tails of the distribution, large-deviation simulations are used [3]. Furthermore, the correlation of the neutral set size to other observables like the number of base-pairs is investigated.

[1] M. Zuker and P. Stiegler, Nucl. Acids Res. 9(1), 133-148 (1981)

[2] T. Jörg, O.C. Martin and A. Wagner, BMC Bioinf., 9:464 (2008)

[3] A.K. Hartmann, Phys. Rev. E 89, 052103 (2014)

BP 19.12 Tue 14:00 P1A

Computational prediction of alternative σ factor control — ●HAO WU, ANGELIKA DIEHL, and GEORG FRITZ — LOEWE Center for Synthetic Microbiology, Philipps University Marburg, Germany

Evolutionary co-variation of residues has been extensively exploited to predict conserved interaction of proteins. Here we used this method to study bacterial alternative σ factors. These subunits of RNA polymerases determine its specificity of promoter recognition and are involved in many gene regulation processes crucial for bacterial survival. One important player in the regulation of σ factor activity are anti-

σ factors, which sequester their cognate σ factors in the absence of a stimulus, but to date the determinants of binding specificity are poorly understood. Our computational analysis revealed the interacting pairs of residues featuring crucial domains in σ factors. The amino acid pairs are either positively and negatively charged, or hydrophobic, depending on the phylogenetic group of the σ factor. Furthermore, a few alternative σ factor groups contain no anti- σ factor and instead feature a protein domain fused C-terminally to the σ factor as well as a highly conserved gene in its genomic context. Our analysis suggests a cluster of interactions interfacing between the σ domain and the C-terminal domain of the σ -factor. The second protein is also predicted to contact a number of residues at the same interface, suggesting a function as a co-factor. This study helps us to deepen our understanding of the specificity of interactions between σ factor and anti- σ factor, and provides novel insights into the regulatory mechanism employed by different alternative σ factor groups.

BP 19.13 Tue 14:00 P1A

Interactions of polyatomic anions with proteins depend strongly on sodium — SADRA KASHEFOLGHETA and •ANA VILA VERDE — MPIKG, Theory and Bio-Systems Dept., Am Mühlenberg 1 OT Golm, 14476 Potsdam, Germany

Polyatomic ions such as sulfates, phosphates or sulfonates are key players in biological processes but the molecular mechanisms by which these ions act are currently incompletely understood. We use molecular simulations and classical, atomistic models with fixed-charge and explicit solvent representation to clarify the molecular mechanisms of interaction between cationic amino acids and sulfates, phosphates and sulfonates, in their methylated and non-methylated forms and in the presence of excess counterions. This work goes beyond prior reports

on the topic in that it uses a newly developed, internally consistent force field for all ions, which correctly captures the energy magnitude and length scale of anion-cation interactions. Our results suggest a possible molecular origin of previously unexplained experimental observations: anions that, according to experiment, differ strongly in the magnitude of their interaction with cationic amino acids have in fact very similar interactions with those amino acids, but different interactions with sodium; the presence of excess sodium in the experiments thus determines the experimental outcome due to competition with the cationic sites on the protein.

BP 19.14 Tue 14:00 P1A

In Silico Model for Vesicle Blebbing — •SEBASTIAN HILLRINGHAUS, DMITRY A. FEDOSOV, and GERHARD GOMPPER — Institute of Complex Systems, Forschungszentrum Juelich, Juelich, Germany

Experiments with vesicles that incorporate an action network show complex behavior and the formation of blebs when they are actively contracted through motor proteins [Loiseau et. al., *Science Advances*, 2016]. To understand the mechanics that lead to this observations, we employ a coarse-grained cell model which incorporates the membrane properties similar to the RBC-model [Turler et. al., *Nature Physics*, 2016] and an elastic inner mesh to include the actin network. The model is formulated in the framework of the dissipative particle dynamics simulation method. To connect both the membrane and the actin network, we use the Two-Pathway Model [Pereverzev et. al., *Biophysical Journal*, 2005] which can model different behavior under tension. We perform various tests to evaluate the best parameters for this model to match the observed experimental data. We observe that the model of Catch-Slip bonds lead to the best fit with the experimental data.

BP 20: Posters - Physics of the Genesis of Life (Focus Session)

Time: Tuesday 14:00–16:00

Location: P1A

BP 20.1 Tue 14:00 P1A

Chemically Driven Ligation Chain Reaction - Towards Protein-free Hypercycles in Sequence Space? — •STEFANIE LEINER, EVGENIYA EDELEVA, and DIETER BRAUN — Systems Biophysics, Physics Department, LMU Munich, Germany

Which mechanism could have fostered the stable emergence of functional sequences for an RNA world? Eigen's hypercycles suggests that cooperating replication leads to hyperexponential selection.

Hypercycle dynamics can be implemented via competitive oligonucleotide ligation in long-term experiments. Under serial dilution, to mimic molecule degradation, this process enhances the replication of majority sequences and allows their emergence from a random sequence pool. Hyperexponential replication arises from the competitive binding kinetics of ligation: oligonucleotides with long-range sequence correlations ligate faster by cooperative hybridization. The mechanism requires thermal cycling - a non-equilibrium boundary condition that could be provided together with accumulation by heat flow across pores of rock [1].

Our investigations show that EDC can be used in an in-situ activated ligation reaction with 80 % yield for temperatures below $\sim 40^\circ\text{C}$ [2][3]. We show preliminary results towards protein-free hypercycles in sequence space.

[1] S. Toyabe, D. Braun, under review. [2] M. Jauker et al. *Angew. Chem. Int. Ed.* 2015, 54, 14559-14563. [3] Taran et al. *J. Sys. Chem.* 2010, 1:9, 1-16.

BP 20.2 Tue 14:00 P1A

Replicating codon sequences only with tRNA — SIMON LANZMICH, THOMAS RIND, and •DIETER BRAUN — Faculty of Physics and Center for Nanoscience, LMU Munich, Germany

The origins of biological information replication constitute a major challenge for understanding the origins of life. Modern life employs a complex tRNA/RNA/protein machinery to build proteins and replicate DNA [1,2,3]. We present a purely thermally driven replication mechanism that selectively replicates sequences of short codons. It does not depend on a particular base-by-base replication chemistry, but only requires the hybridization of short complementary domains. Codons are carried by molecules very similar to tRNA [4]. Upon a few point mutations, the latter adopt secondary structures where the

anticodon is framed by two stem-loops [5]. The stem-loops of different molecules are pairwise complementary, such that sequences of strands can form supramolecular chains. Replication of a template succession of these proto-tRNAs is facilitated by temperature oscillations and implements (1) binding of strands with matching anticodons to the template (2) fluctuations in the bound strands' hairpins hybridize to neighboring tRNA and (3) heating splits the replicate from the template. Experiments show that this purely physical ligation chain reaction proceeds exponentially and amplifies the template codons severalfold within a few temperature cycles.

[1] IUBMB Life 61, 99 (2009) [2] Science 244, 673 (1989) [3] RNA 16, 1469 (2010) [4] J.Comput.Chem. 32, 170 (2010) [5] PRL 108, 238104 (2012)

BP 20.3 Tue 14:00 P1A

The efficiency of driving chemical reactions by a physical non-equilibrium is kinetically controlled — •TOBIAS GÖPPEL, VLADIMIR V. PLYULIN, and ULRICH GERLAND — Physics of Complex Biosystems, Physics Department, Technical University of Munich, James-Frank-Strasse 1, D-85748 Garching, Germany

An out-of-equilibrium physical environment can drive chemical reactions into thermodynamically unfavorable regimes. Under prebiotic conditions such a coupling between physical and chemical non-equilibria may have enabled the spontaneous emergence of primitive evolutionary processes. Here, we study the coupling efficiency within a theoretical model and focuses on generic effects arising whenever reactant and product molecules have different transport coefficients in a flow-through system. The physical non-equilibrium is represented by a drift-diffusion process, which is a coarse-grained description for the interplay between thermophoresis and convection, as well as for many other molecular transport processes. As a simple chemical reaction, we consider a reversible dimerization process, which is coupled to the transport process by different drift velocities for monomers and dimers. Within this minimal model, the coupling efficiency between the non-equilibrium transport process and the chemical reaction can be analyzed in all parameter regimes. The analysis shows that the efficiency depends strongly on the Damköhler number, a parameter that measures the relative timescales associated with the transport and reaction kinetics.

BP 20.4 Tue 14:00 P1A

Spatial organization of encapsulated circuits — ●AURORA DUPIN, BERTA TINAO, and FRIEDRICH C. SIMMEL — Systems Biophysics and Bionanotechnology - E14, Physics Department and ZNN, Technische Universität München, am Coulombwall 4a, 85748 Garching, Germany

Compartmentalization is at the origin of cellular life as we know it today, although the selective advantage of porous or tight membranes for early cells is debated. The compartmentalization of metabolic circuits can reduce cross-talk by isolating parts of the circuits, and increase the efficiency of the metabolic processes by co-localizing reagents. The effect of compartmentalization on synthetic gene circuits has been studied in isolated water-in-emulsion droplets, where communication was mediated by non-specific diffusion. In contrast, our goal is to build large biomimetic networks exhibiting controlled communication and topology. Such a spatial organization should allow for more complex circuit dynamic behaviors.

To this end, we employ the droplet-interface-bilayer technique to construct spatially organized networks of defined composition. In these networks, protein pores exhibiting chemical selectivity incorporate in lipid bilayer interfaces to mediate the communication between droplets, similarly to natural cell membranes. We implement a variety of RNA-based circuits where the pore-mediated translocation of chemicals is used to induce dynamical behavior. In the future, we envision the implementation of more complex circuits within such networks, including in vitro protein expression systems.

BP 20.5 Tue 14:00 P1A

Elucidating signatures of the genetic code with binding assays — ●EVGENIA EDELEVA, PHILIPP SCHWINTER, and DIETER BRAUN — LMU Munich, AG Braun, Amalienstrasse 54, 80799 Munich, Germany

What defined specific assignment of amino acids to their cognate codons during the emergence of the genetic code? According to the stereochemical theory, the assignments were established based on affinity interactions between amino acids and their codons/anticodons. In the structure of the modern tRNA molecule, the acceptor stem with the amino acid and the anticodon loop with the anticodon triplet are separated by 6 nm in space, making direct interaction impossible. However, two alternative primal tRNA structures have been proposed that bring together in space the amino acid and the codon determinant [1, 2]. Both structures contain tetraloop-like geometries - simple structures that were recently shown to possess enzymatic activity such as ligation, cleavage, and terminal recombination [3].

In this project, we experimentally study the binding of stable AMP activated amino acid analogs to RNA motifs of AMP-binding aptamers as a testbed or to the above mentioned tetraloop-like structures containing corresponding coding triplets using microscale thermophoresis. We aim to elucidate patterns of anticodon-amino acid correlations for the emergence of the genetic code.

[1] J.J. Hopfield, Proc. Natl. Acad. Sci. U. S. A. 75, 4334-8 (1978)

[2] A.S. Rodin et al., Biology Direct 4, 4 (2009)

[3] P. Stadlbauer et al., Chemistry 21, 3596-604 (2015)

BP 20.6 Tue 14:00 P1A

Peptide-based vesicles as precursors to protocells — ●KILIAN VOGELE, MARISA GÖTZFRIED, ELISABETH FALGENHAUER, FRIEDRICH C. SIMMEL, and TOBIAS FIRZ — Systems Biophysics and Bionanotechnology E14, Physics-Department and ZNN, TU Muenchen, 85748 Garching, Germany

Commonly stated requirements for protocells are the maintenance of a metabolism, sensing and responding to the environment, the capability for self-reproduction and Darwinian evolution. In order to meet these requirements compartmentalization is often regarded as an essential aspect. In the lab, protocellular compartmentalization is typically modelled with self-assembled vesicles, for which various molecular components such as fatty acids, lipids or amphiphilic peptides have been utilized. Here we use synthetic elastin-like polypeptides (ELP) to create self-assembled peptide vesicle structures. Among their advantages are tunability in size, permeability and stimuli-responsiveness. The ELP vesicles are fabricated by rehydration from glass beads and have a size of about 200 nm, as observed by DLS and TEM. Using flow cytometry and spectroscopy, we demonstrate successful encapsulation of GFP and fluorescent DNA in the polymersomes, and we also show transcription of the fluorescent RNA aptamer dBrocColi inside of the vesicles. On the long run, we aim at the self-reproduction of ELP vesicles by expression of ELP encoding genes in an artificial transcription-

translation (TX-TL) system.

BP 20.7 Tue 14:00 P1A

Phospholipids and the prebiotic formation of vesicles — ●MARIA TSANAKOPOULOU, CECILE CAUMES, CLAUDIA PERCIVALLE, BHAVESH PATEL, COLM DUFFY, and JOHN SUTHERLAND — MRC Laboratory of Molecular Biology, Francis Crick Avenue, Cambridge Biomedical Campus, CB2 0QH, UK

Glycerol-2-phosphate, which, along with the 1-phosphate, can readily be synthesised by phosphorylation of glycerol, was used as the substrate for the prebiotically plausible formation of alkyl chain phospholipids (1,3-bisacylated and 1-monoacylated glycerol-2-phosphate esters). All the alkyl chain acids were produced selectively in two steps from the aldol reaction of acetaldehyde and reduction by macroporous nickel and hypophosphite - known corrosion products of iron-nickel meteorites. The corresponding acyl imidazolides were used as activated forms of the acids for the formation of the phospholipids. Solutions of different concentrations of the phospholipids bearing the longer chain acyl groups were studied and were found to form vesicles, which could have played a role in the origins of the prokaryotic cells. If the mixture of the phospholipids contains a lot of the shorter chain derivatives, vesicles are not formed. In this case, it was found that recycling - iterative partial selective hydrolysis and reacylation - changes the composition of the mixture in favour of the longer chain derivatives with the result that vesicles can then be observed.

BP 20.8 Tue 14:00 P1A

High-resolving chemical analysis of products formed under hydrothermal vent conditions — ●JESSICA SOBOTTA¹, ALEXANDER RUF^{2,3}, WOLFGANG EISENREICH¹, PHILIPPE SCHMITT-KOPPLIN^{2,3}, and CLAUDIA HUBER¹ — ¹Biochemistry, Technische Universität München, Garching Germany — ²Analytical BioGeoChemistry, Helmholtz Zentrum München, Munich Germany — ³Analytical Food Chemistry, Technische Universität München, Munich Germany

Hydrothermal vents offer a continuous supply of reactive nutrients which react with transition metal minerals. The combination of high pressure, a temperature gradient and a nearly neutral pH can lead to a high diversity of organic molecules including amino acids, hydroxy acids, fatty acids and small peptides [1-3]. In depth analysis of these complex reaction mixtures requires high-resolving analytical tools [4,5] and sophisticated approaches [6]. The combination of FT-ICR-MS, GC-MS and NMR methods have provided a complementary profile of the products for both low and high molecular weight compounds, including an unexpected variety of CHOS derivatives. In summary, high-resolving analytical methods expand our view into the fascinating chemistry of a potential origin of life scenario under hydrothermal vent conditions. [1] C. Huber, G. Wächtershäuser, Science (2006) 314:630-632. [2] C. Huber, W. Eisenreich et al. (2003) Science 301:938-940. [3] C. Scheidler, J. Sobotta et al. (2016) Sci. Rep. 6. [4] Schmitt-Kopplin et al. (2010) PNAS 107:2763-2768. [5] Popova et al. (2013) Science 342:1069-1073. [6] Tziotis et al. (2011) EJMS 17.4: 415-421

BP 20.9 Tue 14:00 P1A

Modeling a mechanism for pre-biotic selection and organization — ●VARUN GIRI¹ and SANJAY JAIN^{2,3} — ¹Department of Biological Experimental Physics, Saarland University, Saarbrücken, Germany — ²Department of Physics and Astrophysics, University of Delhi, Delhi, India — ³Santa Fe Institute, Santa Fe, New Mexico, United States of America

Large molecules such as proteins are crucial for life. Production of these molecules requires good catalysts, and the only good catalysts known today are themselves large molecules. For the origin of life this presents a chicken-and-egg problem in chemistry. We use a mathematical model based on an artificial but pre-biotically plausible chemistry to investigate how certain specific chemical species can be selected out of a large set of possible combinations. We further describe a cascading mechanism by which large and improbable molecules are formed relatively easily in our system, thereby making more plausible the appearance of macromolecules like proteins, RNAs, etc., in pre-biotic settings. We start by considering a set of small molecules and construct a network of chemical reactions amongst these molecules and their reaction products. We find that under certain circumstances, autocatalytic sets (ACSs) come to dominate the chemistry in that the concentrations of the molecules belonging to an ACS are much higher than the background. We study the conditions under which large catalysts can appear starting from chemistries comprising of small molecules and later dominate the system.

BP 20.10 Tue 14:00 P1A

Spatial fractionation of RNA in an inhomogeneous temperature gradient — •PRASANNA PADMANABAN, JUAN IGLESIAS ARTOLA, and MORITZ KREYSING — MPI of Molecular Cell Biology and Genetics, Dresden

Thermal gradients across small pores are able to accumulate nucleic acids from dilute aqueous solutions, e.g. a pre-biological ocean, pond, or puddle [1]. More recently it was found that an open pore of this kind can even act as length selective filter for nucleic acids that are delivered by a steady hydrodynamic flow through this pore. This results in the deposition of long, rare and potentially functional nucleic acids inside this small porous compartment [2]. It was shown that this selection pressure towards increasing molecular complexity is capable of stabilizing long replicators in the presence of short parasites.

Here, we investigate the accumulation characteristics of spatially varying, rather than homogenous, temperature gradients. We present simulation results that indicate distinct, RNA-length dependent accumulation zones. We interpret this as a spatially varying fitness landscape and present an experimental strategy to map it. Our finding implies the possibility of a continuous evolutionary process over multiple levels of innovation in a single compartment, and without the need for temporal changes of the system.

- [1] Baaske et al., PNAS 104(22), 9346*9351 (2007)
[2] Kreysing et al., Nat Chem, 7(3), 203*208 (2015)

BP 20.11 Tue 14:00 P1A

Strong accumulation in a 3D printed thermal trap — •MATTHIAS MORASCH, JONATHAN LIU, CHRISTOF B. MAST, and DIETER BRAUN — Systems Biophysics, Physics Department, Ludwig-Maximilians-Universität München, Amalienstrasse 54, 80799 München, Germany

Thermogravitational traps were shown to be a plausible solution for the concentration problem of the origin of life (1,2,3). In order to simulate the conditions in porous rock more closely, we developed a new microfluidic chamber in which we can accumulate molecules with full optical readout and a wide range of geometries.

Using this technique, we could show a strong accumulation of DNA at water-air interfaces (4). A combination of capillary flow and continuous evaporation-condensation cycles of water pushes the molecules towards the meniscus of the interface, reaching up to 1000-fold accumulation. This robust mechanism may be common for many naturally occurring fluid systems and therefore lead to an accumulation of various kinds of molecules.

In addition, we use the technique to grow crystals from RNA precursor materials inside the chamber. Our goal is to grow a small amount of single, pure crystals from a racemic mixture and measure the chirality of these crystals inside the chamber. We hereby aim to show a plausible scenario for a symmetry breaking process in water-filled porous rocks.

- (1) Braun & Libchaber, PRL 89, 188103 (2002) (2) C. B. Mast et al., PNAS 110, 8030-8035 (2013) (3) M. Kreysing et al., Nat. Chem. 7, 203-208 (2015) (4) J. Liu et al., under review

BP 20.12 Tue 14:00 P1A

Microthermal Approaches to the Origin of Life — •LORENZ KEIL¹, DAVID HORNING², FRIEDERIKE MÖLLER¹, and DIETER BRAUN¹ — ¹Systems Biophysics, LMU Munich, Amalienstrasse 54, 80799 Munich, Germany — ²Department of Chemistry, The Scripps Research Institute, La Jolla, CA 92037

All known living systems are built around information stored in RNA and DNA. To protect this information against molecular degradation and diffusion, the second law of thermodynamics imposes the need for a non-equilibrium driving force. We have shown that heat gradients in millimeter sized pores can drive an accumulation, replication, and selection of ever longer molecules, implementing all the necessary parts for Darwinian evolution. Here, we show that heat gradients can also form pH gradients of at least 1-2 units. Thermophoresis accumulates individual species of a buffer solution differentially at the bottom. Since the accumulation of the proton acceptor is mostly stronger compared to the proton donor, the pH increases towards the bottom of the trap. The result is the formation of a pH gradient facilitated by a temperature difference. This finding opens the door for various reaction pathways to the origin of life that involves pH oscillations. We also found that laminar thermal convection can efficiently drive an

ribozyme-based form of polymerase chain reaction. The RNA polymerase ribozyme replicates short RNA strands up to 10 nucleic acids, enabling the propagation of information in a natural environment and the absence of proteins.

BP 20.13 Tue 14:00 P1A

Reversible cooperation of molecular replicators — •GEORG URTEL^{1,2}, THOMAS RIND², and DIETER BRAUN² — ¹Université Pierre et Marie Curie, Laboratoire Jean Perrin, 4 place Jussieu, 75005 Paris, France. — ²Braun Lab, LMU Munich, Amalienstraße 54, 80799 München, Germany.

For evolution to occur, information-carrying molecules have to replicate their information into new molecules before their own degradation. One class of prebiotically plausible molecules capable of carrying information are oligonucleotides. In random sequences, hairpin molecules are ubiquitous [1]. Replication mechanisms typically require an initiation site on the template to start replication (e.g. [2]). Due to their self-complementarity, hairpins replicate exponentially using only one primer. But, the secondary structure inhibits the initiation site and the hairpin replicators grow slow and go extinct even when degradation is weak. Our experiments show how two hairpin species with similar loop sequence can overcome this problem by a reversible cooperation termed 'crossbreeding'. In this mechanism, new species emerge which lose the secondary structure, but keep the sequence information. These crossbreeds replicate more efficient, outgrow the hairpins and survive strong dilutions. The mechanism can be reversed and hairpins can regrow under changed conditions, showing that their information is preserved in the process. [1] B. Obermayer et al., PRL, 107, 018101 (2011). [2] D. P. Horning et al., PNAS, 21, 9786 (2016).

BP 20.14 Tue 14:00 P1A

Globular Protein Design from Ancestral Supersecondary Structures — •MOHAMMAD ELGAMACY, MURRAY COLES, and ANDREI LUPAS — Max Planck Institute for Developmental Biology, Tuebingen, Germany

Combinatorial reshuffling of subdomain-sized peptides may have provided a very economic means for sequence space navigation and thus protein fold evolution. Previously, through a bioinformatic study we identified a set of highly conserved, subdomain-sized motifs recurring across distant folds, a cue that such motifs may have predated the existing pedigree of folds. This has led to the hypothesis that these ancestral fragments may have provided the basic building blocks for modern protein folds. We also demonstrated repetition of these fragments as a mechanism in creating new folds. The aim of this work was to investigate an alternative mechanism via recombination of heterologous fragments, especially that we were unable to detect any such recombination incidents between the ancestral fragments in modern proteins. To provide an exemplar, we attempted to reconstruct a polymerase-beta N-terminal domain out of two conserved supersecondary structures derived from two unrelated folds. We have done so using a computational strategy that introduces a minimal number of mutations to the constituting fragments. The resulting NMR structure agreed with the designed coordinates with atomic accuracy, demonstrating that a recombination event and a few mutation are sufficient to evolve a new domain.

BP 20.15 Tue 14:00 P1A

On the Physical Origin of Biological Communication — •MATTHIAS F. SCHNEIDER — Medical and Biological Physics, Otto Hahn Str. 4, Dortmund, Germany

Life is full of hydrated interface that all have to obey the 2nd Law. The enormous power of this approach was first pointed out by K. Kaufmann starting in the late 80ties when following Einstein's approach to thermodynamics. This work is strongly inspired by his theory.

From a thermodynamic state to (biological) function. With Einstein's approach one finds, that state and state changes regulate morphological transitions, interface conductivity, catalytic rates etc..

On communication. Pulses that propagate in interfaces can modulate the state and hence the aforementioned functions, especially the activity of enzymes. This is in striking contrast to all known biological communication models where diffusion is the key element for transport.

The waves observed can be driven into a non-linear regime, where excitation only occurs over a critical threshold. The striking similarity with the nervous impulse is in support of Kaufmann and Heimburg's work.

Specificity. Finally I present a model where specificity arises naturally from physics and does NOT need to be introduced by structural

compatibilities (lock & key).

In conclusion: Excitation, Propagation and Fluctuations arising from physics and lead to phenomena we ultimately name "function". Importantly, this mind set is in strong contrast to the molecular/structural approach.

BP 20.16 Tue 14:00 P1A

Reactivity of ribonucleotides in hydrothermal prebiotic conditions: an approach from ab-initio molecular dynamics and NMR experiments — ●ANDREA PÉREZ-VILLA¹, THOMAS GEORGELIN², JEAN-FRANÇOIS LAMBERT², BAPTISTE RIGAUD², MARIE-CHRISTINE MAUREL³, FRANÇOIS GUYOT^{1,3}, MARCO SAITTA¹, and FABIO PIETRUCCHI¹ — ¹IMPMC/UPMC (Paris, France) — ²LRS/UPMC (Paris, France) — ³UPMC/MNHN (Paris, France)

The "RNA world" is one of the most accepted hypothesis of origins of life, due to the versatility of RNA in several chemical processes. Previous studies have investigated the RNA formation in different prebiotic scenarios, like the exposure to drying/wetting cycles and the role of mineral surfaces. However, the spontaneous synthesis of RNA monomers (ribonucleotides), in the primitive Earth is still a key question in the prebiotic chemistry field. In this work, we model the reactions involved in ribonucleotide formation/breakdown under hydrothermal prebiotic conditions, by means of ab initio molecular dynamics in explicit water. We exploit free-energy methods combined with a topological approach developed in our group able to accurately describe variations of chemical bonds. From this framework, we explore different reaction pathways for the nucleotide synthesis/degradation as well as quantitatively reconstruct the free energy surface. We also present a series of NMR experiments for the nucleotide to characterize the different substrates and products and determine the kinetics of the reaction, providing complementary information to the simulations and validating the predicted values from the free-energy calculations.

BP 20.17 Tue 14:00 P1A

Driving early biochemical reactions by the thermal accumulation of ATP over ADP/AMP? — ●ALEXANDRA KÜHNLEIN¹, CHRISTOF B. MAST¹, AMELIE BENK², JOACHIM P. SPATZ², and DIETER BRAUN¹ — ¹Systems Biophysics and Center for NanoScience, LMU Munich — ²MPI for Intelligent Systems, Stuttgart

Life is in non-equilibrium. And all prevalent biochemical reactions use ATP as energy source. Can this chemical driving be accomplished from prebiotic gradients? Interestingly, a simple thermal gradient is capable to accumulate ATP over ADP/AMP due to its difference in charge. This mechanism provides a modern energy source with prebiotic mechanisms. With this hypothesis, we can allow previously studied thermal replication and selection systems [1,2] to use ATP as the energy currency of its biochemical reactions. No highly evolved and complex ATP synthase would be necessary for life in its first steps.

Experimentally, we feed the thermal trap with an equilibrium concentration ratio of ATP and ADP. The local accumulation of the energy-rich species is monitored by the fluorescent protein PercevalHR [3] that was generously provided by the Spatz lab.

[1] PRL (2010) doi:10.1103/PhysRevLett.104.188102; [2] Nat. Chem. (2015) doi:10.1038/nchem.2155; [3] Nat. Comm. (2013) doi:10.1038/ncomms3550

BP 20.18 Tue 14:00 P1A

Temporal climatic fluctuations frozen into chemical non-equilibrium: appearance of high-energy biomolecules — ●JEAN-FRANÇOIS LAMBERT¹, MAGUY JABER², THOMAS GEORGELIN¹, MARIAME AKOUCHE¹, YURIY SAKHNO¹, and MARIE-CHRISTINE MAUREL³ — ¹Sorbonne Universités, UPMC Univ Paris 06, LRS (UMR7197) Case Courrier 178, 4 Place Jussieu, 75005 Paris, France — ²Sorbonne Universités, UPMC Univ Paris 06, LAMS (UMR8220) Case Courrier 225, 4 Place Jussieu, 75005 Paris, France — ³Sorbonne Universités, UPMC and MNHN, ISYEB (UMR 7205), 57 Rue Cuvier, 75005 Paris, France

Life relies on metastable molecules: prebiotic biopolymers synthesis was thermodynamically upfield in water. Chemical energy had to be extracted from the environment and stored in the system to synthesize them. This can be done by adsorbing precursor molecules on mineral surfaces and submitting them to drying-wetting cycles. When water activity is low, anabolic condensation reactions become favorable and complex biomolecules are formed. We evidenced the generation of peptides from single amino acids, and of nucleotides from ribose, nucleobases, inorganic phosphate, using in - and ex situ analysis techniques. When higher water activity is restored, complex biomolecules become thermodynamically metastable, but for kinetic reasons are not necessarily degraded. One must study the catalytic effect of surface sites on both condensation and hydrolysis, and maintain a clear distinction between thermodynamics and kinetics. In many cases macroscopic fluctuations of water activity can result in chemical energy storage.

BP 20.19 Tue 14:00 P1A

Bridging the RNA and lipid worlds — ●JAMES SAENZ — B CUBE, Technical University Dresden, Arnoldstrasse 18, 01307 Dresden

How did the first cells arise? Primitive life would have relied on simple systems that could self-assemble from prebiotic molecules and segregate biomolecules through compartmentalization. It is clear that membranes can self-assemble to form compartments. But what selective advantage would membranes have provided to reaction networks of primitive biomolecules? Prebiotic lipid membranes may have been crucial for the emergence of early cells by providing a surface to concentrate and enhance the catalytic activity of primitive ribozymes. To this end, we are exploring how membrane-RNA interactions can lead to an RNA-lipid world on the path to life.

BP 21: Posters - Membranes and Vesicles

Time: Tuesday 14:00–16:00

Location: P1A

BP 21.1 Tue 14:00 P1A

Direct proof of spontaneous translocation of lipid-covered hydrophobic nanoparticles through a phospholipid bilayer — YACHONG GUO¹, EMMANUEL TERAZZI², RALF SEEMANN³, ●JEAN-BAPTISTE FLEURY³, and VLADIMIR BAULIN¹ — ¹Universitat Rovira i Virgili, Tarragona, Spain. — ²University of Geneva, Geneva, Switzerland. — ³Universität des Saarlandes, Saarbrücken, Germany.

It is generally accepted that small hydrophobic nanoparticles are blocked by lipid bilayers and accumulate in the bilayer core, whereas big nanoparticles can only penetrate cells through slow energy-dependent processes, such as endocytosis, lasting minutes. In contrast to expectations, we demonstrate that lipid-covered hydrophobic nanoparticles may translocate through lipid membranes by direct penetration within milliseconds. We identified the threshold size for translocation: nanoparticles with diameters smaller than 5 nm stay trapped in the bilayer, whereas those with diameters larger than 5 nm insert into the bilayer, opening pores in the bilayer. The direct proof of this size-dependent translocation was provided by an in situ observation of a single event of a nanoparticle quitting the bilayer. This was achieved with a specially designed microfluidic device combining

optical fluorescence microscopy with simultaneous electrophysiological measurements. A quantitative analysis of the kinetic pathway of a single nanoparticle translocation event demonstrated that the translocation is irreversible and that the nanoparticle can translocate only once.

Science Advances 2, e1600261 (2016)

BP 21.2 Tue 14:00 P1A

Shear-thinning and shear-thickening of a confined suspension of vesicles — ●ABDESSAMAD NAIT OUHRA^{1,2}, MARINE THIÉBAUD¹, OTHMANE AOUANE^{1,3}, HAMID EZ-ZAHRAOUI², ABDELILAH BENYOUSSEF², CHRISTIAN WAGNER³, and CHAOUQI MISBAH¹ — ¹Université Grenoble Alpes France — ²Université Mohammed V Rabat Maroc — ³Experimental Physics, Saarland University, Saarbrücken, Germany

Widely regarded as an interesting model system for studying flow properties of blood, vesicles are closed membranes of phospholipids that mimic the cytoplasmic membranes of red blood cells (RBCs). In this study we analyse the rheology of a suspension of vesicles in a confined geometry: the suspension, bound by planar planes on each side, is subjected to a shear flow. Flow properties are then analyzed as a function

of shear rate $\dot{\gamma}$, the concentration of the suspension ϕ and the viscosity ratio $\lambda = \eta_{in}/\eta_{out}$, where η_{in} and η_{out} are the fluid viscosities of the inner (hemoglobin solution for RBC) and outer fluids, respectively. We find that the apparent (or effective viscosity) of the suspension exhibits either shear-thinning (decreasing viscosity with shear rate) or shear-thickening (increasing viscosity with shear rate). The shear thinning or thickening behaviors appear as subtle phenomena, dependant on viscosity contrast λ . We provide arguments about the possible sources of these phenomena.

BP 21.3 Tue 14:00 P1A

Analytical description of nanoparticle motion near an elastic membrane — ●REBECCA BENELLI, ABDALLAH DADDI-MOUSSA-IDER, and STEPHAN GEKLE — Biofluid Simulation and Modeling, Fachbereich Physik, Universität Bayreuth

We investigate analytically the motion of an extended nanoparticle near an elastic membrane endowed with shearing rigidity. For the simpler case of a point particle or rather a particle distant to the membrane this has been done recently¹. Taking the conditions resulting from an elastic membrane and combining them with the description of the motion of an extended spherical particle near a fluid-fluid-interface² leads to a linear equation system. This can be solved numerically in order to get the frequency dependent mobility of the particle.

¹ A. Daddi-Moussa-Ider, A. Guckenberger and S. Gekle. Long-lived anomalous thermal diffusion induced by elastic cell membranes on nearby particles. *Phys. Rev. E*, **93**(1):012612, 2016

² SH. Lee and LG. Leal. Motion of a sphere in the presence of a plane interface. *J. Fluid Mech.*, **98**(01):193-224, 1980

BP 21.4 Tue 14:00 P1A

Monte Carlo lattice modelling of a bilayer system — ●FABIAN KELLER, DAVIT HAKOBYAN, and ANDREAS HEUER — Institute of Physical Chemistry, Corrensstraße 28/30 48149 Münster, Germany

Recently, a lattice model has been developed which allows one to describe the properties of lipid bilayer mixtures, containing DPPC and/or DLiPC [1]. It was introduced to examine the local phase separation and aggregation behavior of the respective lipids. The free energy functional is based on the lipid interaction enthalpy and lipid conformational chain entropy. All contributions can be extracted from short atomistic simulations. The model approach has proven to be able to correctly reproduce phase separation behavior and predict melting temperatures of gel phases for the lipid binary mixtures.

As cholesterol plays a crucial role in the dynamics of lipid bilayers, especially being prominent for its property to form the basis of lipid rafts, we present an extension of the lattice model by incorporation of cholesterol. We have to deal with different challenges, related, e.g., to the different sizes of cholesterol and DPPC/DLiPC. Adding cholesterol to the model will allow one to gain deeper insight into the fundamental mechanics of lipid raft formation and the basics of lipid-cholesterol interaction.

[1] D. Hakobyan, A. Heuer, submitted to J. Chem. Phys.

BP 21.5 Tue 14:00 P1A

Flat-to-curved transition of clathrin-mediated endocytosis — ●FELIX FREY^{1,2}, DELIA BUCHER³, KEM SOCHACKI⁴, JUSTIN TARASKA⁴, KARL ROHR^{2,5,6}, STEVE BOULANT³, and ULRICH SCHWARZ^{1,2} — ¹Institute for Theoretical Physics, Heidelberg University, Germany — ²BioQuant, Heidelberg University, Germany — ³Department of Infectious Diseases, Virology, Heidelberg University, Germany — ⁴National Institutes of Health, Bethesda, U.S.A. — ⁵Department of Bioinformatics and Functional Genomics, Heidelberg University, Germany — ⁶DKFZ, Heidelberg, Germany

The self-assembly of proteins into supramolecular complexes is essential for many cell functions. Examples are the growth of cell adhesion contacts, the formation of the cytoskeleton or the assembly of clathrin-coated vesicles mediating endocytosis. Here we investigate the assembly of flat clathrin arrays at the cell membrane that subsequently reshape to form curved pits. By combining metal replica electron microscopy, correlative light and electron microscopy, live fluorescence microscopy, image analysis and mathematical modeling we demonstrate that acquisition of membrane curvature during clathrin-mediated endocytosis in mammalian cells does not show a linear correlation with clathrin coat assembly. Instead we show that clathrin structures first grow flat and then undergo a substantial ultra-structural reorganization prior to invagination of the plasma membrane. We determine at what stage of coat assembly curvature occurs and demonstrate

a relation to plasma membrane tension.

BP 21.6 Tue 14:00 P1A

Diffusion of membrane-bound ligand-receptor bonds — ●HENNING STUMPF¹, DANIEL SCHMIDT¹, and ANA-SUNCANA SMITH^{1,2} — ¹PULS Group, Institut für Theoretische Physik I, Friedrich-Alexander-Universität Erlangen-Nürnberg — ²Division of Physical Chemistry, Institute Ruder Bošković, Zagreb

Protein-mediated membrane adhesion plays a crucial role in a number of biological processes including the immune response and morphogenesis. We aim to understand the effect of lateral interactions between two adhesion bonds on the mobility of the bonds. In the current work, we address this problem by numerical and simulation means. In principle, we find that two adhesive bonds strongly attract each other at short distances and repel at large distances. Naturally such an interaction has a barrier at intermediate separations. We calculate the time it takes for one bond to escape from the attractive well. We also determine the effective diffusion constant of a bond diffusing through an adhesion domain represented by a periodic arrangement of affixed ligand-receptor constructs. This is an important step in understanding the diffusion of bonds, which have recently been measured, and consequently understand the role of the membrane in the process of cell adhesion.

BP 21.7 Tue 14:00 P1A

Element-specific Density Profiles in Single and Interacting Solid-supported Biomembrane Models — ●GEORGI GOCHEV^{1,2}, ERNESTO SCOPPOLA¹, IGNACIO RODRIGUEZ-LOUREIRO¹, LUCA BERTINETTI¹, DMITRI NOVIKOV³, OLEG KONOVALOV⁴, PHILIPPE FONTAINE⁵, and EMANUEL SCHNECK¹ — ¹Max Planck Institute Colloids and Interfaces, Potsdam, Germany — ²Institute of Physical Chemistry, Sofia, Bulgaria — ³Deutsches Elektronen-Synchrotron, Hamburg, Germany — ⁴European Synchrotron Radiation Facility, Grenoble, France — ⁵Synchrotron SOLEIL, Gif-sur-Yvette, France

Surface interactions involving biomembranes, such as cell-cell interactions or membrane contacts inside cells play important roles in numerous biological processes. Structural insight into the interacting surfaces is a prerequisite to understand the interaction characteristics as well as the underlying physical mechanisms. Here, we work with simplified planar experimental models of membrane surfaces, composed of lipids and lipopolymers. Their interaction is quantified in terms of pressure-distance curves using ellipsometry at controlled dehydrating (interaction) pressures. For selected pressures, their internal structure is investigated by standing-wave x-ray fluorescence (SWXF). This technique yields specific density profiles of the chemical elements P and S belonging to lipid headgroups and polymer chains, as well as counter-ion profiles for charged surfaces. Along this line we further establish methodology for the element-specific structural characterization of lipid monolayers at the solid/liquid interface with atom-scale resolution.

BP 21.8 Tue 14:00 P1A

Preparation and characterization of 2D phospholipid and copolymer nanomembranes — ●ROLAND HILLMANN¹, DOMINIC GILZER², MARLÉN-VIVIANE EICKMANN¹, NIKLAS BIERE¹, MARTINA VIEFHUES¹, TILMAN KOTTKE², and DARIO ANSELMETTI¹ — ¹Experimental Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University, Germany — ²Physical and Biophysical Chemistry, Department of Chemistry, Bielefeld University, Germany

We investigated Langmuir-Blodgett (LB) nanomembranes (NM) of UV-polymerized phospholipids and of copolymers as free-standing as well as substrate-supported 2D-systems. As a model for artificial and robust biological membranes, they will serve for various applications, such as for artificial filters or for the functional incorporation of channel proteins. The diacetylene phospholipids (PTPE and DC(8,9)PC) as well as the PB-PEO copolymers were prepared by spreading them at an air-water interface and consecutively transferred to a TEM-grid as well as onto mica and graphite substrates. UV-polymerizing of the phospholipids was performed by a 4W 254nm UV lamp. Successful formation of pore-spanning monolayers up to 2µm x 8µm was verified by helium-ion-microscopy. Further investigation of the UV-polymerized nanomembranes with attenuated total reflection infrared (ATR-IR) spectroscopy allowed us to monitor the polymerization process.

BP 21.9 Tue 14:00 P1A

Biological Signaling by Sound. A Physics Approach. — ●CARINA FEDOSEJEVS and MATTHIAS SCHNEIDER — TU Dortmund,

Germany

Lipid bilayers build up all biological interfaces in cells. We study the prediction that perturbations can propagate and have characteristics of acoustic waves. These perturbations can be local changes of parameters like pH, temperature or density. The pulses increase also the activity of embedded enzymes during their propagation. We examine whether these acoustic pulses can explain how intercellular communication happens. For lipid monolayers this is already proven. Here we attempt to study the propagation in bi-/ multilayers because of their biological relevance. To measure these pulses a Langmuir Trough is used with two pressure sensors holding a Wilhelmy Plate. With the Langmuir-Blodgett Technique lipid layers are transferred onto a glass slide. The bi-/multilayer results by connecting the slide to the monolayer on the subphase. The excitation happens with the embedding of e.g. ethanol molecules in the layer, which causes a local density change. Pulses were measured in bilayers for different phospholipids in varied phase states. By using more layers a correlation between number of layers and velocity is expected. Additionally the lipid dynamics on the glass slide are investigated with fluorescence measurements. A correlation between diffusion velocity in the outer layer and number of layers could show the influence of the glass slide in the experiments. We could prove that our assumptions are also true for lipid bilayers, which is an important step transferring this theory to the living system of cells.

BP 21.10 Tue 14:00 P1A

Electro-mechanical Coupling during Action Potentials — ●JULIA MUCHOWSKI, CHRISTIAN FILLAER, and MATTHIAS SCHNEIDER — TU Dortmund, Germany

Action potentials are a classical phenomenon in biological cells. Their electrical component has been studied in detail whereas little is known about other components. Action potentials were investigated in excitable plant cells (*Chara Braunii*).

The membrane potential was monitored by intracellular recording. The cell membrane was separated from the cell wall by plasmolysis and observed by light microscopy. During a pulse not only the electrical potential of the membrane changed (depolarization) but also a mechanical displacement of the cell membrane was observed. The displacement of the membrane took place on a timescale of 1-2 min. The electrical signal preceded the mechanical displacement by $2+/-0.5$ s. To further study the mechanical properties of the excitable membrane, one method was established to obtain large plasma membrane vesicles ($r=50-100$ micrometer) from the cell. This was achieved by plasmolysing the cell, cutting the cell wall, deplasmolysing the cell and extracting a membrane vesicle via osmotic pressure. Size and stability of the vesicles depended on the length of the cut and the speed of plasmolysis and deplasmolysis.

Our results demonstrate electro-mechanical coupling during an action potential. Further work aims at obtaining thermodynamic state diagrams of the excitable membrane.

BP 21.11 Tue 14:00 P1A

Nonlinear fractional waves in elastic membranes — ●JULIAN KAPPLER¹, SHAMIT SHRIVASTAVA², MATTHIAS F. SCHNEIDER³, and ROLAND R. NETZ¹ — ¹Freie Universität Berlin, Germany — ²University of Oxford, United Kingdom — ³TU Dortmund, Germany

Recently, there has been experimental interest in nonlinear sound waves in interfaces. In our contribution, we provide a theory for such sound waves. Starting from standard hydrodynamics, we derive a nonlinear fractional wave equation for interfacial sound waves in an elastic membrane on a viscous fluid. Our result constitutes the first derivation of a physical fractional wave equation from first principles. In addition, we compare predictions of our theory to experimental data and find that our model reproduces several key experimental features, such as an abrupt increase in both range and velocity as a function of excitation amplitude.

BP 21.12 Tue 14:00 P1A

Detachment of membrane bound virions by competitive ligand-binding induced receptor depletion — ●NAGMA PARVEEN¹, STEPHAN BLOCK², VLADIMIR ZHDANOV^{1,4}, GUSTAF

RYDELL³, and FREDRIK HÖÖK¹ — ¹Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — ²Department of Chemistry and Biochemistry, Freie Universität Berlin, Berlin, Germany — ³Department of Infectious Diseases, Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden — ⁴Boriskov Institute of Catalysis, Russian Academy of Sciences, Novosibirsk, Russia

Multivalent interactions between virions and receptors in a lipid membrane can be weakened using competitive non-pathogenic ligand binding. In particular, the subsequent binding of such ligands can induce detachment of bound virions, a phenomena of crucial relevance for the development of new antiviral drugs. Focusing on the simian virus 40 (SV40) and recombinant cholera toxin B subunit (rCTB), and using (monosialotetrahexosyl)ganglioside (GM1) as their common receptor in a supported lipid bilayer (SLB), we present the first detailed investigation of this phenomenon by employing the quartz crystal microbalance with dissipation (QCM-D) and 2D single particle tracking (SPT) techniques. Analysis of the QCM-D-tracked release kinetics made it possible to determine the binding strength of a single SV40-GM1 pair. The release dynamics of SV40, monitored by SPT, revealed that a notable fraction of SV40 become mobile just before the release, allowing to estimate the distribution of SV40-bound GM1 receptors just prior to release.

BP 21.13 Tue 14:00 P1A

Cancer specific plasma membrane association of Hsp70-1A - AFM and fluorescence imaging of model membranes —

●CONSTANZE LAMPRECHT¹, JOSEF MADL^{2,3}, WINFRIED RÖMER^{2,3}, MATHIAS GEHRMANN⁴, and ANDREAS EBNER¹ — ¹Institute of Biophysics, Johannes Kepler University Linz, Austria — ²Centre for Biological Signalling Studies (BIOS), University Freiburg, Germany — ³Faculty of Biology, University Freiburg, Germany — ⁴Klinikum rechts der Isar, TU Munich, Germany

Hsp70A1A is the major stress-inducible member of the HSP70 chaperone family and has been implicated in cancer diseases with the development of tumor resistances to standard therapies, increased invasiveness and poor prognosis. In normal cells Hsp70A1A is expressed in response to external stimuli such as physical exertion and heat to deal with denatured proteins and prevent toxic aggregations. In a majority of human tumors the protein is produced permanently in high amounts and a significant fraction of the cytosolic protein is found associated with cellular membranes. In this work we study the cancer specific plasma membrane localization of Hsp70A1A. As the protein lacks a consensus sequence for translocation to the cell membrane as well as known membrane binding domains, its anchorage may follow a new paradigm of protein-lipid interactions that may hold the key for deciphering membrane associated functions of Hsp70A1A in cancer evolution. We conduct AFM investigations in combination with fluorescence microscopy on model membranes to determine the anchoring mechanism and function on the cell surface.

BP 21.14 Tue 14:00 P1A

Functional reconstitution of ion channels in lipid bilayers in a microfluidic device — ●PHILIPP HANNIBAL¹, THOMAS

BAUKROWITZ², STEFAN KLUMPP³, and CHRISTOPH F. SCHMIDT¹ — ¹III. Physikalisches Institut, Universität Göttingen, Germany — ²Physiologisches Institut, Christian-Albrechts-Universität zu Kiel, Germany — ³Institut für Nichtlineare Dynamik, Universität Göttingen, Germany

Membrane channel proteins play crucial roles for signaling and sensory processes across the cell membrane. We work with potassium-selective K2P channels that are sensitive to temperature, voltage, pH, drugs or mechanical forces. Several of these K2P channel proteins show diode-like current-voltage-dependencies when they are embedded in lipid bilayers [1].

The goal of this work is to create a microfluidic device with reconstituted lipid bilayers and inserted functional channels with electrical access so that channel currents can be measured in simple and complex geometries.

[1] Schewe, M. et al., A Non-canonical Voltage-Sensing Mechanism Controls Gating in K2P K⁺ Channels, *Cell*, 2016, Vol. 164-5, pp. 937-949.

BP 22: Posters - Biomaterials and Biopolymers

Time: Tuesday 14:00–16:00

Location: P1A

BP 22.1 Tue 14:00 P1A

Humidity-controlled gelatin bioactuator — ●STEFANIE RIEDEL¹, BENEDIKT HEYART¹, KATHARINA APEL¹, and STEFAN G. MAYR^{1,2} — ¹Leibniz-Institut für Oberflächenmodifizierung e. V., Leipzig, Germany — ²Fakultät für Physik und Geowissenschaften, Universität Leipzig, Leipzig, Germany

Natural hydrogels such as gelatin are of particular interest in biology and medicine. Due to their strong biocompatibility and biodegradability, they are highly attractive materials in regenerative medicine as extracellular matrix component. Furthermore, stimuli responsiveness of hydrogels attracts considerable interest due to the potential use in sensor and actuator applications. In regard to these applications, adaption of stimuli-responsiveness is an interesting aspect of gelatin modification. Modification of hydrogels can be achieved by crosslinking for which several methods exist. An important method is high energy irradiation by using highly energetic electrons. In contrast to several other crosslinking methods, electron irradiated gelatin is non-toxic and thus beneficial for biological applications. In the presented poster, we show a stimuli-responsive system made up from electron irradiated gelatin that becomes actuated upon exposure to humidity. Furthermore, we demonstrate how adjustment of system's and environmental properties such as gel concentration, irradiation dose, pH and salt concentration allows fine-tuning of the system's response.

BP 22.2 Tue 14:00 P1A

A Self-Assembled Active Plasmonic Waveguide with a Peptide-Based Thermomechanical Switch — KILIAN VOGEL¹, JONATHAN LIST¹, GÜNTHER PARDATSCHER¹, NOLAN B. HOLLAND², FRIEDRICH C. SIMMEL¹, and ●TOBIAS PIRZER¹ — ¹Systems Biophysics and Bionanotechnology E14, Physics-Department and ZNN, TU Muenchen — ²Department of Chemical and Biomedical Engineering, Cleveland State University

Nanoscale plasmonic waveguides composed of metallic nanoparticles are capable of guiding electromagnetic energy below the optical diffraction limit. Signal feed-in and readout typically requires the utilization of electronic effects or near-field optical techniques, whereas for their fabrication mainly lithographic methods are employed. Here we developed a switchable plasmonic waveguide assembled from gold nanoparticles (AuNPs) on a DNA origami structure that facilitates a simple spectroscopic excitation and readout. The waveguide is specifically excited at one end by a fluorescent dye and energy transfer is detected at the other end via the fluorescence of a second dye. The transfer distance is beyond the multi-color FRET range and below the Abbé limit. The transmittance of the waveguide can also be reversibly switched by changing the position of an AuNP within the waveguide, which is tethered to the origami platform by a thermo-responsive peptide. High yield fabrication of the plasmonic waveguides in bulk was achieved using silica particles as solid supports. Our findings enable bulk solution applications for plasmonic waveguides as light-focusing and light-polarizing elements below the diffraction limit.

BP 22.3 Tue 14:00 P1A

Time dependent fluoride uptake in hydroxyapatite from aqueous NaF solution - How long should we brush our teeth? — ●THOMAS FAIDT¹, CHRISTIAN ZEITZ¹, SAMUEL GRANDTHYLL¹, MICHAEL HANS², MATTHIAS HANNIG³, KARIN JACOBS¹, and FRANK MÜLLER¹ — ¹Experimental Physics, Faculty of Natural Sciences and Technology, Saarland University, 66123 Saarbrücken, Germany — ²Functional Materials, Faculty of Natural Sciences and Technology, Saarland University, 66123 Saarbrücken, Germany — ³Clinic of Operative Dentistry, Periodontology and Preventive Dentistry, Faculty of Medicine - Clinical Medicine, Saarland University Hospital, 66421 Homburg, Germany

The application of fluoride containing products to protect tooth enamel from caries has been daily practice for many decades. However, to this day little is known about the time dependence of fluoride uptake in hydroxyapatite (HAP) which is the mineral component of human enamel. In our study, we use HAP pellet samples as a model system for the crystallites of tooth enamel. To investigate the time dependence of the fluoride uptake, samples were exposed to a fluoride solution (NaF, 500 ppm) for different times, resembling the tooth brushing process. XPS depth profiling revealed a saturation behavior both for the overall

amount of fluoride taken up by the sample and for the thickness of the formed fluoridated layer. Our results show that the usual application times of about 2 minutes for, e. g., toothpastes are already in a range to ensure the maximum uptake of fluoride.

BP 22.4 Tue 14:00 P1A

Magnetic nanoparticles-filled carbon nanotubes as potential thermo-seed for Hyperthermia — ●RASHA GHUNAIM¹, SEBASTIAN SCHULZ², CHRISTIAN KOBROW², SILKE HAMPEL¹, RUEDIGER KLINGELER², and BERND BUECHNER^{1,3} — ¹IFW-Dresden, Germany — ²Kirchhoff Institute for Physics, Heidelberg, Germany — ³TUD-Dresden, Germany

Hyperthermia can be considered as a promising tool for cancer treatment; based on the prolonged and controlled exposure of the body tissues to a temperature in the range of 40-43 °C. Magnetic nanoparticles (MNPs) are considered as promising tools for an effective therapeutic approach against cancer. These MNPs can be heated up in a (AC) magnetic field, which leads to their use as hyperthermia candidates, this magnetic-based hyperthermia is called magnetic fluid hyperthermia (MFH). However, to consider these MNPs safe and effective for the patient, they are encapsulated inside the hollow cavity of carbon nanotubes (CNTs). These nano-carriers are chemically stable (protect MNPs from oxidation due to interaction with the biological system), biocompatible (can easily penetrate biological barriers) and have functionalizable surface (for better bonding with matrix elements and compounds). In this work, the current candidates for MFH are mainly binary alloys of Fe-Co, Fe-Ni, Ni-Cr, Ni-Cu and Co/Ni-ferrites. Their feasibility for magnetic hyperthermia therapies is exploited by investigating induced heating under AC magnetic field. Quantitatively, their Specific Absorption Rate (SAR) can give a hint about the amount of heat released by unit mass of material per unit time

BP 22.5 Tue 14:00 P1A

functionalized DNA origami nanostructures for molecular electronics — ●TÜRKAN BAYRAK^{1,2}, BEZU TESCHOME^{1,2}, TOMMY SCHONHERR¹, and ARTUR ERBE¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany. — ²Technische Universität Dresden, cfaed, 01062 Dresden, Germany.

The DNA origami method provides a programmable bottom up approach for creating nanostructures of any desired shape, which can be used as scaffolds for nanoelectronics and nanophotonics devices. (1,2,3) This technique enables the precise positioning of metallic and semiconducting nanoparticles along the DNA structures. (4) In this study, two nanostructures, i.e. DNA origami nanotube and DNA origami molds (5), are used for the fabrication of nanoelectronic devices. To this end, the DNA origami nanotubes are modified to assemble 14 gold nanoparticles (AuNPs) along them. Then electroless gold deposition is used to selectively grow the AuNPs and create eventually continuous nanowires. Similarly, AuNPs are also grown within the DNA origami molds. In order to investigate the transport properties of the so-fabricated nanostructures, a method is developed by electron beam lithography. Additionally, the assembly of heterogeneous nanostructures, i.e. AuNPs and quantum dots (QDs), on a single DNA origami nanotube is demonstrated and further metallized, thus representing a first step toward the fabrication of DNA origami-templated quantum dot transistors. 1Rothmund, Nature 440.7082 (2006) 2Teschome, et al. Langmuir 32.40 (2016) 3Samanta, et al. Nanoscale 7.6 (2015) 4Teschome, et al. Langmuir 31.46 (2015) 5Helmi, et al. Nano letters 14.11 (2014)

BP 22.6 Tue 14:00 P1A

Novel Hybrid hydrogel substrates with non-linear elastic response — ●CHRISTINA JAYACHANDRAN and FLORIAN REHFELDT — Third Institute of Physics, Georg-August Universität

It has been shown in the recent past that the responses of cells depend upon their environment's physical and chemical properties. Cultured on conventional collagen coated polyacrylamide (PA) gels, cells only feel the linear elastic behaviour, in contrast to native extracellular matrix's non-linear elastic response.

Here, we present novel hybrid hydrogels that mimic the heterogeneous structure and the non-linear elastic behaviour of connective tissue by incorporating collagen fibrils into PA hydrogels. We tuned the

Young's modulus over a broad physiologically relevant range and investigated the responses of adult human mesenchymal stem cells (hMSC). On soft hybrid gels, hMSCs behave significantly different than on collagen coated gels of the same stiffness, exhibiting a typical morphology known from stiff environments. Fluorescence imaging of hybrid gels revealed that stem cells locally re-organize the underlying collagen fibrils. These findings implicate that the responses of stem cells are largely dependent on the non-linear elasticity of their environment.

BP 22.7 Tue 14:00 P1A

Liquid crystalline ordering of amyloid-iron(II,III) oxide hybrid fibrils under magnetic field — •JIANGUO ZHAO¹, SREENATH BOLISETTY¹, STEPHANE ISABETTINI², JOACHIM KOHLBRECHER³, JOZEF ADAMCIK¹, PETER FISCHER², and RAFFAELE MEZZENGA¹ — ¹Laboratory of Food and Soft Materials, D-HEST, ETH Zurich — ²Laboratory of Food Process Engineering, D-HEST, ETH Zurich — ³Laboratory of Neutron Scattering and Imaging, PSI

Magnetic field is a promising approach to induce spatial ordering in the originally disordered suspension of magneto-responsive rod-like particles. By loading iron(II,III) oxide nanoparticles with amyloid fibrils, we fabricated hybrid fibrils having high magneto-responsiveness, high aspect ratio (length-to-diameter, L/D) and flexibility. An apparently increased orientation was obtained upon increasing magnetic field strength and fibrils volume fraction (ϕ). At constant dimensionless concentration ($\phi \cdot L/D$), stiff hybrid fibrils with varied aspect ratios and volume fractions displayed identical degree of ordering at constant magnetic field; while the semiflexible fibrils with contour length close to persistence length exhibited a lower degree of alignment. To the best of our knowledge, this is first direct experimental proof of Khokhlov-Semenov theory, which predicts that the ordered phase for anisotropic colloidal particles is highly restricted by the semiflexible nature of the particles under external fields. We believe these findings are detrimental for the fundamental understanding and applications of liquid crystalline phases in numerous external fields. *current address: Drittes Physikalisches Institut, Georg-August-Universität Göttingen.

BP 22.8 Tue 14:00 P1A

Zno nanowires application in controlling the wettability for biomedical uses — •AMITENDER SINGH and SARAVJEET SINGH — Deenbandhu Chhotu Ram University of Science and Technology Murthal, Sonapat-131039, India

Hydrophobic materials are widely used for different biological applications and nanostructures are mainly used for preparation of hydrophobic surfaces. Mainly used materials and polymers for these studies are

silicone, polydimethylsiloxane (PDMS) and poly (methyl methacrylate) (PMMA) etc. To achieve this hydrophobicity, various attempts have been made recently to improve the surface properties by various chemical and physical methods. The host-material interactions take place through the surface of the material. So, the material's biocompatibility is mainly related to its surface properties more as compared to its bulk properties. Further, Wang et al. showed that ZnO nanowires are completely bio-safe and biocompatibility when used in various concentrations below $100\mu\text{g/ml}$. This study is aimed to develop facile method to prepare hydrophobic coating on various substrates for different biomedical applications. Here, we report the variations in contact angle on various substrates like; glass, quartz, Si and PDMS where CA measurements were done before and after ZnO nanowires coating. A drastic change in CA was found after ZnO nanowires coating on various substrates. It was found that the surface wetting properties can be tuned further for various biomedical applications like wound dressing, surgical tools and bio implants.

BP 22.9 Tue 14:00 P1A

Tuning synthetic semiflexible networks by bending stiffness — •CARSTEN SCHULDT^{1,2}, JÖRG SCHNAUSS^{1,2}, TINA HÄNDLER^{1,2}, MARTIN GLASER^{1,2}, JESSICA LORENZ², TOM GOLDE¹, JOSEF A. KÄS¹, and DAVID M. SMITH² — ¹Institute for Experimental Physics I, Leipzig University, Germany — ²Fraunhofer IZI, Leipzig, Germany

The mechanics of complex soft matter such as cells or tightly-entangled biopolymer networks cannot be understood in the classical physical frame of flexible polymers or rigid rods. Instead, the underlying filaments are semiflexible, with their finite bending stiffness leading to non-trivial bulk mechanical responses. A natural model for such polymers is the protein actin. Experimental studies of actin networks, however, are limited since the persistence length cannot be readily tuned.

Here, we experimentally investigated this parameter for the first time through bulk rheological and single-filament measurements of entangled networks formed by structurally tunable DNA nanotubes. This de novo model system enabled the validation of numerous characteristic properties inherent to semiflexible polymers and networks thereof, i.e. persistence length, inextensibility, reptation, and mesh size scaling. The scaling of the elastic plateau modulus with concentration is consistent with previous measurements and established theories. In contrast, we showed that the elastic plateau modulus scales linear with the persistence length, which drastically opposes the predominant theoretical predictions [1].

[1] Schuldt et al.: Tuning synthetic semiflexible networks by bending stiffness, Phys. Rev. Lett. 117, 197801 (2016)

BP 23: Posters - Statistical Physics of Biological Systems

Time: Tuesday 14:00–16:00

Location: P1A

BP 23.1 Tue 14:00 P1A

Generic transport mechanisms for molecular traffic in cellular protrusions — •ISABELLA KRÄMER and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität, München, Deutschland

Transport of molecular motors along protein filaments in a half-closed geometry is a common feature of biologically relevant processes in cellular protrusions. Using a lattice-gas model we study how the interplay between active and diffusive transport and mass conservation leads to localised domain walls and tip-localisation of the motors. We identify a mechanism for task sharing between the active motors (maintaining a gradient) and the diffusive motion (transport to the tip), which ensures that energy consumption is low and motor exchange mostly happens at the tip. These features are attributed to strong nearest-neighbour correlations that lead to a substantial reduction of active currents, which we calculate analytically using an exact moment-identity.

BP 23.2 Tue 14:00 P1A

The architecture of bacterial biofilms depends on biofilm age and active force generation — •ANTON WELKER, NADZEYA KOUZEL, and BERENIKE MAIER — Biophysik, Köln, Deutschland

Many bacterial species aggregate in communities, called biofilms. In contrast to individual bacteria, bacterial biofilms show a complex structure, which makes them resistant against a variety of environmen-

tal factors and causes environmental, industrial and medical problems. Bacteria can adjust the three dimensional structure of their biofilms to varying environmental conditions. However, the molecular mechanisms governing biofilm structure are unclear. Here, we characterized the three-dimensional structure of biofilms formed by the human pathogen *Neisseria gonorrhoeae* at cellular resolution. In particular, the local density distribution, radial distribution function and parameters describing ordering and defects were implemented. We found that force-generating and force-defective bacterial microcolonies show significant differences in microcolony shape and density. The radial distribution function showed a significant difference in local ordering dependent on biofilm age, indicating that the density and the fraction of diplococci increased with biofilm age.

BP 23.3 Tue 14:00 P1A

Interference of deleterious and beneficial mutations in spatial habitats — •PHILIPP KLATT and JOACHIM KRUG — Institute for Theoretical Physics, Cologne, Germany

One of the fundamental questions of population genetics is that of the rate at which beneficial or deleterious mutations are generated and incorporated into asexual populations. The quantity which describes this process is the speed of evolution. We here study a spatially structured model in which individuals of a population only compete locally on the time scale of a generation. In contrast to well-mixed models, where individuals compete with the whole population, the speed of evolu-

tion tends to a finite value in the limit of infinite habitat size when all mutations are either beneficial or deleterious [1,2]. We consider the general case where both types of mutations are present and map out the dependence of the speed of evolution on several parameters by interpreting analytical and numerical results. In contrast to the well-mixed case, we find that large populations undergoing a fitness decline caused by the accumulation of deleterious mutations (Muller's ratchet) cannot be rescued by a small rate of beneficial mutations. Moreover, the effects of deleterious and beneficial mutations on the speed of evolution are generally not additive, suggesting a nontrivial interference between the two types of mutational effects.

[1] Martens, E.A. and Hallatschek, O. (2011). Interfering waves of adaptation promote spatial mixing. *Genetics* 189:1045-60.

[2] Otwinowski, J. and Krug, J. (2014). Clonal interference and Muller's ratchet in spatial habitats. *Physical Biology* 11:056003.

BP 23.4 Tue 14:00 P1A

Recombination and Speciation on Fitness Landscapes — ●ALEXANDER KLUG and JOACHIM KRUG — Institut für Theoretische Physik, Universität zu Köln, Germany

Deterministic evolution models with selection, mutation and recombination display multiple stable stationary states in one realisation of a fitness landscape [1]. These distinct stationary states are mostly sharply peaked, which implies that the major part of the population of one stationary state has the same genotype, even in the presence of mutation. The populated genotypes of different stationary states can then be thought of as different species, because they differ in a number of loci and are stable. We are investigating various aspects of these stationary states, such as the number of distinct stationary states that exist in different landscapes models (House-of-Cards model, percolation model [2]) and the properties of their basins of attraction under the deterministic dynamics. The results are interpreted in the context of the concepts of Dobzhansky-Muller incompatibility [1] and mutational robustness [3].

[1] T. Paixao, K. E. Bassler, R. B. R. Azevedo, bioRxiv 008268

[2] S. Gavrilits, *Trends Ecol. Evol.* 12:307-12 (1997)

[3] E. van Nimwegen, J. P. Crutchfield, M. Huynen, *PNAS* 96:9716-9720 (1999)

BP 23.5 Tue 14:00 P1A

Non-equilibrium dynamics of heterogeneous biological systems — ●FEDERICA MURA and CHASE BROEDERSZ — Department of Physics, Ludwig-Maximilians-University Munich, Theresienstrasse 37, 80333 Munich, Germany

Recent experiments indicate that many biological systems, including the cytoplasm, actin-myosin networks, and chromosomal loci can be driven out of thermodynamic equilibrium. The active dynamics of these systems is governed by local stochastic forces resulting from enzymatic processes. To provide insight into the non-equilibrium dynamics of such systems, we propose a simple stochastic model of a d-dimensional bead-spring network subject to a heterogeneous distribution of random driving forces. By using a combination of numerical simulations and analytical results we investigate how this non-equilibrium setting affects the system's steady state dynamics. We discuss how detailed balance is broken in the stochastic dynamics of different degrees of freedom and use this to quantify the rate of entropy production. Ultimately, this model could help to establish a systematic and more general method to extract information from a trajectory analysis of the stochastic dynamics of biological systems.

BP 23.6 Tue 14:00 P1A

Quantification of polymer loop shapes in application to chromosome oscillations — ●WENWEN HUANG and VASILY ZABURDAEV — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In this contribution, we model the chromosomes in meiotic fission yeast by pinned bead-rod loops in external force field. The 3D gyration tensor containing information of all beads positions is calculated. Based on the gyration tensor, the shape of polymer loops is quantified under different strength of the external force field. We show that the resulting shape is more rod-like and prolate under strong force and more sphere-like and oblate under weak force. Our study provides a quantitative description of the shape of pinned polymer loops under external field and may help us to describe the relevant biological processes in fission yeast such as chromosome oscillations and their alignment during meiosis.

BP 23.7 Tue 14:00 P1A

From flexible to stiff: a homopolymer model state diagram and its morphologies — ●BENNO WERLICH and WOLFGANG PAUL — Institut für Physik, MLU Halle-Wittenberg, Germany

A hard-sphere homopolymer model with attractive interaction potential can be varied in its stiffness by modification the bondlength. According to this variation, thermodynamic functions and geometric observables undergo changes which are presented in a state-diagram for a chain length of $N=40$. The morphologies, e.g. in the low temperature range, show peculiar changes in monomer ordering towards stiffer chains. We use a Stochastic-Approximation Monte-Carlo (SAMC) method for our off-lattice model simulations and generate an estimation to the microcanonical entropy $S(E)$. This entropy is our statistical weight for canonical production runs.

BP 23.8 Tue 14:00 P1A

Predictability of mutational trajectories in evolutionary rescue — ●JAN SCHMIDT and JOACHIM KRUG — THP, Cologne

Predictability of evolutionary pathways has been considered in terms of the strong selection weak mutation model (SSWM), where the whole population moves monomorphically along pathways with increasing fitness while maintaining a constant population size [1,2]. We compare these trajectories to pathways that are taken by a population which is on the verge of extinction. Here, conceptually, the assumption of SSWM is no longer valid. Dropping the constraint of fixed population size, where the population does not fixate the intermediate types before the rescuing type is reached, this process is described in terms of a branching process [3].

[1] D.M. Weinreich et. al., *Science* 312, 111 (2006)

[2] J. Franke et. al., *PLoS Comput Biol* 7, e1002134 (2011)

[3] B. Bauer and C. Gokhale, *Scientific Reports* 5, 9607 (2015)

BP 23.9 Tue 14:00 P1A

Local optima in NK fitness landscapes — ●BENJAMIN SCHMIEGELT, SUNGMIN HWANG, and JOACHIM KRUG — Institute for Theoretical Physics, University of Cologne

Fitness landscapes, the assignment of fitness values to genotypes, determine the structural impact of selection on population dynamics. Populations will, especially under strong selection pressure, cluster around local optima. The number of local optima is also considered a measure of ruggedness, complexity and difficulty for a population to move on the landscape. The NK model models landscapes with parameter-controlled ruggedness and many possible interaction schemes between loci, sharing similarities with p-spin glass models. For a quasi-one dimensional circular interaction layout the expected number of local optima is well established. We consider instead the case of random interaction networks, mean field and other variations and find, contrary to traditional assumptions, quantitatively different asymptotics for the expected numbers of local optima from the circular case.

[1] Weinberger, E. D. (1991). Local properties of Kauffman's N-k model: A tunably rugged energy landscape. *Physical Review A*, 44(10), 6399.

[2] Limic, V., & Pemantle, R. (2004). More rigorous results on the Kauffman-Levin model of evolution. *The Annals of Probability*, 32(3), 2149-2178.

[3] Schmiegelt, B., & Krug, J. (2014). Evolutionary accessibility of modular fitness landscapes. *Journal of Statistical Physics*, 154(1-2), 334-355.

BP 23.10 Tue 14:00 P1A

Stochastic switching of Min proteins in short Escherichia coli cells — ●LUKAS WETTMANN¹ and KARSTEN KRUSE² —

¹Theoretische Physik, Saarland University, Saarbrücken, Germany —

²NCCR Chemical Biology, Department of Biochemistry, Department of Theoretical Physics, University of Geneva, Geneva, Switzerland

Intracellular processes are subjected to noise, be it through thermal fluctuations or, for example, molecular noise. The latter case is especially true when the total number of involved molecules inside the cell is low. More interesting than the, for the case of gene expression, local changes in protein number is the stochastic behavior of spatially inhomogeneous protein distributions inside the cell.

To this end, we study the influence of noise on the dynamics of the Min system. The Min proteins are a family of proteins which through self-organization are able to exert spatial pole-to-pole oscillations in rod-shaped E. coli cells. These oscillations cause the division site to be located along the symmetry axis of the cell, ensuring equal-sized

daughter cells. In contrast, for short cells, the oscillations are replaced by stochastic switching of the proteins between two stable polar configurations. This behaviour can cause the emergence of mini cells if the residence times are sufficiently long.

We developed a mechanism based on the underlying molecular pro-

cesses to study the dynamics of the Min proteins. With this mechanism, we are able to use a framework developed in earlier work to analyze the behaviour of the Min proteins in the limit of weak noise and calculate the residence times as a function of the cell length.

BP 24: Posters - Protein Structure and Dynamics

Time: Tuesday 14:00–16:00

Location: P1A

BP 24.1 Tue 14:00 P1A
NMR Investigation of Protein Aggregation in Concentrated Solutions of Eye Lens Crystallins. — ●MARIA CAMILLES, SUSANNE LINK, ALEXEY KRUSHELNITSKY, JOCHEN BALBACH, and KAY SAALWÄCHTER — Institute of Physics, Faculty of Natural Sciences II, Betty-Heimann-Str. 7, 06120 Halle/Saale, GERMANY

Crystallins are the major vision-related (i.e. refractive) proteins found in the eye lens. The mammalian lens consist of three classes of proteins, i.e alpha-, beta- and gamma-crystallins, which are structural proteins. The former also acts as chaperone. Commonly, proteins are subject to a continuous degradation and replacement process, but the eye lens proteins have to remain stable and soluble for a lifetime. Heat, shock or other stressors can cause aggregation and lead to cataract, thus the major chaperone function is to prevent aggregation. The conventionally used methods to study aggregation include observations by optical techniques applied mostly to dilute solutions. Here we demonstrate the use of 1H pulsed field gradient (PFG) NMR as an alternative to study the aggregation kinetics of crystallin proteins in highly concentrated protein solutions. PFG-NMR provides self-diffusion coefficients and is thus sensitive to aggregate size. We have studied the thermal denaturation and aggregation kinetics of gammaB-crystallin in the absence and presence of alphaB-crystallin. The components can be easily distinguished by their rather different sizes, thus their self diffusion coefficients. Our data demonstrate qualitative changes in the thermal degradation of gammaB-crystallin in the presence of alphaB-crystallin.

BP 24.2 Tue 14:00 P1A
Molecular dynamics study of the mechanical stability of dimeric coiled-coils under strain — ●CHUANFU LUO, ANA VILA VERDE, and REINHARD LIPOWSKY — Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

Coiled-coils (CCs) are ubiquitous folding motifs found in proteins. Dimeric CCs consist of two alpha-helices wrapped around each other in a super helix configuration. In biological systems, CCs are highly versatile: they play an important role in various intracellular regulation processes as well as in membrane fusion. Their unusual structure suggests that it may also be possible to use them as biological force sensors to detect forces involved in biochemical processes *in vivo*. We investigated this possibility by carrying out Steered Molecular Dynamics to simulate the shear pulling of *de novo* designed coiled-coils with different lengths. We found that the pulling force at slow pull appears to be independent of either the initial length or the contact length of the coiled-coils. Analysis shows that there are two pathways when pulling CCs: "opening of helices" at fast pulling speeds, and "step-wise sliding" at slower speeds.

BP 24.3 Tue 14:00 P1A
Characterization of open and closed beta 2 glycoprotein I conformation — ●INA BUCHHOLZ, PETER NESTLER, FLORIAN BERG, and MIHAELA DELCEA — University of Greifswald, ZIK HIKE, Fleischmannstr. 42, 17498 Greifswald, Germany

The antiphospholipid syndrome (APS) is an autoimmune disease characterized by the presence of anti-beta 2 glycoprotein I (b2GPI) antibodies circulating in blood of patients. b2GPI exists in at least two different conformations: the closed form which is found circulating in blood and the open form which exposes a cryptic binding site (i.e. epitope). This antigenic conformation leads to formation of antibody-protein complexes which induce thrombotic events and recurring pregnancy loss. To identify the conditions that direct to the development of APS, a conversion protocol is used to prepare the open and closed forms of b2GPI. Therefore, the structures of b2GPI are studied by circular dichroism spectroscopy, fluorescence spectroscopy and atomic force microscopy in varying buffer systems. First results indicate in-

herent differences between open and closed conformation. Some experimental conditions also provide mixed conformational populations. These findings will be handled as a basic reference for further experiments aiming for the alteration of b2GPI protein structure. For this, the influence of different stress conditions like pH shift, temperature change or ionic strength, as well as the binding of various ligands to b2GPI will be investigated and will be further correlated with APS antibody binding to b2GPI.

BP 24.4 Tue 14:00 P1A
Biophysical characterization of integrin alpha IIb-beta3 under physiological and stress conditions — ●UNA JANKE, PETER NESTLER, and MIHAELA DELCEA — University of Greifswald, ZIK HIKE, Fleischmannstr. 42, 17498 Greifswald, Germany

The heterodimeric transmembrane platelet receptor integrin alpha IIb-beta 3 (α IIb β 3) plays a crucial role in haemostasis and is involved in the autoimmune disease Immune Thrombocytopenia (ITP). ITP patients develop a higher bleeding risk due to autoantibody mediated platelet destruction. The immunogenicity (i.e. capacity of the immune system to induce an immune response) depends strongly on the conformation of the α IIb β 3. Thus, we aim to study the influence of closed, opened and intermediate conformations on the binding properties of α IIb β 3 to ITP patient autoantibodies. Here we present a strategy to investigate the effect of mutations, external stress factors and binding partners on the α IIb β 3 conformation. The interaction under physiological conditions, e.g. in a membrane environment, is investigated using surface plasmon resonance (SPR) and quartz crystal microbalance (QCM) after incorporating α IIb β 3 into liposomes. Different incorporation protocols are compared with regards to liposome- α IIb β 3 conjunction. First results indicate that pH, manganese ions and temperature are important influence factors.

BP 24.5 Tue 14:00 P1A
Identification of reaction coordinates for functional dynamics: understanding the molecular pacman T4 Lysozyme — ●MATTHIAS ERNST, STEFFEN WOLF, and GERHARD STOCK — Biomolecular Dynamics, University of Freiburg, Germany

T4 Lysozyme is a model system for both experimental and computational investigations of functional protein dynamics. The major functional dynamics is a hinge-bending motion between its two domains which occurs on a timescale of 10-20 μ s[1]. Yet, the Free energy landscape based on widely applied reaction coordinates like the radius of gyration or the root mean square deviation to the crystal structure shows a barrier that is much too small to explain this timescale. Hence, there must be mechanistic details that require other reaction coordinates.

Using a combination of distance-based principal component analysis[2] on a 50 μ s long equilibrium trajectory of T4L and inverse targeted molecular dynamics simulations[3], we could identify new reaction coordinates describing local structural rearrangements which act as a locking mechanism. We find two intermediate states on the path between "open" and "closed" which slow down the process. Thus, we propose a hierarchical four-state model that can explain the observed timescales semi-quantitatively.

- [1] R.B. Yirdaw and H.S. Mchaourab, *Biophys.J.* **2012**, 103(7), 1525.
- [2] M. Ernst, F. Sittel and G. Stock, *J.Chem.Phys.* **2015**, 143, 244114.
- [3] J. Schlitter, M. Engels and P. Krüger, *J.Mol.Graph.* **1994**, 12, 84.

BP 24.6 Tue 14:00 P1A
Fast liquid DSC - a novel tool to study protein solutions — ●JANA RÜDEL, PATRIZIA KRUSE, and MARIA OTT — Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany

Fast scanning calorimetry with heating rates up to 10000 K/s allows to

study rapid non-equilibrium processes which remain invisible in standard DSC experiments. The available sensor chips, however, which were successfully used in polymer science [1] restricted the use to dry or highly viscous samples. If this technique could be extended to liquid samples, fast scanning calorimetry would give a unique access to study the time dependencies of processes in biology.

We extensively tested novel, recently introduced liquid Flash DSC sensors [2] by studying aqueous protein solutions with scanning rates up to 500K/s. We will illustrate the potential of using fast scanning calorimetry and discuss current challenges and limitations.

[1] V. Mathot et al., *Thermochim Acta* 522 (2011), 36-45

[2] R. Splinter et al., *Thermochim Acta* 603 (2015), 162-171

BP 24.7 Tue 14:00 P1A

Thermophoretic trapping of single molecules — TOBIAS THALHEIM, MARCO BRAUN, ANDREAS BREGULLA, and •FRANK CICHOS — Molecular Nanophotonics Group, Institute of Experimental Physics I, University of Leipzig, Germany

We present a force-free trapping method which is capable of confining the Brownian motion of single molecules by applying the actual fuel of Brownian motion: temperature. A focused laser beam is used to optically heat a plasmonic structure generating dynamical temperature gradients. Single molecules migrate in these temperature gradients typically to colder regions due to an effect known as thermophoresis or Ludwig-Soret effect. An optical feedback algorithm utilizes this behavior to reposition the focused laser beam and, hence, restricts the Brownian motion of the single molecule. As a first biological model system, double-stranded lambda-DNA is investigated in the thermophoretic trap. The macromolecular conformational changes due to the inhomogeneous temperature gradients are evaluated with the help of a principal component analysis. Furthermore, the Soret coefficient of single 6-helix bundle DNA origami structures has been measured in the trap.

BP 24.8 Tue 14:00 P1A

Small-angle X-ray scattering study of aqueous Trypsin solutions and the influence of pressure on interaction potential — •JAN LATARIUS, JULIAN SCHULZE, MICHAEL PAULUS, CHRISTIAN STERNEMANN, JAN NYSAR, GÖRAN SURMEIER, and METIN TOLAN — Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund

Proteins as most important components of life show complex and non-intuitive behaviour regarding the interaction with themselves and each other under high pressure. Using the method of small-angle X-ray scattering we explore the properties of soluted Trypsin exposed to hydrostatic pressure and compare the findings to studies on aqueous solutions of Lysozyme and RNase. By altering the pressure in a range from 1 to 4000 bar with constant pH and adding co-solvents like TMAO and TMACl to differently concentrated protein solutions we hope to reveal the influence of co-solvents and pressure on the interaction potential.

BP 24.9 Tue 14:00 P1A

MD Simulation Studies of Protein Dynamics in Neutral Confinement — •TIMOTHY WOHLFROMM, MATTHIAS BARTELMESS, TATJANA THIEL, and MICHAEL VOGEL — Institut für Festkörperphysik, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt, Germany

We report on recent findings regarding dynamics of the elastin like protein model (VPGVG)₅₀ and its surrounding hydration shell in a neutral pore. Despite recent progress we lack understanding of dynamics of complex systems, such as proteins, specifically when studied in confinement. To isolate direct effects of confining geometries on protein dynamics the pore consists of the same atom type as the solvent, in most cases water, restrained in position by harmonic potentials of varying restoring forces to simulate confining surfaces with differing rigidity. Varying the hydration level of the confined protein we find that the minimal degree of hydration as ratio of water mass to protein mass for the protein to show bulk behaviour is 1 g/g. Moreover, we observe in spatially resolved analyses that with decreasing distance to the pore wall the correlation times of water increase by more than one order of magnitude. This effect is drastically reduced with reduced rigidity of the pore wall. In addition the protein acts as a soft confinement to water in vicinity to its surface. Finally, we systematically investigate changes in the dynamics of the elastin model when water is replaced by other solvents.

BP 24.10 Tue 14:00 P1A

Chiral effects in CH₃->CF₃ mutations in amino acids de-

termine hydrophobicity — JOAO ROBALO¹, SUSANNE HUHMANN², BEATE KOKSCH², and •ANA VILA VERDE¹ — ¹MPIKG, Theory and Bio-Systems Dept., Am Mühlenberg 1 OT Golm, 14476 Potsdam, Germany — ²Freie Universität Berlin, Institute of Chemistry and Biochemistry, Takustr. 3, 14195 Berlin

Protein fluorination is a promising avenue to modify protein properties. Predicting the impact of protein fluorination on protein stability based on simple heuristics - e.g., changes in amino acid apolar surface area or polarity - has proven impossible because of the interplay between the fluorinated site and its neighboring environment. Ultimately understanding and predicting how fluorination impacts proteins can best be done using molecular simulations and classical, atomistic models. Here we present such a model for fluorinated amino acids. We apply this force field to investigate how CH₃->CF₃ mutations alter the hydrophobicity of apolar amino acids. Our results show that these mutations increase the hydrophobicity of the amino acid directly, by increasing the apolar surface area, and indirectly, by decreasing the number of backbone-water hydrogen bonds. Strikingly, stereoisomeric effects strongly impact the conformational orientation and the flexibility of the amino acid side chain and ultimately determine the magnitude of changes in hydrophobicity. We demonstrate that the commonly accepted notion that CH₃->CF₃ mutations alter protein stability only via changes in apolar surface area is incorrect, and show that different fluorinated stereoisomers may be exploited for particular purposes.

BP 24.11 Tue 14:00 P1A

Metadynamics Simulations of the Fibrinogen Protomer — •TIMO SCHÄFER^{1,2}, LORENZ RIPKA¹, FRIEDERIKE SCHMID¹, and GIOVANNI SETTANNI^{1,3} — ¹Johannes Gutenberg-University Mainz — ²Graduate School Materials Science in Mainz — ³Max Planck Graduate Center with the Johannes Gutenberg-University Mainz

Fibrinogen is a dimeric multi-chain serum protein that polymerizes into fibrin when activated by thrombin as part of the coagulation cascade. Fibrinolysis, the cleavage of fibrin by the enzyme plasmin, controls the dissolution of blood clots. While the major factors contributing to fibrin formation and dissolution have been identified, the atomistic details of these mechanisms are largely unknown.

Here, the connection between structure and function of fibrinogen is studied using classical atomistic molecular dynamics simulations coupled to metadynamics, a technique that allows for a thorough exploration of the important degrees of freedom of the system. Based on our previous characterization of a hinge along the coiled-coil region of the fibrinogen protomer, we used metadynamics to explore the major degrees of freedom related to this hinge, represented by the two largest principal components of motion. The simulations reveal the presence of two specifically distinct modes of bending, characterized by a different loss of secondary structure and exposure of plasmin cleavage sites.

BP 24.12 Tue 14:00 P1A

Chemical Selective Preparation of Native Proteins on Surfaces by Mass Spectrometry for High Resolution, Single Molecule Imaging — •STEPHAN RAUSCHENBACH¹, JEAN-NICOLAS LONGCHAMP¹, JOSEPH GAULT³, SABINE ABB², HANS-WERNER FINK², and KLAUS KERN¹ — ¹Max Planck Institute for Solid State Res., Stuttgart, Germany — ²Univ. of Zuerich, Switzerland — ³Oxford Univ., UK

The structural characterization of proteins relies on extensive preparation efforts; once to obtain and purify the molecule, and second to bring it in the required form and environment. With free electron lasers or low energy electron holography/1/ new single molecule methods for structural analysis are in sight. They, too, require matching preparation methods, in particular ensuring chemical purity, specificity and compatibility with the vacuum environment. Preparative mass spectrometry, specifically soft-landing electrospray ion beam deposition/2/ is in the unique position to fulfill these requirements. We can generate intense beams of native proteins, protein complexes, and even membrane proteins and deposit them on solid surfaces. The imaging by scanning tunneling microscopy on metal surfaces confirms the protein is deposited as a three-dimensional object. In the future, relevant structural information is to be expected by using free-standing graphene/3/ as a substrate and low-energy electron holography/4/ for imaging. /1/ PRL 110,255501(2013) /2/ Annu. Rev. Anal. Chem. 9, 16.1 (2016) /3/ J. Vac. Sci. Technol. B31, 020605 (2013) /4/ arXiv:1512.08958 (2015)

BP 24.13 Tue 14:00 P1A

Polarization anisotropy of IR spectra reveals geometry of a protonated water cluster — ●JAN DALDROP¹, MATTIA SAITA¹, MATTHIAS HEYDEN², JOACHIM HEBERLE¹, and ROLAND NETZ¹ — ¹Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — ²MPI für Kohlenforschung, 45470 Mülheim an der Ruhr

Infrared spectra for protonated and unprotonated water chains, water slabs and water drops are calculated from ab initio Molecular Dynamics trajectories. For all three water cluster geometries we obtain a pronounced IR continuum band over a wide frequency range in the presence of an excess proton. This continuum band exhibits a strong polarization anisotropy for chains and slabs with maximal adsorption for IR polarization along the water cluster long axes. The continuum band for protonated water chains is shown to be due to charge fluctuation dynamics of the Zundel state ensemble linked to pronounced friction memory effects that decay over 100fs. For proton-conducting proteins, where a water chain traverses the membrane-spanning protein, this anisotropy allows to distinguish proton motion along the water chain from proton motion along the protein or membrane surfaces by the use of polarization and time-resolved IR adsorption spectra. We use the results to interpret our experimental data for the continuum band around $\nu = 1900 \text{ cm}^{-1}$ of aligned bacteriorhodopsin proteins in membranes during laser-flash initiated proton transfer. Polarization-resolved IR spectroscopy thus allows for the interpretation of IR continuum bands and in particular furthers the microscopic understanding of water-mediated proton-transfer processes.

BP 24.14 Tue 14:00 P1A

Global Langevin model of multidimensional biomolecular dynamics — ●BENJAMIN LICKERT, NORBERT SCHAUDINNUS, MITHUN BISWAS, and GERHARD STOCK — Albert Ludwigs University, 79104 Freiburg, Germany

Biomolecular processes, recorded by molecular dynamics simulations, are often treated as diffusive motions on low-dimensional free energy landscapes $F(\vec{x})$. A theoretical basis of such an interpretation is provided by Zwanzig's system-bath Hamiltonian approach which allows to derive a memory-free Langevin equation describing the motion of the system $\vec{x}$ on the free energy landscape $F(\vec{x})$.

While the theoretical framework of Zwanzig generally assumes a highly idealised form of the bath Hamiltonian and the system-bath coupling, it would be desirable to apply the approach to realistic data-based biomolecular systems. Here, we propose a practical method to construct an analytically defined global model of structural dynamics. On basis of molecular dynamics simulations and suitable system coordinates our approach uses an "empirical valence bond"-type model to represent the multidimensional free energy and an approximate description of the friction. We show for several systems that the resulting Langevin models reproduce the results of the underlying all-atom simulations. Since the Langevin equation can also be shown to satisfy the underlying assumptions of the theory (e.g., delta-correlated Gaussian noise), the analytically defined model provides a correct realisation of Zwanzig's formulation.

BP 24.15 Tue 14:00 P1A

Temperature dependence of the self-diffusion of BSA in solution with trivalent ions — ●CHRISTIAN BECK^{1,2}, MICHAEL BRAUN¹, MARCO GRIMALDO², NIINA H. JALAVARO³, FELIX ROOSEN-RUNGE², FAJUN ZHANG¹, TILO SEYDEL², and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — ²Institut Laue-Langevin, Grenoble, France — ³Neutron Sciences Directorate, Oak Ridge National Laboratory, USA

Recent studies focused on the salt-induced slowing down of the short-time self-diffusion of bovine serum albumin (BSA) in aqueous solutions (D_2O) at constant temperature [1] using quasi-elastic neutron scattering. The diffusion coefficients of the clusters, induced by the presence of trivalent yttrium ions, can be described independently of the protein concentration as a function of the ratio of salt ions per protein.

With experiments at BASIS (SNS, ONRL, Oak Ridge, TN) we determined the temperature-dependence of the system. For each tem-

perature, a master curve is observed. In samples with trivalent salts, the diffusion coefficients increase less with increasing temperature than predicted by the Stokes-Einstein relation. The different master curves were used to determine the temperature dependent binding probabilities between the proteins using the Flory-Stockmayer theory. An increasing binding probability with increasing salt concentration and increasing temperature was found. This observation on the microscopic scale is in agreement with the observed lower critical solution temperature (LCST) on macroscopic scale.

[1] M.Grimaldo et al. J. Phys. Chem. Letters, **6** (2015) 2577

BP 24.16 Tue 14:00 P1A

Effect of disulfide bridges on denatured protein dynamics investigated by neutron spin-echo spectroscopy — ●FELIX AMESSEDER¹, AUREL RADULESCU², PETER FALUS³, ANDREAS STADLER¹, and DIETER RICHTER¹ — ¹Forschungszentrum Jülich GmbH, JCNS-1/ICS-1, Germany — ²Forschungszentrum Jülich GmbH, JCNS Outstation at MLZ, Germany — ³Institut Laue-Langevin, France

The dynamics of proteins in solution is highly dependent on the presence of covalent bonds acting as internal crosslinks between different domains. Here, we investigate the denatured Bovine Serum Albumin (BSA) protein in solution at 6 molar guanidine hydrochloride first with active disulfide bridges, and secondly with reduced disulfide bridges using β -mercaptoethanol as additional chemical denaturant. The results are interpreted with common polymer models that include hydrodynamic interactions like the Zimm model.

The protein structure was investigated beforehand with small angle neutron scattering SANS and small angle x-ray scattering SAXS. A distinct power law scaling behavior could be retrieved for both cases. The dynamics of the protein was investigated with dynamic light scattering, and neutron spin-echo spectroscopy NSE. The NSE results reveal distinct differences of the internal dynamics between the both cases that will be discussed in detail in the talk.

BP 24.17 Tue 14:00 P1A

Principal Component Analysis of Circular Data: Theory and Application — ●FLORIAN SITTEL, THOMAS FILK, and GERHARD STOCK — Uni Freiburg/BrsG.

Principal Component Analysis (PCA) is a widely adopted technique for dimensionality reduction. However, being a linear transform it is not directly applicable to circular data, like the dynamics of protein backbone dihedral angles. There have been several attempts already in modifying PCA to circular data (Dihedral angle-based PCA, GeoPCA, Principal Geodesic Analysis), yet none addressed the special geometry of the underlying space (N-dimensional Tori) to full extent, resulting in projection errors. Here we present a theoretical analysis of this geometry and identify the pitfalls given by the periodicity of the data. Based on our analysis, we derive a new formulation of PCA of circular data and demonstrate its performance in the context of protein dynamics.

BP 24.18 Tue 14:00 P1A

The influence of non-Markovian effects on reaction coordinate quality — ●FLORIAN BRÜDIG, JAN DALDROP, and ROLAND NETZ — Freie Universität Berlin, Germany

Defining appropriate low-dimensional reaction coordinates remains a crucial task in molecular-dynamics data analysis. Quantification of reaction-coordinate quality by analyzing transition-path probabilities is a commonly applied method, but it is based on Markovian theory. However, non-Markovian effects, arising from inertia, friction memory or orthogonal degrees of freedom, cannot be neglected in relevant biophysical systems.

We investigate the applicability of this method to non-Markovian processes by two model systems that allow to continuously introduce non-Markovian effects: Langevin dynamics in a two dimensional potential and generalized Langevin dynamics with a friction memory kernel in a doublewell potential. Results are discussed with respect to data obtained from molecular-dynamics simulations.

BP 25: Posters - Cytoskeletal Filaments

Time: Tuesday 14:00–16:00

Location: P2-EG

BP 25.1 Tue 14:00 P2-EG

Investigations of the cytoskeleton of squamous cell carcinoma cells and oral keratinocytes — ●NINA BARTELS¹, MAJA STRUGACEVAC¹, SUSANNE STEEGER¹, JAN LIETZ¹, JULIA KRISTIN², MARCEL GLAAS², JÖRG SCHIPPER², and MATHIAS GETZLAFF¹ — ¹Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf, Deutschland — ²Hals-Nasen-Ohrenklinik, Universitätsklinikum Düsseldorf, Deutschland

In order to investigate differences between oral carcinoma cells (HNSCC) and oral keratinocytes (DOK) two different techniques, Atomic Force Microscopy (AFM) and fluorescence microscopy, were used.

By means of AFM the mechano-elastic properties of carcinoma cells were investigated, because a possible cause for the differences between HNSCC and DOK cells are modifications in the cytoskeleton of cancer cells. To calculate the elasticity of the cells, the Young's Modulus was determined using the Hertzian Model.

The cytoskeleton of HNSCC and DOK was examined using confocal fluorescence microscopy. This contribution is focused on the comparison of the cytoskeleton and its staining for the two cell lines. For the staining of the cytoskeleton, SiR-actin and SiR-tubulin were used. An optimized staining process for both, actin and tubulin, was found for the collective staining of HNSCC and DOK.

BP 25.2 Tue 14:00 P2-EG

Non-Equilibrium Dynamics in Critical Biological Networks — ●FEDERICO GNESOTTO and CHASE BROEDERSZ — Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, D-80333 München, Germany

Biological networks such as the actin cytoskeleton of a cell are inherently out of equilibrium. ATP-driven molecular motors constantly exert local stochastic forces on the fibers in these networks, thereby driving them into a non-equilibrium steady state. Recent studies have proposed that such systems might be poised near a mechanical stability (isostatic) threshold, where the system exhibits critical behavior.

To investigate how this criticality affects the non-equilibrium dynamics of such marginal networks, we propose a minimal model of a diluted triangular lattice with tunable connectivity and local motor activity. With this model we study how non-equilibrium behavior manifests on different length scales.

This minimal framework allows us not only to capture interesting non-equilibrium features, but also to intuitively understand the underlying mechanisms.

BP 25.3 Tue 14:00 P2-EG

A Time-Resolved Study of Intermediate Filament Assembly — ●MANUELA DENZ, GERRIT BREHM, CLÉMENT HÉMONNOT, ANDREW WITTMEIER, OLIVA SALDANHA, CHARLOTTA LORENZ, and SARAH KÖSTER — Institute of X-Ray Physics, University of Göttingen, Göttingen, Germany

The cytoskeleton of eukaryotes is primarily composed of three different types of filaments, namely microfilaments (MF, diameter 8 nm), microtubules (MT, diameter 25 nm) and intermediate filaments (IF, diameter 10 nm) along with cross-linkers and motor proteins. The assembly of IFs follows, in contrast to the MF and MT assembly, a hierarchical pathway and is not nucleotide driven. Furthermore, the resulting filaments lack polarity. For different IF types, the assembly process underlies the same general model, however, the details may vary. For example, two monomers of the most studied IF protein vimentin first assemble into a homodimer, whereas the monomers of another IF protein, keratin, form heterodimers. Until now, the assembly process of IFs is not completely known. Therefore, this project aims on studying the assembly of keratin and vimentin. Experiments are performed using a combination of small angle X-ray scattering (SAXS) and microfluidics. To do so, we first test different microfluidic device types by characterizing them with gold colloids. In a second step, we analyze the weaker-scattering proteins. With the above mentioned combination of techniques we are able to perform time-resolved studies and gain deeper insights into the assembly process of IFs.

BP 25.4 Tue 14:00 P2-EG

The challenges of a FEM simulation of an intermediate filament network — ●RALF SCHUSTER, OTHMAR MARTI, and KAY GOTTSCHALK — Institute of Experimental Physics, Ulm University

Our aim is to build a 3D numerical finite element model of the cytoskeleton. The point of interest is the interplay between intermediate filament network and mechanical properties. The cytoskeleton is one of the key elements responsible for stiffness and deformability of cells. Changes in structure and shape of cells, caused by external forces, play an important role for cell migration and proliferation. They trigger reorganizations of the cytoskeleton systems. Metastasizing cancer cells can have a softer cytoskeleton through changes in the network. This leads to a reduced drag resistance when passing through narrow constrictions.

There exist numerical models for the cell deformation, but they are either modelling the cytoplasm as a continuum, or limit the simulations to microtubules and actin filaments. In contrast we look at the behavior and influence of intermediate filament networks, but the implementation of such a model is challenging. Due to the high disparity of scale for the different components of the model, many difficulties arise concerning the mesh and the element quality. Unfortunately, the geometry specifications do not allow simultaneously a coarse mesh with a good quality, thus leading to long computation times. Different approaches to simulate a heterogeneous interior of the cell will be presented and discussed. Models with 3D rod shaped elements for the network structure, as well as with 1D beam elements, were created and tested.

BP 25.5 Tue 14:00 P2-EG

Modelling collective microtubule and kinetochore dynamics — ●FELIX SCHWIETERT and JAN KIERFELD — TU Dortmund, Lehrstuhl für Theoretische Physik I

We investigate the cooperative dynamics of microtubules, which are elastically coupled to kinetochores in the mitotic spindle. The model includes the dynamic instability of microtubules, forces on microtubules and kinetochores from elastic linkers and, eventually, an external force on the kinetochore. We use stochastic simulations and analytical Fokker-Planck equations to analyze one hemisphere of the mitotic spindle consisting of an ensemble microtubules coupled to one kinetochore under constant external force. In simulations of this one-sided spindle model, kinetochore movement exhibits bistable behavior as a function of the applied force [1]. Solving the Fokker-Planck equations for the microtubule-kinetochore distance distribution, we can derive the bistable behavior analytically and obtain conditions for the occurrence of bistability. This allows us to quantify the bistable regime in the parameter plane of linker stiffness and microtubule numbers. The bistable behavior can explain stochastic chromosome oscillations in metaphase, which have been observed in several experiments.

[1] E. J. Banigan: Minimal model for collective kinetochore-microtubule dynamics. (2015) PNAS 112.41:12699-12704.

BP 25.6 Tue 14:00 P2-EG

Derivation of continuous equations for an isotropic active elastic network — ●KARIN JOHN and ERIC BERTIN — Laboratoire Interdisciplinaire de Physique Grenoble, France

The standard active gel theory postulates phenomenological continuous equations for the density, stress, and local orientation fields on the basis of symmetry and linear irreversible thermodynamics arguments. In most cases, the gels considered behave as liquids on long time scales, but 'solid' active gels, which do not flow at long time under an externally applied shear, have also been studied. In this work, we derive the large-scale continuous description of an isotropic elastic network in the presence of force dipoles (a crude modeling of an actin network with molecular motors) which generate an active stress. The main results of this explicit coarse-graining procedure are two-fold. First, the derivation yields non-linear terms able to saturate the instability reported in linear active gel theory. Second, activity (i.e., the strength of force dipoles) not only generates new 'active' terms with respect to the passive case, but also 'renormalizes' the passive elastic properties of the medium. This change of the elastic properties leads to an instability for extensible force dipoles, while standard active gel theory yields an instability for contractile dipoles.

BP 25.7 Tue 14:00 P2-EG

Force-dependent Self-Assembly of Myosin II Minifilaments — ●JUSTIN GREWE and ULRICH S. SCHWARZ — Institute for Theoretical Physics, Heidelberg, Germany

Non-muscle myosin II plays an important role in cytokinesis and cell migration by generating tension in the actin cytoskeleton. Because myosin II is a non-processive motor, it cannot generate appreciable levels of force by itself, but needs to work in larger ensembles. In non-muscle cells, it assembles into myosin II minifilaments, which are approximately 300 nm large and contain around 30 myosin II molecules.

In order to investigate the coupling between myosin II self-assembly and force generation, we introduce a crossbridge model. Using mean-field methods the qualitative behavior of the theoretical model is investigated and compared to stochastic simulations.

The catch-slip bond that is introduced in the model leads to a bimodal distribution of minifilament sizes when retaining a constant force, where minifilaments attached to actin are larger than the ones that are not attached. This is a reasonable mechanism that could be used by nature to efficiently utilize a given amount of motor proteins to retain a force.

BP 25.8 Tue 14:00 P2-EG

Dynamics of circular dorsal ruffles and their role in cancer — ERIK BERNITT^{1,2,3}, JULIA LANGE¹, ●MALTE OHMSTEDT¹, NIR GOV², ARIK YOCHELIS³, and HANS-GÜNTHER DÖBEREINER¹ — ¹Institut für Biophysik, Universität Bremen — ²Department of Chemical Physics, Weizmann Institute of Science, Israel — ³Department of Solar Energy and Environmental Physics, Ben-Gurion University of the Negev, Israel

Cells utilize the actin cytoskeleton to actively remodel their morphologies. This enables them to internalize extracellular fluid and activated membrane receptors via macropinocytosis. To form large vesicles this endocytotic mechanism relies on the contraction and closure of actin-based, ring-shaped vertical protrusions at the dorsal cell membrane that are known as Circular Dorsal Ruffles (CDRs). CDRs are essential to a range of vital and pathogenic processes alike. We show that CDRs are propagating fronts of actin polymerization in a bistable system. A new model assigns the expansion and contraction of waves to distinct counter-propagating fronts of different velocities. Under a change in biochemical conditions, CDRs may be pinned and fluctuate near the cell boundary or result in complex spiral wave dynamics due to a wave instability. Indeed, both phenomena are found in our data [1] pointing at the conditions for which macropinocytosis is suppressed. The latter scenario is valid for, e.g., confined CDRs on quasi one-dimensional tracks. We investigate the stochastic dynamics of these states as a function of biochemical conditions and find evidence of stochastic resonance. [1] E.Bernitt, C.G.Koh, N.Gov, HG Döbereiner, PLOS One 10 (1), e0115857 (2015)

BP 25.9 Tue 14:00 P2-EG

Forces generated and transmitted by the diffusible, microtubule-crosslinking motor protein kinesin-14 — ●ANNE-MARIE LÜDECKE^{1,2}, MARCUS BRAUN^{1,2}, ZDENEK LANSKY^{1,2,3}, ANJA-MARIA SEIDEL¹, and STEFAN DIEZ^{1,2} — ¹B CUBE, TU Dresden, Arnoldstraße 18, 01307 Dresden, Germany — ²MPI-CBG, Pfotenhauerstraße 108, 01307 Dresden, Germany — ³CAS, BIOCEV, Prumyslova 595, Vestec 25250, Czech Republic

Faithful cell division critically depends on the ability of the spindle apparatus to exert and withstand high force while dynamically remodeling its entire architecture during mitosis. In this context, microtubule (MT) contacts, facilitated by MT-crosslinking proteins are of vital importance. Crosslinking motors control spindle shape by (i) sliding newly nucleated MTs towards the spindle poles, thereby focusing MTs at the poles, but also by (2) crosslinking MTs from opposing spindle poles in the midzone of the spindle thereby mechanically stabilizing the spindle apparatus. Recently, force contributions of several types of crosslinkers have been described (e.g. of kinesin-5, ase1), but others remain elusive. Here, we quantified both the force generation of kinesin-14 motor domains as well as the force transmission of kinesin-14 full-length proteins in between MTs. We show that force generation by the motor domains is linearly dependent on motor number and that forces above 10 pN can be reached. Furthermore, we show that force transmission as well as sliding velocity are critically regulated by the diffusivity of the kinesin-14 tail domains on the MTs. Our results have implications in the force balance of the mitotic spindle.

BP 25.10 Tue 14:00 P2-EG

The shape of k-fibers reveals the existence of torques at the spindle poles — ●MAJA NOVAK^{1,2}, BRUNO POLAK², ZVONIMIR BOBAN¹, IVA M. TOLIC², and NENAD PAVIN¹ — ¹Faculty of Science, University of Zagreb, Zagreb, Croatia — ²Rudjer Boskovic Institute, Zagreb, Croatia

During cell division, the mitotic spindle made of microtubules drives segregation of the genetic material into two nascent cells. Bundles of microtubules known as k-fibers pull on kinetochores, protein complexes on the chromosomes. Recently, by investigating bundles of microtubules at the outer part of the spindle, we have found that bridging microtubules, which link sister k-fibers, attain a C-shape and balance the forces at the kinetochores (Kajtez et al, Nat Commun 2016). However, it is unknown what forces and torques are present in the inner part of the spindle. To answer this question, we have developed a theoretical model, where sister k-fibers are represented as an elastic slender rod shaped by forces and torques generated at the spindle poles. We found that k-fibers attain a general helical shape, whose projection on a plane can be identified as C-, S- and M- shape. By live-cell imaging experiments, we observed these three characteristic shapes, indicating a helical shape of k-fibers and consequently torques in the direction of the major axis. In addition, we found that helical shapes can exist under both tension and compression. We conclude that torques, as well as forces at the spindle poles determine the shape of mitotic spindle.

BP 25.11 Tue 14:00 P2-EG

Composite networks of actin and intermediate filaments — ●TOM GOLDE¹, MARTIN GLASER¹, TINA HÄNDLER¹, CARSTEN SCHULDT¹, JÖRG SCHNAUSS¹, HARALD HERRMANN², and JOSEF KÄS¹ — ¹University of Leipzig, Leipzig, Germany — ²German Cancer Research Center, Heidelberg, Germany

Mechanical properties of cells are mainly determined by the cytoskeletal components actin, microtubules, and intermediate filaments (IF). F-actin networks have been extensively studied both experimentally and theoretically. They are the most common model system for semiflexible polymer networks. IF feature network properties such as strain stiffening and a weak concentration dependency of the plateau modulus that are not covered by simple actin models. Although these proteins co-localize *in vivo*, the interplay between actin and cytoskeletal IF is widely unknown.

We used bulk rheology to study simplified *in vitro* networks comprised of actin and one type of IF, namely vimentin. Composite networks revealed physical properties between pure actin and vimentin networks in both the linear and non-linear regime. These properties can be tuned via the mixing ratio of these proteins. Fluorescence microscopy was employed to measure the network mesh size as well as the persistence length and reptation behavior of tracer filaments. Thus, we were able to link the properties of single filaments with the macro rheological properties of composite networks.

BP 25.12 Tue 14:00 P2-EG

Transition from a linear to a harmonic potential in collective dynamics of a multifilament actin bundle — ●JÖRG SCHNAUSS^{1,2}, TOM GOLDE¹, CARSTEN SCHULDT^{1,2}, B.U. SEBASTIAN SCHMIDT¹, MARTIN GLASER^{1,2}, DAN STREHLE¹, TINA HÄNDLER^{1,2}, CLAUS HEUSSINGER³, and JOSEF A. KÄS¹ — ¹Institute for Experimental Physics I, Leipzig University, Germany — ²Fraunhofer IZI, Leipzig, Germany — ³Institute for Theoretical Physics, Georg-August University of Göttingen, Germany

Modeling approaches and recent experimental data have shown that depletion forces between suspended, rod-like particles display different signatures depending on the orientation of these particles. It has been shown that depletion-driven, axial attraction of two rods yields a constant contractile force of 0.1 pN, which corresponds to a linear energy potential. We extended these pairwise interactions to a multi-filament level by investigating arising dynamics within actin bundles. Without any additional proteins such as crosslinkers or molecular motors, we found contractile forces in a biologically relevant regime of up to 3 pN. Generated forces due to bundle relaxation were not constant as in a two filament case, but decayed exponentially with a mean decay time of 3.4 s. These different dynamics are explained within the frame of a mathematical model (and supported by simulations) by taking pairwise interactions to a multi-filament scale [1].

[1] Schnaß et al.: Transition from a Linear to a Harmonic Potential in Collective Dynamics of a Multifilament Actin Bundle, Phys. Rev. Lett. 116, 108102 (2016)

BP 26: Posters - Cell Adhesion

Time: Tuesday 14:00–16:00

Location: P2-EG

BP 26.1 Tue 14:00 P2-EG

Fracture test of epithelial monolayers — •DAVE AHRENS¹, GEORG DREISSEN¹, MATTHIAS RÜBSAM², BERND HOFFMANN¹, WOLFGANG ZIEGLER³, CARIEN NIESSEN², and RUDOLF MERKEL¹ — ¹Institute of Complex Systems, ICS-7: Biomechanics, Forschungszentrum Jülich, 52425 Jülich, Germany — ²Department of Dermatology, Center for Molecular Medicine Cologne, University of Cologne, 50931 Cologne, Germany — ³Hannover Medical School, Dept. of Paediatric Kidney, Liver and Metabolic Diseases, 30625 Hannover, Germany

One vital function of epithelial tissue is providing a physical barrier against high mechanical loads in order to protect underlying tissues. Due to experimental limitations for mechanical characterizations of cell layers we developed a monolayer cell-sheet model on highly elastic silicone rubber chambers. These chambers allow single cell and cell sheet straining by 150% and more in single as well as cyclic tensile straining events. Furthermore, cell-cell contact formation and epithelial cell sheet maturation was induced by Ca²⁺ for different time periods before stretching. We could show that epithelial cells completely change their mechanical behavior in response to strain with increasing incubation times in Ca²⁺ containing media. Previously acting as a system whose components respond largely independent from each other, cells mechanically function as unit after sheet maturation. Stretching epithelial cells lacking vinculin as a component of cellular adhesion could prove the importance of vinculin for mechanical resistance in cell-matrix adhesions on single cell level while vinculin KO cell sheets were rarely affected in their mechanical integrity.

BP 26.2 Tue 14:00 P2-EG

Revealing contact formation characteristics of bacteria — •NICOLAS THEWES, CHRISTIAN SPENGLER, FRIEDERIKE NOLLE, and KARIN JACOBS — Experimental Physics, Saarland University, Germany

Bacteria exhibit an outstanding ability to adhere to various kinds of surfaces. Single cell AFM force spectroscopy has proven to be a powerful tool to quantify the acting forces if combined with a clever choice of substrates. On hydrophobic surfaces, the hydrophobic interaction plays the main role for the adhesion of bacteria and the contact formation process is dominated by the longest cell wall macromolecules. In our AFM study, we were able to observe the process of making contact by observing the snap-in process in detail [1]. To interpret the data, Monte Carlo simulations were set up, involving a simple model for a bacterium. The simulations yield strikingly matching results, corroborating the interpretation that the contact formation of *S. aureus* relies on thermally fluctuation cell wall proteins that tether to a surface and subsequently pull the bacterium to the surface. That way, e.g. *S. aureus* is able to attach to surfaces over distances far beyond the range of classic surface forces! Our results therefore suggest that the bacterial adhesion process in general, can be described by solely taking into account the tethered macromolecules between a bacterium and a surface.

[1] N. Thewes et al, Stochastic binding of Staphylococcus aureus to hydrophobic surfaces, Soft Matter 2015, 11, 8913 - 8919

BP 26.3 Tue 14:00 P2-EG

Microbial Adhesion Influenced by Nanoroughnesses — CLAUDIA LÜDECKE-BEYER^{1,3}, MARTIN ROTH^{2,3}, NATHALIE STEFANI^{2,3}, •CHRISTIAN HELBING¹, JÖRG BOSSERT^{1,3}, and KLAUS D. JANDT^{1,3} — ¹Chair of Materials Science, Otto Schott Institute of Materials Research, Friedrich Schiller University, Jena, Germany — ²Leibniz Institute for Natural Product Research and Infection Biology, Bio Pilot Plant, Hans Knöll Institute, Jena, Germany — ³Jena School for Microbial Communication (JSMC), Excellence Graduate School, Friedrich Schiller University, Jena, Germany

An advanced understanding of the microbe-material-interaction is required for the current development and progress in nanoscale structuring of materials surfaces to control microbial adhesion. This study aimed to investigate the nanostructure of the microbe-material-interface and to link it to microbial adhesion kinetics as a function of the titanium surface nanoroughness. A statistically significantly reduced microbial adhesion on titanium surfaces, prepared by physical vapor deposition, with a nanoroughness of 6 nm compared to 2 nm was observed. Direct insight into the microbe-titanium-interface

was gained by cross-sectioning of the microbial cells with a focused ion beam. High resolution scanning electron microscopy images gave first evidence that the surface peaks are the loci of initial contact between the microbial cells and the materials surface which is proposed in a qualitative model. This new understanding will help towards the design of materials surfaces for controlling microbial adhesion.

BP 26.4 Tue 14:00 P2-EG

Cell-cell adhesion in the optical stretcher - Methods for experimental and analytical force measurements — •PABLO GÖTTHEIL, STEFFEN GROSSER, and JOSEF KÄS — Germany, University of Leipzig, Faculty of Physics and Earth Sciences, Institute of Experimental Physics I, Soft Matter Physics Division

The optical stretcher is a dual-beam laser trap used to micromanipulate single cells in order to measure their viscoelastic properties. Here however, we use it to measure cell-cell adhesion forces, by stretching them apart from each other. The experimental way of approximating this force is to track the cells in the stretcher chamber and measure the speed in order to calculate the Stokes' law. Calculate the beam propagation and its diffraction by the cells can be used to analytically get the momenta in the whole cell chamber respectively before and after the diffraction. Comparing these two methods would give a nuanced view on the cell-cell adhesion forces.

BP 26.5 Tue 14:00 P2-EG

Mechanosensitivity of Murine Kidney Epithelial Cells — •THERESA HOPPE and FLORIAN REHFELDT — Third Institute of Physics, University of Göttingen

Recent experiments have shown that cell adhesion and subsequent spreading is dictated by the elasticity of the underlying substrate. Additionally, the ligand density and type of ligand employed result in differences in a cell's spreading behavior.

Here we investigate cellular spreading on two different types of collagen (Collagen I and IV) and by way of using two cell types. Collagen I is a major component of the connective tissue extracellular matrix (ECM), whereas collagen IV is primarily prominent in the ECM of epithelial tissue cells. Previous studies have well established optimal ligand concentrations of Collagen I for hMSC's. In this study, we determined the optimal collagen IV concentration for the maximal spreading of human mesenchymal stem cells (hMSC) on 10kPa polyacrylamide (PA) gels. We also studied the adherence of primary murine tubular epithelial cells on PA gels of varying elasticity coated with the same concentrations of collagen I and IV as for the hMSCs. We analyzed cell spreading via fluorescence microscopy.

Results indicate that on comparison with collagen I hMSC's spread area is lower on collagen IV for the same 10kPa PA gels. Surprisingly murine cell adherence seems to be ligand specific. On varying substrate stiffness, collagen I promotes spreading of these cells whereas collagen IV failed to supply sufficient adhesion sites.

BP 26.6 Tue 14:00 P2-EG

Measuring Cell Dynamics at the Substrate-Interface with Surface Plasmon Resonance Microscopy — •EVA KREYSING, HOSSEIN HASSANI, and ANDREAS OFFENHÄUSSER — ICS8/PGI8, Forschungszentrum Jülich, 52425 Jülich

In neuroelectronics the cell-electrode distance is one of the most critical parameters during cell recordings. Cardiomyocyte-like cells are among the most popular model systems because they periodically generate an action potential. This feature also leads to a cell contraction which affects the cell-electrode distance. To achieve a qualitative and quantitative characterization of the dynamics at the interface in vitro and label-free, we built a surface plasmon resonance microscope (SPRM). Using gold coated sapphire chips as the substrate for cell culture it is possible to excite plasmons in the gold layer due to specific illumination. The resonance frequency of the plasmons depends strongly upon the dielectric constant of the gold's environment. In turn the angle spectrum of the reflected light depends upon said resonance frequency. Due to these dependencies it is possible to deduce the cell-substrate distance. Our microscope is capable of imaging the interface in a live-imaging mode where we can observe cell dynamics qualitatively. A scanning mode uses localized surface plasmons to measure the cell-substrate distance. The resolution in z-direction lies in the nanometer

range. This allows us to measure the movement of the cell membrane at each scanning point with a time resolution of 150 ms. Using this method we have been able to record the dynamics of multiple cardiomyocytes.

BP 26.7 Tue 14:00 P2-EG

Microbial adhesion forces on nanostructured surfaces — ●CAROLIN DEWALD^{1,2,3}, CLAUDIA LÜDECKE-BEYER¹, MARTIN ROTH^{2,3}, JÖRG BOSSERT¹, and KLAUS D. JANDT^{1,3} — ¹Chair of Materials Science, Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena — ²Bio Pilot Plant, Leibniz Institute for Natural Product Research and Infection Biology, Hans Knöll Institute Jena, Beutenbergstraße 11, 07745 Jena — ³Jena School for Microbial Communication, Neugasse 23, 07743 Jena

Often only qualitative adhesion properties are analyzed limiting the quantitative information about adhesion forces between microbial cells and materials surfaces. Force-distance curves are one option to measure adhesion forces. Therefore, the aim of this study is to investigate the adhesion kinetics and forces of *Candida albicans* as function of nanoparticle structured materials surfaces. The investigated surfaces with different AuNPs densities as well as unstructured control surfaces showed no statistically significant differences in contact angle and surfaces chemistry. A reduced microbial adhesion was observed on the nanostructured surfaces compared to the control surface. The AuNPs act as contact points for initial microbial adhesion which was confirmed by force-distance curves. A lower AuNP density led to a reduced microbial adhesion due to reduced adhesion forces between microbial cells and materials surfaces. This study will provide new

insight into microbial adhesion on materials surfaces structured in the nanometer range.

BP 26.8 Tue 14:00 P2-EG

Morphological, Mechanical and Adhesion Properties of Neutrophil Extracellular Traps — ●RICARDO H. PIRES^{1,2,3}, MIHAELA DELCEA^{2,3}, STEPHAN B. FELIX^{2,3}, and OLIVER OTTO^{1,3} — ¹Universität Greifswald, Greifswald, Germany — ²Universitätsmedizin Greifswald, Greifswald, Germany — ³DZHK, Greifswald, Germany

Neutrophils are immune system cells that have recently been found to engage in a suicidal pathway that leads to the extrusion of partially decondensed chromatin, or neutrophil extracellular traps (NETs). In the circulatory system, NETs bind and capture pathogens thus limiting their spread, but they have also been associated with thrombus formation, as well as other cardiovascular disorders. Despite their relevance, little is known about the molecular mechanisms behind their adhesive and mechanical properties. In this work we combine fluorescence and atomic force microscopies with force spectroscopy to obtain detailed information on the morphology of NETs, on parameters that affect their mechanical behavior and their adhesive properties. We report that NETs are not a simple bundle of chromatin fibers, but exhibit an order evidenced by its web-like appearance with openings in the sub-micron range. Partial proteolysis assays further indicate that the protein content of NETs is not only relevant to its mechanical behavior but to its morphology as well, thus highlighting the inextricable role of proteins in defining the architecture of NETs. In addition, force spectroscopy also indicates that the adhesive mechanism of NETs may in part be governed by unspecific electrostatic interactions.

BP 27: Posters - Microswimmers

Time: Tuesday 14:00–16:00

Location: P2-EG

BP 27.1 Tue 14:00 P2-EG

A bacterial swimmer with two alternative movement patterns — VERONIKA WALJOR, MARIUS HINTSCHE, ●ZAHRA ALIREZAEIZANJANI, and CARSTEN BETA — Institute of Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany

The soil bacterium *Pseudomonas putida* is a bacterial swimmer that propels itself with the help of several flagella that are polarly arranged at one end of the cell body. Through its chemosensory system, which is coupled to the rotary motors that drive the flagella, *P. putida* senses changes in its environment and responds by altering its motility.

When growing in a medium that offers only minimal amounts of nutrient, *P. putida* exhibits a motion pattern characterized by persistent runs that are interrupted by reversals in the swimming direction. In contrast, when growing under rich medium conditions, the reversal rate is drastically reduced and the swimming pattern is dominated by stopping events that interrupt the episodes of persistent runs.

Additional experiments in microfluidic gradient chambers suggest that the reversals are signatures of a chemotactic strategy, which is activated when food is sparse but not required under rich growth conditions.

BP 27.2 Tue 14:00 P2-EG

Curvature-Guided Motility of Single Microalgae in Geometric Confinement — TANYA OSTAPENKO, FABIAN SCHWARZENDAHL, ●THOMAS BÖDDEKER, CHRISTIAN T. KREIS, JAN CAMMANN, MARCO G. MAZZA, and OLIVER BÄUMCHEN — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

Microorganisms often live in habitats consisting of a liquid phase and a variety of curved interfaces. Understanding the precise way in which such organisms behave in their environment finds technological relevance with regards to surface colonization leading to biofilm formation. Using experiments, simulations, and analytics, we study the motility of a single *Chlamydomonas* cell in an isolated microhabitat with controlled geometric properties. We provide evidence that the local wall curvature controls the cell's navigation in confinement, where there is an enhanced probability of finding the cell in the vicinity of a wall with high curvature. This probability scales linearly with the curvature of the interface, as seen for both circular and elliptical chambers. Our theory utilizing a dumbbell model of the organism captures our ex-

perimental data quantitatively, with no free parameters, evoking only steric wall interactions and the cell's torque at the wall during an interaction event with finite time. Thus, hydrodynamics are not necessary to describe the statistical behavior of the cell's swimming on the compartment length scale. (T. Ostapenko, et al. arXiv:1608.00363, 2016)

BP 27.3 Tue 14:00 P2-EG

Inertial effects in microswimming — ●OLEG TROSMAN^{1,2}, JAYANT PANDE^{1,2}, and ANA-SUNČANA SMITH^{1,2,3} — ¹PULS group, Department of Physics, Friedrich-Alexander-University of Erlangen-Nuremberg, Germany — ²Cluster of Excellence: Engineering of Advanced Materials, Department of Physics, Friedrich-Alexander-University of Erlangen-Nuremberg, Germany — ³Division of Physical Chemistry, Ruđer Bošković Institute, Zagreb, Croatia

Increased theoretical study in the past few decades has enabled scientists to gain a deeper insight into the motion of micro-swimmers, yet most theoretical approaches addressed the domain of negligible Reynolds number Re , ignoring inertia. In nature, however, in an intermediate range of Re , before turbulences arise, the inertial effects become important. In this work we conduct a theoretical study of how this regime emerges. For this we extend the swimmer model by Golestanian and Najafi, which has three beads attached in series in a fluid and moving along the axis of the swimmer, by inclusion of the beads' masses. We do this by combining the Oseen-Stokes equations for the coupled motion of distant spheres in a fluid with Newton's force-mass relations and obtain a coupled system of first-order differential equations. Solving these equations allows us to derive a closed-form expression for the velocity of the swimmer which explicitly takes inertia into account. This velocity expression compares considerably better to results obtained from lattice-Boltzmann simulations of the swimmer, for intermediately high bead masses or driving forces, than the inertia-free model of Golestanian and Najafi.

BP 27.4 Tue 14:00 P2-EG

Light-activated flagella dynamics of *Chlamydomonas* in contact with a surface — ●CHRISTINE LINNE, CHRISTIAN KREIS, and OLIVER BÄUMCHEN — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, D-37077 Göttingen, Germany

The photoactive microalga *Chlamydomonas reinhardtii* typically lives in complex environments such as soil and has two modes of locomotion: freely swimming in liquid and gliding on a surface. By performing in-

in vivo force spectroscopy experiments we discovered that light stimulation regulates the transition between both motility modes, since the adhesiveness of the flagella can be reversibly switched on and off by light [1]. We held a *Chlamydomonas* cell with a micropipette force sensor in close proximity to a substrate, such that the flagella tips can physically sense the surface during every beating cycle. After light stimulation, the flagella provide adhesive contacts with the surface

and actively pull the cell body towards the substrate. Time-resolved *in vivo* micropipette experiments reveal the forces exerted by the cell during this process. We explain the flagella dynamics using a model which takes into account the activity of the molecular motors within the flagella. [1] C. Kreis, M. Le Blay, C. Linne, M. Makowski, and O. Bäümchen, in review (2016).

BP 28: Posters - Cell Migration & Contraction

Time: Tuesday 14:00–16:00

Location: P2-EG

BP 28.1 Tue 14:00 P2-EG

Connecting cell jamming with adhesion, contractility and cell stiffness — ●JÜRGEN LIPPOLDT, PAUL HEINE, STEFFEN GROSSER, LINDA OSWALD, and JOSEF KÄS — Soft Matter Physics, University of Leipzig, Germany

Our collaborators, Lisa Manning and Cristina Marchetti have developed a coarse grained model of cell jamming in elastic tissues. The constitutive equation has a harmonic term for the cell area, which promotes volume conservation due to cell stiffness and osmotic pressure, and one for the cell perimeter, which expresses the interplay between cell adhesion and cell contractility. In simulations with self-propelled cells and Voronoi tessellation a phase transition between a jammed and an unjammed phase was observed.

We examine this model with cancer cell lines, which undergo the epithelial-mesenchymal transition. To determine, whether the cell layers are jammed, we use glassy metrics like the mean-square displacement, Bayes statistics of individual tracks and an analysis of the neighbourhood change. The shape of the cells can be determined by image analysis of phase contrast or actin labelled fluorescence images.

This framework is well suited to explore changes in collective cell migration for different cell types, varying conditions and the use of drugs. Changing physical properties of the cells will lead to a different target shape parameter and should change their motility. This will provide insights in how cells can change their collective behaviour by altering their individual properties and how observed collective phenomena like cellular streaming emerge.

BP 29: Posters - Multi-Cellular Systems

Time: Tuesday 14:00–16:00

Location: P2-EG

BP 29.1 Tue 14:00 P2-EG

Stress-Strain Relation in Reconstituted Tissue — ●SIMONE GEHRER¹, DAMIR VURNEK¹, SARA KALIMAN¹, MARYAM ALIEE¹, DIANA DUDZIAK², BERND HOFFMANN³, RUDOLF MERKEL³, and ANA-SUNČANA SMITH^{1,4} — ¹Puls Group, Institute for theoretical Physics, FAU Erlangen — ²University Clinic Erlangen — ³ICS-7:Biomechanics, Forschungszentrum Jülich — ⁴Division of Physical Chemistry, IRB Zagreb

Epithelial cells form active two-dimensional sheets that are involved in variety of functions like morphogenesis, embryogenesis, wound healing and organ development. Mechanical stress stimulates i.e. processes like growth, proliferation and remodeling of the surfaces.

To study the stress-strain relation in model tissues Madin-Darby canine kidney II cells were seeded on fibronectin coated polydimethylsiloxane elastomer chambers in a droplet wise manner. The resulting surface was uniaxially stretched with amplitudes of 0, 10, 20 and 30%. Subsequently the reaction and growth of clusters was imaged in phase contrast on timescales from minutes to days.

We present a comprehensive study of tissue growth after stretching. The change in cell size, elongation and orientation as well as connectivity and relaxation was investigated.

BP 29.2 Tue 14:00 P2-EG

Predicting cell colony growth from single cell proliferation and migration behavior — ●NICO WUNDERLING, JULIAN ÜBELACKER, JANINA LANGE, BEN FABRY, and CLAUS METZNER — Biophysics, University of Erlangen, Germany

The macroscopic growth of cell colonies on planar substrates is driven by the division and migration of individual cells. Experiments show that many qualitative features of the colony growth dynamics, such as a linear growth of the colony radius with time, are universal among many different cell types, thus pointing to a generic mechanism behind this collective phenomenon. Here, we describe colony growth by a cell-density-dependent proliferation and diffusion. Using cells seeded at different confluences (30-100%), we measure how the proliferation rate and the diffusion constant vary with cell density for three differently metastatic tumor cell lines (HT1080 fibrosarcoma, MDA-MB-231 epithelial breast carcinoma, and MCF-7 epithelial breast carcinoma). We find that cell proliferation saturates at high cell densities in HT1080 and MDA-MB231 cells, but shows a maximum at intermediate cell densities for MCF-7 cells. Cell diffusion is independent of cell density in MDA-MB-231 and MCF-7 cells, but linearly increases with cell

density in HT1080 cells. With these experimentally obtained density-dependent proliferation and diffusion profiles, we numerically predict the cell colony growth over several days. In each case, we find a linear growth of the colony radius versus time with a growth speed that closely matches the experimental data, thus demonstrating that colony growth can be predicted from single cell behavior.

BP 29.3 Tue 14:00 P2-EG

Theoretical Model for Absorption Profiles in Xylem Networks — ●FELIX MEIGEL and KAREN ALIM — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Plant leaves receive their supply of nutrients from the soil through sap flow traveling up the plant stem and then being spread out within the leaf through the leaf's vascular network. Within sap flow nutrients are transported by advection and diffusion while they are readily absorbed into the leaf's cells. Assuming that all leaf cells require the same amount of nutrients one would expect the ideal case to be homogeneous absorption of nutrients throughout the entire leaf. Yet, the entire leaf only has one inflow of sap through the single vein connecting it to the plant stem. How must the leaf vascular network be set up such that a single inflow can give rise to homogeneous absorption of nutrients throughout a leaf? We present a model for the sap flow and the resulting absorption pattern in a leaf vascular network. We find that the sap influx rate is the dominating factor. There exists an optimal influx rate that corresponds to the most homogeneous absorption profile. We simplify the flow dynamics in an extended vascular network to a simple leaky pipeline. This toy model allows us to determine a simple scaling law for the optimal influx rate.

BP 29.4 Tue 14:00 P2-EG

Coalescence of bacterial microcolonies reveals liquid-like dynamics — ●TOM CRONENBERG, ENNO R. OLDEWURTEL, NADZEYA KOUZEL, and BERENIKE MAIER — Department of Physics, University of Cologne, 50539 Cologne, Germany

Many bacteria are able to form communities called microcolonies. Within these structured communities they benefit from various advantages including facilitated gene transfer and increased antibiotic resistance. The human pathogen *Neisseria gonorrhoeae* is able to aggregate into spherical microcolonies due to active retraction of its type 4 pili, which is the first step of biofilm formation. Once two microcolonies are within a minimal range, an actively driven fusion process is initiated. To test if the fusion of microcolonies shows liquid-like

dynamics, we acquired time lapsed microscopy data of newly formed microcolonies in liquid environment. The contour of fusing colonies was extracted and fitted by an ellipse to calculate the ratio between minor and major axis. According to a model developed by Young, the deformation of a liquid droplet from an ellipse to a sphere is driven by surface tension σ and resisted by viscosity η . Therefore, we used Young's model to characterize the spatio-temporal dynamics of colony fusions quantitatively by calculating the ratio σ/η .

BP 29.5 Tue 14:00 P2-EG

A Computational model of nuclei ordering in early *Drosophila* embryos — ●FRANZ KAISER¹, ZHIYI LV², JÖRG GROSSHANS², and KAREN ALIM¹ — ¹Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ²Institute for Biochemistry and Molecular Cell Biology, University of Göttingen, Göttingen, Germany

During interphase, nuclei in early *Drosophila melanogaster* syncytial embryos actively arrange in an ordered fashion. Interaction between nuclei in this syncytial embryo through F-actin and microtubule networks is assumed to play an important role for the establishment of nuclei order. However, the observed patterns still lack a physical explanation. Here we develop a theoretical model including passive interactions mediated by the extracellular matrix and active elements arising from microtubule dynamics to explain the observed ordering. We perform computer simulations and quantify the observed degree of orientational order. Results are compared to experimental recordings of tracked nuclei to identify mechanical model parameters. We observe how mechanical properties and nuclei order change between subsequent interphases.

BP 29.6 Tue 14:00 P2-EG

Controllability of discrete pattern formation by local inputs — ●STEPHAN KREMSE¹, TIAGO RAMALHO¹, HAO WU², and ULRICH GERLAND¹ — ¹Physics of Complex Biosystems, Physics Department, Technical University of Munich, James-Frank-Str. 1, 85748 Garching, Germany — ²LOEWE Zentrum für Synthetische Mikrobiologie, Philipps-University-Marburg, Hans-Meerwein-Str. 6, 35043 Marburg, Germany

Controllability is a fruitful concept to explore the extent to which a dynamical system can be steered by external inputs or internal feedback signals. Although it has been applied to a diverse range of problems in science and engineering, the controllability of a large class of dynamical systems, those that describe pattern formation processes, is not well understood, despite the fundamental role of controlled pattern formation in biology and technology. Here, we propose a minimal system for studying the control of discrete patterning, based on a one-dimensional cellular automaton model, which has only a finite set of possible update rules that specify its dynamics. The control signals are given by individual cells that are located either within the system or at its boundary. We consider two different control schemes and determine the extent to which the pattern formation process is controllable under a given control scheme.

BP 29.7 Tue 14:00 P2-EG

Direct measurements reveal significant improvement in retinal light transmission due to photoreceptor nuclear inversion — ●KAUSHIKARAM SUBRAMANIAN¹, MARTIN WEIGERT¹, IRINA SOLOVEI², and MORITZ KREYSING¹ — ¹Max Planck Institute of Molecular Cell Biology & Genetics, Dresden, Germany — ²Department of Biology, Ludwig Maximilian University, Munich, Germany

The vertebrate retina bears the odd evolutionary heritage of being inverted, necessitating photons to travel through hundreds of microns of living neuronal tissue before detection by photoreceptor cell (PRC) outer-segments. The large number of PRCs results in densely packed nuclei in the tissue which can potentially scatter light. Postnatal retinal PRC nuclei in nocturnal mammals undergo a hallmark process of inversion in their chromatin architecture [1]. Interferometric measurements and simulations, suggested that this chromatin rearrangement could lead to reduced light scattering and that each nuclei possess optical quality of lenses [2]. Using the concept of modulation transfer, we show that optical transmission of wild type (WT) mouse adult retina is significantly better than a WT retina in its postnatal development stages. Also, WT retina has a significantly higher strehl ratio than retina of a transgenic mouse where this inversion does not take place. We also complement these results with simulations to develop a mechanistic understanding of the light propagation in these tissues and visual behavioral studies. References [1] Solovei et al, Cell, 137(2)

(2009) [2] Błaszczyk et al, Opt Express, 22(9) (2014)

BP 29.8 Tue 14:00 P2-EG

Cell Jamming: Connecting the Shape and Density Dependences — ●STEFFEN GROSSER, LINDA OSWALD, JÜRGEN LIPPOLDT, PAUL HEINE, and JOSEF A. KÄS — Universität Leipzig, Germany

Cellular dynamics has been shown to display characteristics of jamming transitions which originally had been observed as a function of cell number density (Angelini et al., PNAS 2011). Recently, the Self-Propelled Voronoi (SPV) model has predicted a density-independent transition as a result of the counterplay of adhesion and contractile forces (Bi et al., Nat. Phys. 2015), visible in the dimensionless shape parameter.

We present experimental data for MCF-10A and MDA-MB-231 showing that shape and number density actually evolve in close concert; shape parameters decrease under increasing cell density. This feature, not predicted by the SPV model, happens in both the epithelial and mesenchymal cell lines, albeit with different consequences. Mesenchymal cells strongly delay their jamming transition even under high densities.

BP 29.9 Tue 14:00 P2-EG

Probing liquid-liquid phase transitions via fast and localized temperature stimuli — ●ANATOL FRITSCH¹, MATTHÄUS MITTASCH¹, ANDRÉS DIAZ¹, FRANK JÜLICHER², ANTHONY HYMAN¹, and MORITZ KREYSING¹ — ¹MPI of Molecular Cell Biology and Genetics, Dresden — ²MPI for the Physics of Complex Systems, Dresden

Recent studies report membrane-less organelles (MLO) to show liquid-like behavior formed by phase transition of aqueous solutions. These organelles foster a dynamic, spatially separated platform for important biochemical reactions inside the cell. In *C. elegans* embryos MLOs called P granules segregate asymmetrically and play a key role in the specification of the germ cell fate. We want to shed light on the physical principles underlying this segregation process.

Since liquid-like organelles are formed by phase separation, they should respond to variations in their environment such as changes in pH, salt concentration or temperature. To study the kinetics of MLO phase transition we use temperature as a control parameter for defined changes between the mixed and demixed state. For fast and localized temperature control, we use a custom build IR-laser scanning microscopy setup combined with a Peltier controlled sample stage. Experiments on *in vivo* P granules and corresponding *in vitro* reconstituted systems show fast transition times and allow for the characterization of growth and melting kinetics of the phase separated domains. Furthermore, specific temperature patterns can be used to capture the thermodynamics of P granule segregation inside the embryo.

BP 29.10 Tue 14:00 P2-EG

Mode structure of morphogen transport — ●DANIEL AGUILAR-HIDALGO^{1,2}, MARIA ROMANOVA-MICHAELIDES², MARCOS GONZÁLEZ-GÁITAN², and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems — ²University of Geneva

Concentration profiles of specific signaling molecules, also called morphogens, have been identified that control patterning and growth of developing tissues. In this regard, the morphogen transport dynamics defines the shape of the morphogen profile, which has been highlighted as a key factor in a number of growth control mechanisms, hence the importance to understand how molecules are transported in tissues. We propose a general theoretical framework and a novel approach for the study of morphogen transport dynamics in cell monolayer tissues. In particular, we analyze the mode structure of a transport model, where we allow molecules to spread by free diffusion and transcytosis that is a trafficking process in which molecules travel long distances by subsequent rounds of internalization and externalization at different positions in cells. Our theory reveals different transport modes in the system. We discuss how seemingly contradictory interpretation of experiments that measure morphogen transport dynamics (FRAP, FCS) may capture different dynamical modes in the system. Our theoretical framework allows quantifying effective transport parameters as well as rates for elementary transport events, unifying measures from different experimental assays. As a particular case of study, we apply our theory to quantitatively describe the transport of the morphogen Dpp in the *Drosophila* wing disc.

BP 29.11 Tue 14:00 P2-EG

Scaling of peristaltic waves in slime moulds by a feedback between actin contractions and flow — ●JEAN-DANIEL JULIEN,

NATALIE ANDREW, and KAREN ALIM — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The coordination of movements over macroscopic organisms lacking in any neural circuit, such as slime moulds, fungi or plants, is a fascinating yet poorly understood phenomenon. Plasmodial slime moulds grow as networks of tubes whose extent can vary on several orders of magnitude. The coordinated contractions of the tubes lead to the transport of biomass and nutrients over the network. Recent studies of *P. polycephalum* have demonstrated that those waves of contraction scale with the size of the organism in order to optimise the transport. How such a giant cell can perform this scaling independently of its size is unclear. *F. Septica*, another slime mould, displays similar patterns of contractions, and also builds simple networks constituted of a single loop, thus making it ideal to theoretical analysis. By modelling the turnover of the actin cortex at the periphery of the tube and the flow generated by the contractions, we show that a positive feedback between the flow and the wavelength of the peristaltic wave can explain how the mechanical wave scales with the extent of the network.

BP 29.12 Tue 14:00 P2-EG

Protein-protein interactions in developmental cell-cell fu-

sion quantified by fluorescence fluctuation spectroscopy — ●VALENTIN DUNSING¹, BENJAMIN PODBILEWICZ², and SALVATORE CHIANTIA¹ — ¹Cell Membrane Biophysics, Institut für Biochemie und Biologie, Universität Potsdam — ²Department of Biology, Technion - Israel Institute of Technology, Haifa

Cell-cell fusion is a universal process in development which is involved in the formation of various organs and tissues. Failure of fusion leads to severe morphogenic disorders. The epithelial fusion failure protein EFF-1 was shown to be necessary and sufficient for fusion in the small nematode *C.elegans* and cell culture systems. However, its mechanism of action remains poorly understood.

Using fluorescence fluctuation microscopy approaches (Number&Brightness, Scanning FCS) we study the cis- and trans- interactions of EFF-1 and its dynamics in the plasma membrane. We observe a concentration dependent cis-trimerization of the protein in living cells and monitor cell-cell (i.e. protein-protein) trans-interactions by calculating cross-correlation of spectrally separated fluctuations.

Finally, we present an experimental setup to investigate EFF-1 interactions in vivo, i.e. epithelial cell-cell fusions in developing *C.elegans* embryos.

BP 30: Posters - Neurosciences

Time: Tuesday 14:00–16:00

Location: P2-OG1

BP 30.1 Tue 14:00 P2-OG1

Self-organized criticality in a binary neural network model with local rules — ●STEFAN LANDMANN and STEFAN BORNHOLDT — Institute for Theoretical Physics, University of Bremen, D-28359 Bremen, Germany

Since the seminal work of Beggs and Plenz [1] which gave strong evidence for criticality in neural systems there is a growing interest in how criticality may emerge in neural networks.

Extending previous work of our group [2,3] we present and investigate a simple but biologically plausible neural network model which exhibits self-organized criticality (SOC). Based on local rules only the network evolves towards criticality, showing typical power-law distributed avalanche statistics. This behavior is independent of initial conditions and robust under noise. Due to its biological plausibility the model could help to understand mechanisms leading to criticality in neural systems.

[1] J. M. Beggs and D. Plenz, *Journal of Neuroscience* 23(35): 11167 (2003)

[2] S. Bornholdt and T. Rohlf, *Phys. Rev. E* 67: 066118 (2003)

[3] M. Rybarsch and S. Bornholdt, *PLoS ONE* 9(4): e93090 (2014)

BP 30.2 Tue 14:00 P2-OG1

Mechanotransduction in the pentamere chordotonal organ

of the *Drosophila* larva — ●ACHINTYA PRAHLAD¹, CHRISTIAN SPALTHOFF², BEN WARREN², DEQING KONG³, JÖRG GROSSHANS³, MARTIN GÖPFERT², and CHRISTOPH SCHMIDT¹ — ¹Third Institute of Physics, Georg August University, Göttingen — ²Schwann-Schleiden Research Centre, Georg August University, Göttingen — ³Institute of Biochemistry and Molecular Cell Biology, University Medical Centre, Göttingen

Chordotonal organs perform mechanosensory functions across diverse insect species. How these organs transduce mechanical stimuli is so far unknown. Our organ of interest is the *lch5* organ, which plays a key role in coordinating locomotion in the *Drosophila* larva. This organ consists of neurons and accessory cells. We applied tension to the whole organ in situ by transverse deflection. Upon release, the organ displays overdamped relaxation with two widely separated time constants, a rapid snap-back followed by a slow relaxation. When the muscles covering the *lch5* organ were excised, the slow relaxation was absent and the fast time constant was faster. Most of the strain in the stretched organ is localized in the cap cells, which account for 66% of the length of the entire organ, and could be stretched to increase the length by ~10% without apparent damage. In laser ablation experiments we found that cap cells severed from the neurons retracted over 100 microns indicating considerable stress and strain in these cells. Given that myosins are abundant in the cap cells, the results point to a mechanical regulatory role of the cap cells in the *lch5* organ.

BP 31: Posters - Biotechnology and Bioengineering

Time: Tuesday 14:00–16:00

Location: P2-OG1

BP 31.1 Tue 14:00 P2-OG1

Synthesis and characterization of magnetite nanoparticles with aminosilane coating — ●STEFANIE FUCHS, MARYAM YOHANNAYEE, and MATHIAS GETZLAFF — Institute of Applied Physics, Heinrich-Heine-Universität, Düsseldorf, Germany

The interest in magnetic nanoparticles grew in the recent years due to a wide range of possible applications in technology and medicine. The most important ones in medical and biomedical science are their use as MRI contrast agent, in targeted drug delivery and in hyperthermia treatment. They show superparamagnetic property at room temperature from the aspect of magnetic properties and also biocompatibility and low toxicity from a biomedical point of view. Magnetite nanoparticles are synthesized from Ferric Chloride and Ferrous Sulphate via wet chemical coprecipitation method. In order to functionalize them we have tried three different methods to coat them with N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (AEAPS). The aminosilane ligand shell increases the stability of magnetite nanoparticles in solution and also

biocompatibility of iron seeds through injection. The obtained particles have been characterized with Fourier transformed infrared spectroscopy (FTIR), X-ray powder diffraction (XRD) and transmission electron microscopy (TEM) to study the morphological structure of particles.

BP 31.2 Tue 14:00 P2-OG1

Bionic electrolocation strategy of objects in fluids based on superposition of numerically extracted and shifted EEVs — ●SABINE WOLF-HOMEYER¹, JACOB ENGELMANN², and AXEL SCHNEIDER¹ — ¹Bielefeld University of Applied Sciences, Germany — ²Bielefeld University, Germany

Additionally to visual sense, weakly electric fish use electrolocation for navigation and to find food even in dark or turbid waters. Specialized muscle cells in the tail region generate a weak electric field around the fish's body. Sensed by electroreceptors on the animals' skin, distortion of the self-generated electric field, caused by objects, is

perceived. Furthermore the fish executes scanning behavior to obtain additional sensory information like size, shape and material properties of detected objects in their vicinity. Inspired by the biological model, a fixed minimal scanning strategy, composed of active receptor-system movements, is developed. The aim of this strategy is the unique identification of object-positions. With the aid of a bio-mimetic abstraction of the receptor-system, a scanning-method for active electrolocation is developed. The method is based on the superposition of numerical extracted EEV- (Ensemble of Electrosensory Viewpoints) contour-rings [Solberg et al., International Journal of Robotics Research, 27(5), pp. 529-548], which are previously simulated by means of FEM. To identify an optimal scanning strategy, the uniqueness of object positions for permutations of sensor movement sequences was evaluated. The best resulting concatenation of receptor-system movements consists of the combination of a linear shift, a rotation and the original EEV.

BP 31.3 Tue 14:00 P2-OG1

Neutron Reflectometry Reveals Structural Aspects of Blood Protein Adsorption to Polymer Brushes — ●VICTORIA LATZA¹, IGNACIO RODRIGUEZ LOUREIRO¹, IRENA KIESEL², AVRAHAM HALPERIN³, GIOVANNA FRAGNETO², and EMANUEL SCHNECK¹ — ¹Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Deutschland — ²Institut Laue-Langevin, Grenoble, Frankreich — ³Université Joseph Fourier, Grenoble, Frankreich

Protein adsorption to biomedical surfaces, for example of implants, is a major issue because it can lead to harmful foreign body reactions. Surface functionalization with hydrophilic polymer brushes is a common strategy to suppress undesired protein adsorption. However, numerous cases where this approach failed are reported and further investigation of the molecular mechanisms is required. Here, we use neutron reflectometry (NR) to characterize the adsorption of blood proteins to poly(ethylene glycol) (PEG) brushes grafted to planar phospholipid surfaces. The unique structural insights provided by NR allows distin-

guishing between different adsorption modes. For whole human blood serum the reflectivity curves show significant primary adsorption into the lipid head group region and suggest the presence of a low amount of ternary adsorption at the brush periphery. In context with the commonly neglected antigenicity of PEG we systematically characterize the structural aspects of antibody binding to polymer brushes with various chain lengths and grafting densities. To this end we obtained qualitatively different results for antibodies specific to the PEG end points and to the backbone.

BP 31.4 Tue 14:00 P2-OG1

The muscle lever arm: a key factor to muscle effectiveness in biomechanical models — ●MARIA HAMMER and SYN SCHMITT — SimTech, Universität Stuttgart

Pulling actuators play an important role in biomechanical simulations. In most animals, muscles are the actuators exerting torques onto the joints. These torques highly depend on the muscles' line of action or, in other words, muscle lever arms. Common methods focus either on single-joint movements, on two-dimensional problems, or on imitating physiological lever arms only in a small working range. However, especially in complex multibody simulations, where reduced descriptions of muscles as massless, visco-elastic bands are used, a correct representation of lever arms is mandatory for a large range of joint angles for all degrees of freedom.

To address these issues, we developed a new design and computational algorithm for modeling the path of linear pulling actuators. The method is based on finding the minimum potential energy path while the actuator is lead through a small number of two-dimensional shapes. It allows for multiple degree of freedom and high-amplitude movements as well as combinations of both, ensuring reasonable lever arms at all possible joint configurations even for muscles spanning more than one joint. We applied this method to a multibody model of the human musculoskeletal system.

BP 32: Posters - DNA/RNA

Time: Tuesday 14:00–16:00

Location: P2-OG1

BP 32.1 Tue 14:00 P2-OG1

Condensation of DNA Brush Networks — ●GÜNTHER PARDATSCHER¹, DAN BRACHA², SHIRLEY S. DAUBE², OHAD VONSHAK², ROY H. BAR-ZIV², and FRIEDRICH C. SIMMEL^{1,3} — ¹TU München, Garching, Germany — ²Weizmann Institute of Science, Rehovot, Israel — ³Nanosystems Initiative Munich, München, Germany

DNA condensation via interaction with multivalent salts or histones is known for the regulation of genes and metabolism, and for the generation of self-assembling rod-like, spheroidal or toroidal DNA nanostructures. We here investigated the condensation of e-beam patterned, surface-bound DNA brushes into arbitrarily shaped DNA bundles. DNA molecules of 1 micron length (3 kbp) were immobilized on lines as thin as 100 nm in width, before condensation was induced by addition of spermidine. Starting at a nucleation site, DNA condensates grew via an inverted domino effect by adsorbing neighboring DNA chains.

The confinement of DNA brushes to widths below the contour length of the DNA resulted in changes in condensation dynamics and condensate morphology from two-dimensional dendritic to a single, straight one-dimensional DNA bundle. In contrast to condensation from solution or extended 2D brushes, 1D DNA bundles can be guided along predefined, arbitrary pathways, while persisting over tens of micrometers. We further applied the process in unconventional approaches to computational problems, e.g. in determining possible solutions for a maze.

BP 32.2 Tue 14:00 P2-OG1

Transcription by RNA polymerase II establishes DNA microstructure — ●LENNART HILBERT^{1,2,3}, YUKO SATO⁴, ALF HONIGMANN², FRANK JÜLICHER³, HIROSHI KIMURA⁴, NADINE L VASTENHOUW², and VASILY ZABURDAEV^{3,1} — ¹Center for Systems Biology Dresden — ²MPI Molecular Cell Biology and Genetics — ³MPI Physics of Complex Systems — ⁴Tokyo Institute of Technology

In interphase cell nuclei, DNA forms a microstructure of interspersed high concentration and low concentration regions. Transcription of DNA is carried out by RNA Polymerase II (Pol II) in low DNA density regions. While this organization reflects a need to unfold DNA for Pol II access, the causal origin of this spatial organization remains unclear. Here, we investigate if and how transcribing Pol II organizes DNA. Using zebrafish embryo cells, we found that Pol II needs to fill nuclei with RNA to induce segregation of DNA and RNA into a fine microstructure of mutually exclusive regions. We observed that the global DNA/RNA microstructure collapsed into a coarse pattern upon transcription inhibition. The microstructure originated from individual transcription sites, which locally displaced DNA by an RNA-rich region upon transcription activation. Our experimental results can be recapitulated in a simulated microemulsion. Here, the accumulation of nuclear RNA induces a global phase separation of DNA and RNA. Transcribing Pol II - tethered to both DNA and RNA - acted as a bivalent copolymer, locally dispersing DNA in the RNA phase. In summary, transcription by Pol II appears as a major driver of nuclear organization, which can be understood in the framework of phase separation.

BP 33: Posters - Systems Biology & Gene Expression and Signalling

Time: Tuesday 14:00–16:00

Location: P2-OG1

BP 33.1 Tue 14:00 P2-OG1

Error model estimation by maximum-likelihood methods — ●MIRIAM FEHLING-KASCHEK, DANIEL KASCHEK, and JENS TIMMER — Physikalisches Institut, Universität Freiburg

Mathematical modeling has become an established approach in cell biology to gain information about intracellular processes. Especially for dynamic modeling, time-resolved data is required. Depending on the measurement technique, taking data points is time-consuming and expensive. Therefore, the modeler is often confronted with the problem of low number of replicates from which uncertainties need to be estimated reliably.

Error models provide a way to pool replicate measurements from different time-points and conditions to estimate the contributions from different error sources. Here, two complementary maximum-likelihood approaches to identify error model parameters, (1) from mean-variance tuples and (2) from model residuals, are implemented. Advantages and disadvantages of both approaches are discussed and usecases from different applications presented.

BP 33.2 Tue 14:00 P2-OG1

Impact of reparametrization on fitting of ODE models — ●LUKAS REFISCH¹, JENS TIMMER^{1,2,3}, and CLEMENS KREUTZ^{1,2} — ¹Institute of Physics, University of Freiburg, Freiburg im Breisgau, Germany — ²Center for Biosystems Analysis (ZBSA), University of Freiburg, Freiburg im Breisgau, Germany — ³BIOSS Centre for Biological Signalling Studies, University of Freiburg, Freiburg im Breisgau, Germany

The dynamics of complex biochemical reactions as they occur in living cells can be modeled by ordinary differential equations (ODE). One major task is model calibration, i.e. to estimate parameters like initial concentrations and rate constants based on experimental data. Optimization-based estimation like maximum likelihood is often challenging due to the existence of local minima, the highly nonlinear model responses and the limited precision of numerical ODE solutions.

It has been claimed that parameter transformations are beneficial for fitting of ODE models. Possible parametrizations exploit the model's scaling invariance originating from the free choice of units and the fact, that measurements in molecular cell biology are often taken on a relative scale. However, up to now the impact of reparametrization has not been evaluated in details. For five established models of cellular signaling pathways and infectious diseases with experimental data, we analyze the effect of reparametrization on the performance of optimization. The different influences including the geometry of the likelihood landscape, the choice of initial guesses and the parameter search space are quantified using multivariate statistical analyses.

BP 33.3 Tue 14:00 P2-OG1

Quantitative analysis of the spatial toggle switch that controls *Myxococcus xanthus* motility — ●MANON WIGBERS¹, LUIS CARREIRA², FILIPE TOSTEVIN¹, DOBROMIR SZADKOWSKI², LOTTE SØGAARD-ANDERSEN², and ULRICH GERLAND¹ — ¹Department of Physics, Technische Universität München, Garching, Germany — ²Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

Dynamic control of cell polarity switching is central to the regulation of *Myxococcus xanthus* motility. Each reversal of the direction of motion of a *M. xanthus* cell is preceded by a reversal of its cell polarity, which is marked by an asymmetric distribution of signaling proteins. Key components of this system include MglA, which accumulates at the leading cell pole, and MglB, which localizes to the lagging cell pole. The correct localization of the Mgl proteins is also mutually dependent on other proteins, including RomR. Together, these proteins form an intriguing *spatial toggle switch*. Here, we use quantitative data analysis and biophysical modeling to study the working principle of this system. In particular, we study how the asymmetric protein distributions emerge from the involved interactions and reactions, and how the switching of cell polarity could be brought about by the upstream Frz system. We establish a model that has qualitative agreement with the localization patterns of the MglA/MglB/RomR system, for the wild type and all mutants. Furthermore we perform a systematic search to find possible mechanisms to control polarity switching.

BP 33.4 Tue 14:00 P2-OG1

Communication between bacteria and cell-free expression systems within linear chains of emulsion droplets — ●MATTHAEUS SCHWARZ-SCHILLING, LUKAS AUFINGER, ANDREA MÜCKL, and FRIEDRICH C. SIMMEL — Technical University of Munich, Physics Department E14 and ZNN/WSI, Am Coulombwall 4a, 85748 Garching, Germany.

Position-dependent gene expression in gradients of morphogens is one of the key processes involved in cellular differentiation during development. Here, we study a simple artificial differentiation process, which is based on the diffusion of genetic inducers within one-dimensional arrangements of 50 micrometre large water-in-oil droplets. The droplets are filled with either bacteria or a cell-free gene expression system, both equipped with genetic constructs that produce inducers or respond to them via expression of a fluorescent protein. We quantitatively study the coupled diffusion-gene expression process in gradients of inducers and demonstrate that gene expression can be made position-dependent. The confinement of genetic inducers to diffuse in only one dimension enables strong coupling between neighbouring droplets. Thus, by generating diffusing quorum-sensing signals in situ, we also establish communication between artificial cell-free sender cells and bacterial receivers, and vice versa.

BP 33.5 Tue 14:00 P2-OG1

Deconvolution of luminescence cross-talk in high-throughput gene expression profiling — ●MARCO MAURI, STEFANO VECCHIONE, and GEORG FRITZ — LOEWE-Center for Synthetic Microbiology (SYNMIKRO), Philipps-University Marburg, Germany

In recent years, luciferase has become a standard genetic tool to monitor gene expression. It has a high signal-to-noise ratio, which is, in principle, only limited by the sensitivity of the photo detector. However, at the same time luciferase reporters have the drawback of emitting a constant glow upon induction, which can lead to undesired cross-talk between neighbouring wells on a microplate. Indeed, we find that the scattering light from a highly luminescent well affects more than 50% of the wells even in a black plate. In order to overcome this limitation, we developed a computational method to correct for luminescence bleed-through and estimate the "true" luminescence activity for each well of a microplate. As the sole input to our algorithm the signals measured from a calibration plate is needed, in which the light emitted from a single luminescent well serves as an estimate of the light-spread function. From this the algorithm creates a deconvolution matrix, which can be used to correct any other measurement obtained under the same technical conditions. Here, we demonstrate that our correction preserves low level signals that are close to the background and show that it is universally applicable to different kinds of microplate readers and plate types. From our algorithm, we developed a freely available tool to correct the luminescence cross-talk in high-throughput gene expression analyses.

BP 33.6 Tue 14:00 P2-OG1

Quantitative analysis of bacterial growth and starvation at elevated temperatures — ●MARIEL GARCÍA HUMÁN, SEVERIN SCHINK, MICHAEL SZABO, and ULRICH GERLAND — Technical University of Munich, Physics Department, James-Frank-Str. 1. 85748 Garching

Up to now, the temperature dependence of bacterial behavior regarding growth and viability beyond the physiological temperature is poorly understood. We study the effects of temperature stress on *E. coli* in minimal nutritional environments. At highly elevated temperatures, short-term starvation causes genetically homogeneous bacterial populations to split into two distinct subpopulations, growing and non-growing. This plays a role in bacterial persistence.

BP 33.7 Tue 14:00 P2-OG1

Machine Learning for epigenetic network inference in T cells — ●CHRISTOPH KOMMER^{1,2,3}, QIN ZHANG^{1,2}, AHMED HEGAZY⁴, MAX LÖHNING^{4,5}, and THOMAS HÖFER^{1,2} — ¹German Cancer Research Center (DKFZ), Heidelberg — ²BioQuant Center, University of Heidelberg — ³HGS MathComp, Institute for Scientific Computing, University of Heidelberg — ⁴German Rheumatism Research Center, Berlin — ⁵Charité-Universitätsmedizin, Berlin

T-helper cells direct the cell- and antibody-based arms of the adaptive

immune system via the secretion of signalling proteins. The classical view of naïve T-helper cells differentiating into a small number of stable steady states has recently been challenged by experimental findings that point towards multistable hybrid states away from a bistable fixed-point solution.

To interrogate the underlying regulatory mechanisms, we identified the epigenetic landscape in naïve and differentiated T-helper cells from histone modification patterns by applying different machine learning approaches and found distinct classes of enhancers and repressors according to their regulation by lineage-specifying transcription factors and/or extrinsic differentiation signals which are also cell-type specific. For mapping epigenetic states to target genes we furthermore developed a novel parametrized multivariable correlation measure model. With this approach, we recovered well-known cis-regulatory elements and predicted new ones with comparable confidence.

We discuss the utility of these data to learn epigenetic regulatory network topologies in order to explain multistability.

BP 33.8 Tue 14:00 P2-OG1

Optimizing Network Models of Nucleosome Configurations at the PHO5 Promoter in Yeast — ●MICHAEL WOLFF¹, ANDREA SCHMID², PHILIPP KORBER², and ULRICH GERLAND¹ —

¹Physik-Department TUM and Graduate School of Quantitative Biosciences Munich (QBM), James-Frank-Straße 1, 85748 Garching — ²Molekularbiologie Biomedizinisches Centrum, LMU, Großhaderner Strasse 9, 82152 Planegg-Martinsried

Nucleosomes are histone DNA complexes densely populating the DNA molecule and their positioning is key to a better understanding of the transcriptional regulation of eukaryotic genes. These positions are influenced by DNA sequence, competition with transcription factors and active reorganization by chromatin remodeling enzymes. A textbook example illustrating the role of nucleosome positioning in promoter regulation is the PHO5 gene in *Saccharomyces cerevisiae*. The PHO5 promoter is also one of the few cases in which single molecule data describing the probability that a promoter will adopt a given nucleosome configuration *in vivo* is available, even for different environmental conditions leading to induction or repression of PHO5 transcription. These measured configuration probabilities can be reproduced by Markov processes on nucleosome configuration networks describing remodeler mediated nucleosome assembly, disassembly and sliding along the DNA. Here we explore the space of these Markov models and search for agreement with further experimental data, such as nucleosome turnover rates and nucleosome occupancy after DNA sequence manipulation.

BP 34: Posters - Physics of *Physarum polycephalum* and Other Slime Molds (Focus Session)

Time: Tuesday 14:00–16:00

Location: P2-OG1

BP 34.1 Tue 14:00 P2-OG1

Analyzing the spatial positioning of nuclei in multinuclear giant cells — ●MAIKE STANGE¹, MARIUS HINTSCHE¹, KIRSTEN SACHSE¹, MATTHIAS GERHARDT¹, ANGELO VALLERIANI², and CARSTEN BETA¹ — ¹University of Potsdam, Potsdam, Germany — ²Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The spatial arrangement of organelles and other subcellular components plays a critical role for many functions of life at the cellular level. For example, during cell division, a proper distribution of cellular material onto the daughter cells is vital for their survival. Here, we study the spatial distribution of nuclei in artificial giant cells of the social amoeba *Dictyostelium discoideum*. We performed dual-color confocal imaging of cells that express fluorescence-labeled proteins for the nucleus and the microtubules. Based on this data, we determined the subcellular positions of nuclei, centrosomes, and their associated microtubules. A comparison with model predictions for random positioning in a confined domain suggests that nuclei in the giant cells are indeed randomly distributed, despite the putative steric interactions of neighboring microtubule cytoskeletons. Three-dimensional image reconstructions support our findings.

BP 34.2 Tue 14:00 P2-OG1

Inexpensive Observation System for Decision Experiments with *Physarum polycephalum* — ●ANN-MARIE PARREY¹, NELLY VON PUTTKAMER^{1,2}, ANJA BAMMANN¹, ADRIAN FESSEL¹, ERIK BERNITT¹, and HANS-GÜNTHER DÖBEREINER¹ — ¹Institut für Biophysik, Universität Bremen — ²Hochschule Bremen

A low-priced observation system with automated temperature control and image capturing is presented. The setup is controlled by a Raspberry Pi and can be used for educational purposes. We demonstrate that with this system, the decision-making behaviour of slime molds such as *Physarum polycephalum* can be automatically observed.

Over a period of 24 hours a Raspberry Pi camera module inside the incubator takes pictures of a slime mold growing on an agar plate composed of two sides. One side contains a threat, i.e. salt, while the other side is neutral. The slime mold is prepared on an oatmeal flake and sits in the middle of the agar plate. Varying salt concentration, we observe a strong preference of the slime mold towards the neutral side for high salt concentrations, while this preference weakens for low concentrations. This behaviour can be explained assuming a two state system, where the salt side is represented by a higher energy state and the neutral side is associated with a lower energy state. With these assumptions, the probability $P_N(c)$ to find the slime mold on the neutral side can be calculated: $P_N(c) = 1/(e^{-kc} + 1)$, with c as the salt concentration and a constant k , which is fit to the data. We find theoretically that $k = 1/\Omega \partial\Omega/\partial c$, i.e. the relative loss of the number of

states Ω with increasing salt concentration.

BP 34.3 Tue 14:00 P2-OG1

Decision making in *Physarum polycephalum* as a basis for biomimetical solutions to optimization problems — ●NELLY VON PUTTKAMER^{1,2}, ANN-MARIE PARREY¹, ANJA BAMMANN¹, ADRIAN FESSEL¹, ERIK BERNITT¹, and HANS-GÜNTHER DÖBEREINER¹ — ¹Institut für Biophysik, Universität Bremen — ²IS Bionik, Hochschule Bremen

Everyone of us is faced with multiple decisions daily, ranging from personal ones to those made on headquarters level. Quite often, although the probability of an unpleasant outcome or the impact is not known, making a decision is inevitable. Albeit humans are outfitted with a sophisticated neural system, there is a lot to learn about the biological basis of decision making from simpler life forms. Previous observations of *Physarum polycephalum*, a unicellular, multinucleate slime mold, demonstrated a higher complexity of decision making than expected for a non-conscious organism. In this work we show that, during foraging, the plasmodium of *P. polycephalum* takes a calculated risk, as present in the form of potassium chloride in the substrate. Risk was quantified by measuring the relative plasmodial area intruding regions with varying salt concentration. The corresponding probability was found to decrease with salt concentration. With a higher risk, the variances of the paths taken by the plasmodium decrease as well, hinting at a lower exploration of the substrate presenting a risk. These findings give an insight into decision making on the lowest level and without a central nervous system. We envision our findings to be useful in fields where risky decisions are inevitably made, for example in economics.

BP 34.4 Tue 14:00 P2-OG1

Indentation Analysis of Active Viscoelastic Microplasmodia of *P. polycephalum* — ●ADRIAN FESSEL¹, CHRISTINA OETTMEIER¹, ANG WEI TEH², and HANS-GÜNTHER DÖBEREINER¹ — ¹Universität Bremen, Bremen, Deutschland — ²Nanyang Technological University, Singapore

We present an analysis of force data obtained from indentation testing of vital microplasmodia of the slime mold *Physarum polycephalum*. Approximating the testing scenario as a layer tied to a rigid foundation leads to an estimation of Young's modulus at $E = (16.7 \pm 7.7)$ kPa, which is fairly consistent for various samples and for different time-dependencies of the indentation force. We observe variation of the modulus with the characteristic oscillation of *P. polycephalum*. Further we find a set of superimposed decay times during repeated indentation, which can be attributed to viscoelastic effects and the porous structure of microplasmodia. We demonstrate by extending the Kelvin-Voigt model to include non-linear effects and via FEM simulations, that ap-

parent non-linearities in the stress-strain ellipsoids can be attributed to variations of sample thickness. A detailed theoretical description of the non-linear thickness effect is given in the contribution 'Non-Linear Compliance of Elastic Layers to Indentation' (BP 7.4).

BP 34.5 Tue 14:00 P2-OG1

Pruning to increase transport in *Physarum polycephalum* — ●SOPHIE MARBACH^{1,4}, KAREN ALIM^{2,4}, NATHALIE ANDREW^{2,4}, ANNE PRINGLE³, and MICHAEL BRENNER⁴ — ¹Laboratoire de Physique Statistique, Ecole Normale Supérieure, Paris, France — ²Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — ³Departments of Botany and Bacteriology, University of Wisconsin-Madison, Wisconsin, USA — ⁴School of Engineering and Applied Science, Harvard University, Massachusetts, USA

How do the topology and the geometry of a tubular network affect the spread of particles within fluid flows? We investigate the detailed physical forces responsible for mixing in the hierarchical, biological transport network formed by *Physarum polycephalum*. We introduce an efficient method to build patterns of effective dispersion, taking into

account all the specificities of the individual. We demonstrate that a change in topology - pruning in the foraging state - causes a large increase in effective dispersion throughout the network. By comparison, changes in the hierarchy of tube radii result in smaller and more localized differences. Pruned networks capitalize on Taylor dispersion to increase the dispersion capability. It is fascinating to speculate that pruning in other biological systems, for example, during vessel development in zebra fish brain development [1] or during growth of a large fungal body [2], serve a similar objective of enhanced effective dispersion. Pruning itself might be triggered by the concentration of specific dispersing particles. Pruning is also tightly governed by the initial pattern of hierarchy, and the dynamic entanglement between hierarchy and pruning remains unsolved. Investigating the mechanisms allowing for pruning would be highly instructive in the process of understanding the overall organization of organisms, and is ongoing work.

[1] Chen, Q. et al., PLoS Biol. 10, e1001374 (2012)

[2] Smith, M. L., Bruhn, J. N., and Anderson, J. B., Nature, 356, 428 (1992).

For more details, Marbach, S. et al., Phys. Rev. Lett. 117, 178103 (2016)

BP 35: Posters - Physics of Parasites (Focus Session)

Time: Tuesday 14:00–16:00

Location: P2-OG1

BP 35.1 Tue 14:00 P2-OG1

Monitoring the blood-stage infection and hemozoin clearance in malaria rodent models by a novel malaria diagnostic device — ●MARIA PUKANCSIK¹, AGNES ORBAN¹, PETRA MOLNAR¹, ADAM BUTYKAI¹, MARIA REBELO², THOMAS HANSCHIED², AHMED S I ALY³, and ISTVAN KEZSMARKI¹ — ¹Dept. of Physics, Budapest University of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, HU — ²Instituto de Medicina Molecular, Faculdade de Medicina, Lisbon, PO — ³Tulane University, Dept. of Tropical Medicine, New Orleans, USA

The first prototype of a diagnostic device was developed as a sensitive platform for malaria diagnosis. The rotating-crystal magneto-optical diagnostic technique (RMOD) targets the natural biomarker hemozoin, which is a magnetic microcrystalline heme compound produced by all species of malaria parasites such as *Plasmodium falciparum* and *Plasmodium vivax*. The *in vivo* investigation of the RMOD device was performed using *P. falciparum*-like and *P. vivax*-like species of malaria parasites infecting mice (e.g. *P. berghei*, *P. chabaudi*, *P. yoelii*, *P. vinckei*) in collaboration with the Instituto de Medicina Molecular and with the Department of Tropical Medicine at Tulane University. The lethal and non-lethal rodent malaria parasites that model different human strains and characteristics of the human blood stage were used in order to monitor the onset of the blood stage infection and compare the sensitivity of the device depending on the rodent strains. The hemozoin clearance was also monitored *in vivo* during and following

the drug treatment of infected mice.

BP 35.2 Tue 14:00 P2-OG1

The physical principles of a novel malaria diagnostic device — ●TAMAS PROK¹, ADAM BUTYKAI¹, AGNES ORBAN¹, PETRA MOLNAR¹, MARIA PUKANCSIK¹, TIVADAR ZELLES², STEPHAN KARL³, and ISTVAN KEZSMARKI¹ — ¹Department of Physics, Budapest University of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, HU — ²Department of Oral Biology, Semmelweis University, 1089 Budapest, HU — ³Infection and Immunity Division, Walter and Eliza Hall Institute of Medical Research, Parkville, Victoria, AU

A novel cost-effective, automated, yet sensitive diagnostic method is needed for malaria detection both as an in-field instrument and as a laboratory tool for malaria researchers. Our group has developed the prototype of such device based on the detection of the magnetically induced linear dichroism of the malaria pigment crystals (hemozoin). These micrometer-size crystals are promising malaria-diagnostic targets as they are unique indicators of the infection exhibiting specific magnetic and optical properties. I am going to present our investigations unravelling the details of their anisotropic magnetic properties and linear dichroism; and I am going to show how these findings led us to the development of a highly sensitive detection setup comprising of a cheap laser diode, permanent magnets, simple polarization optics and computer-based data collection and analysis.

BP 36: Plenary Talk

Time: Wednesday 8:30–9:15

Location: HSZ 01

Plenary Talk

BP 36.1 Wed 8:30 HSZ 01

Characterization of Biological Photoreceptors in Space and Time — ●PETER HEGEMANN — Humboldt-Universität zu Berlin

Biological sensory photoreceptors are families of proteins that can be studied with unprecedented precision in space and time. Excited state dynamics, chromophore isomerization and electron transfer reactions, as well as inactivation processes are studied on rhodopsins with retinal chromophores or LOV and BLUF-proteins with flavin chromophores by UV/Vis, Raman and IR spectroscopy on fs to ps time scales. Proton transfer reactions, hydrogen-network changes and structural changes

can nowadays also be studied on fs to second time scales, whereas ion transport or catalytic activities are monitored on microsecond to second scales by biochemical or electrical methods. By employment of these technologies in conjunction with protein engineering and theoretical calculations my group in collaboration with many colleagues has deciphered or at least enlightened the reaction mechanism of light-gated ion channels, light-driven pumps, and photo-activated guanylyl/adenylyl cyclases. These proteins are widely applied in the neurosciences for activation or deactivation of selected neurons in large neuronal networks as the animal brain (Optogenetics).

BP 37: Physics of Collective Mobility (Joint Symposium SOE/DY/BP/jDPG)

Time: Wednesday 9:30–12:15

Location: HSZ 02

Invited Talk

BP 37.1 Wed 9:30 HSZ 02

Mobility in shareability networks — ●MICHAEL SZELL — Centre for Social Sciences, Hungarian Academy of Sciences, Országház utca 30, 1014 Budapest, Hungary — Center for Network Science, Central European University, Nador utca 11, 1051 Budapest, Hungary — Center for Complex Network Research, Northeastern University, 177 Huntington Avenue, 02115 Boston, USA — moovel lab, Hauptstätter Straße 149, 70178 Stuttgart, Germany — Senseable City Lab, MIT, 77 Massachusetts Ave, 02139 Cambridge, USA

We introduce the notion of shareability network, which allows us to model the collective benefits of sharing trips as a function of passenger inconvenience, and to efficiently compute optimal sharing strategies on massive datasets. We apply this framework to a dataset of millions of taxi trips taken in New York City, showing that cumulative trip length can be cut by 40%. This benefit comes with reductions in emissions and split fares, hinting toward a wide passenger acceptance. Shareability as a function of trip density saturates fast, suggesting effectiveness of the taxi sharing system also in cities with much sparser taxi fleets. We compute the shareability curves in several further world cities, and find that a natural rescaling collapses them onto a single, universal curve. We explain this scaling law with a simple model that predicts the potential for ride sharing in any city, using a few basic urban quantities and no adjustable parameters. Finally, we demonstrate how interactive data visualizations of re-ordered city spaces can effectively inform relevant stakeholders and the public about large-scale reductions of parking spaces in future scenarios of wide-spread car-sharing.

Invited Talk

BP 37.2 Wed 10:00 HSZ 02

Trail-following bacteria: from single particle dynamics to collective behaviour — ANATOLIY GELIMSON¹, KUN ZHAO^{2,3}, CALVIN K. LEE³, W. TILL KRANZ¹, GERARD C. L. WONG³, and ●RAMIN GOLESTANIAN¹ — ¹Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3NP, United Kingdom — ²Key Laboratory of Systems Bioengineering, Ministry of Education, School of Chemical Engineering and Technology, Tianjin University, Tianjin, 300072, People's Republic of China — ³Bioengineering Department, Chemistry & Biochemistry Department, California Nano Systems Institute, UCLA, 90095-1600, Los Angeles, CA, USA

Can we learn from bacteria how to coordinate our mobility, and navigate our way towards mutually beneficial collective states? Trail-following bacteria leave behind precious exopolysaccharides as marker of where they been, and use it to accelerate the formation of colonies. We study this phenomenon, by building a stochastic microscopic model for the pili-driven motility of bacteria that interact with trails which could be laid by themselves and others. We discuss its phenomenology both at the level of single bacterium dynamics and collective self-organization into colonies. We validate the model using *Pseudomonas aeruginosa* trajectories, and show that fitting the parameters at the single bacterium level leads to a good quantitative agreement between the predictions of the model for the collective behaviour of the colony and the corresponding experimental observations.

Invited Talk

BP 37.3 Wed 10:30 HSZ 02

Mobility and Self-Organization in Multi-Layer Networks: A Meta-Foodweb example — ●THILO GROSS¹, ANDREAS BRECHTEL², PHILIPP GRAMLICH², DANIEL RITTERSKAMP¹, and BARBARA DROSSEL² — ¹Department of Engineering Mathematics, University of Bristol, Bristol, UK — ²Institut für Festkörperphysik, TU Darmstadt, Darmstadt, Germany

The emergence of structures and patterns from diffusive motion has

long fascinated scientists. This phenomenon is best known from systems in continuous space. In this talk I will propose a general approach for the study of such phenomena in certain multi-layer networks.

I focus on the example of ecological meta-foodwebs, which describe the dispersal of animals across a fragmented landscape. Each individual undergoes diffusive motion on a network where the nodes are habitats and the links are routes of potential migration. Furthermore, the individuals are subject to predator-prey interactions with other individuals, described by a complex food web. The meta-foodweb thus constitutes a large multiplex network-on-network system.

To study the onset of self-organized pattern formation I consider the dynamical stability of steady states. By exploiting the structure of the system it is possible to separate the effects of the food-web and the geographical network and write a master stability function for the system. The result is a reduced system that bears a remarkable resemblance to pattern forming systems in continuous space, but has much richer behaviour.

15 min. break**Invited Talk**

BP 37.4 Wed 11:15 HSZ 02

Temporal Percolation in Critical Collective Mobility Systems — ●ANDREAS SORGE^{1,2,4}, DEBSANKHA MANIK^{1,2}, JAN NAGLER^{3,4}, and MARC TIMME^{1,2,4} — ¹MPI for Dynamics and Self-Organization, Göttingen, Germany — ²Institute for Nonlinear Dynamics, Georg-August-Universität, Göttingen, Germany — ³Computational & Theoretical Physics, IfB, ETH Zürich, Switzerland — ⁴Organization for Research on Complex Adaptive Systems (or-cas), Göttingen, Germany

A collective mobility system is a stochastic dynamical system that operates under opposing objectives. Its function is to both satisfy individual mobility demand in a timely fashion and make efficient use of the available transport vehicles. To understand and design such a system, one must study, devise and assess dispatching rules that bundle individual requests and assign them to vehicles. If overall mobility demand exceeds capacity, the system congests and ceases to function. Determining the capacity is henceforth crucial to assess any given dispatching rule and inform system design for optimized system performance and individual utility. Intriguingly, the brink to congestion constitutes a critical transition reminiscent of percolation in time. We develop a dynamic notion of criticality of such stochastic processes, mapping return times to spatial clusters of percolation theory. We present a method to algorithmically determine the critical point and exponents and its application to collective mobility systems in this temporal percolation paradigm.

Invited Talk

BP 37.5 Wed 11:45 HSZ 02

Modeling the evolution of cities — ●MARC BARTHELEMY — IPHT/CEA, Saclay, France — CAMS/EHESS, Paris, France

The recent availability of data about cities and urban systems opens the exciting possibility of a 'new Science of Cities'. Urban morphogenesis, activity and residence location choice, mobility, urban sprawl and the evolution of urban networks are just a few of the important processes that can be discussed now from a quantitative point of view. In this talk, I will discuss how a data-informed approach can elaborate on urban economics models in order to get predictions in agreement with empirical observations. I will illustrate this approach on the growth of cities and the emergence of a polycentric structure of activity centers. I will conclude by highlighting some important challenges and possible research directions.

BP 38: Membranes and Vesicles I

Time: Wednesday 9:30–13:00

Location: HÜL 386

Invited Talk

BP 38.1 Wed 9:30 HÜL 386

Simulations move toward the understanding of protein-mediated membrane fusion — ●HERRE JELGER RISSELADA — Dept of Theoretical Physics, Georg-August University, Göttingen, Germany — Leibniz Inst. of Surface Modification, Leipzig, Germany

Membrane fusion is fundamental for the cycle of life. From the start (sperm fusion), into being (synaptic fusion and intra cellular fusion reactions), toward a possible end (viral infections). Over the last three decennia the process of membrane fusion has been intensively studied by experiments but also by theory. As a matter of fact, theory—at the time in the form of continuum elastic models—has played a dominant role in envisioning the lipidic fusion reaction and its formed intermediates. These insights have lead to the popular stalk-pore hypothesis which still governs our view on membrane fusion up to today. The role of fusion proteins herein was initially confined to bringing the membranes into close apposition by exerting mechanical force to overcome the activation energy barrier. The subsequently formed transition states were considered to be exclusively lipidic. Recent molecular dynamics simulations have contributed to the emerging consensus that such simple and clear-cut separation between the role of the fusion proteins and that of the pure lipid membrane misses their close coupling, which turns out to be essential for a quantitative understanding of protein mediated membrane fusion. Here, I will highlight possible strategies which fusion proteins or involved helper proteins may evoke to overcome the free energy barriers of membrane fusion up to the final opening of the fusion pore.

BP 38.2 Wed 10:00 HÜL 386

Carbon nanotubes mediate fusion of lipid vesicles — ●STEPHANIE LINKER, RAMACHANDRA BHASKARA, MARTIN VÖGELE, JÜRGEN KÖFINGER, and GERHARD HUMMER — Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Max-von-Laue StraÙe 3, D-60438 Frankfurt am Main, Germany

The fusion of lipid membranes is opposed by high energetic barriers. In living organisms, complex protein machineries carry out this biologically essential process. Here we show that membrane-spanning carbon nanotubes (CNTs) can trigger spontaneous fusion of small lipid vesicles.

In coarse-grained molecular dynamics simulations, we find that a CNT bridging between two vesicles locally perturbs their lipid structure. Their outer leaflets merge as the CNT pulls lipids out of the membranes, creating an hourglass-shaped fusion intermediate with still intact inner leaflets. As the CNT moves away from its symmetry axis, the inner leaflets merge, forming a pore that completes fusion. CNT-mediated vesicle fusion offers a fresh perspective on a poorly understood process. Possible applications include the design of new fusion agents, e.g., for the targeted delivery of drugs or nucleic acids.

BP 38.3 Wed 10:15 HÜL 386

Shape remodeling vesicles by localized actin polymerization — ●KATHARINA HENNEBERG¹, FELIX KEBER¹, CHRISTIAN CYRON¹, JAN FAIX², and ANDREAS BAUSCH¹ — ¹Technical University of Munich, Munich, Germany — ²Hannover Medical School, Hannover, Germany

Interactions between the cytoskeleton and the cell membrane are essential for various cellular processes. Here we reconstitute lamellipodia and filopodia like structures in a bottom up approach inside giant unilamellar vesicles (GUVs). We couple the network from the inside to the lipid membrane of GUVs. By the use of different actin binding proteins (ABPs) we control the binding characteristics of actin to the membrane and the network architecture. One of the key players is Arp2/3, which binds via its activator VCA to the vesicle's membrane. The autocatalytic nature of Arp2/3 and the finite volume of the vesicle result in the formation of patches of a dense actin network, which ultimately leads to pronounced membrane deformations. The capping protein (CP) determines thereby the resulting membrane deformations by finetuning the actin network geometry. We are able to model the formation of the localized networks by kinetic equations, a continuum elastic model suffices to describe the resulting membrane shape deformations.

BP 38.4 Wed 10:30 HÜL 386

Distance-Dependent Structures of Interacting Membranes Displaying Synthetic Polymers and Wild-Type Bacterial Lipopolysaccharides — ●IGNACIO RODRIGUEZ LOUREIRO¹, ERNESTO SCOPPOLA¹, VICTORIA LATZA¹, LUCA BERTINETTI¹, AURELIO BARBETTA^{1,2}, GIOVANNA FRAGNETO³, and EMANUEL SCHNECK¹ — ¹Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — ²Institut de Chimie Séparative de Marcoule, France — ³Institut Laue-Langevin, Grenoble, France

Polymer brushes are found on the surfaces of important classes of biological membranes, such as lipopolysaccharides on bacterial outer membranes. The latter mediate the interaction with other bacteria and thus influence the physical properties of bacterial biofilms. But interacting polymer brushes are also of technological relevance, for instance in the field of surface lubrication. The interaction between polymer-decorated surfaces is coupled to the distance-dependent conformation of the polymer chains. This problem has been addressed by theory, but accurate experimental data on polymer conformations under confinement are rare. Here, we utilize neutron reflectometry (NR) to determine the distance-dependent structure of interacting lipid membrane surfaces decorated with hydrophilic poly(ethylene glycol) (PEG) brushes. To gain insight into bacterial interactions in biofilms we also investigate the structure of two interacting surfaces formed by wild-type bacterial lipopolysaccharides with strain-specific O-side chains.

BP 38.5 Wed 10:45 HÜL 386

Pure Protein Bilayers and Vesicles from Native Fungal Hydrophobins — HENDRIK HÄHL¹, JOSE NABOR VARGAS¹, ALESSANDRA GRIFFO², PÄIVI LAAKSONEN², GÉZA SZILVAY³, MICHAEL LIENEMANN³, KARIN JACOBS¹, RALF SEEMANN¹, and ●JEAN-BAPTISTE FLEURY¹ — ¹Saarland University, 66123 Saarbrücken, Germany — ²Aalto University, 00076 Aalto, Finland — ³VTI Technical Research Centre of Finland, 02150 Espoo, Finland

In this study, a microfluidic approach to generate free-standing, protein bilayers and protein vesicles is presented, which are composed solely of the hydrophobin HFBI, which is a small, amphiphilic protein produced by filamentous fungi. The amphiphilicity of the proteins allows them to self-assemble at any hydrophilic/hydrophobic interface in very stable monolayers. These monolayers are used to generate free-standing bilayers. Employing different fluids in a microfluidic setup, the stability of bilayers in both possible orientations (i.e. in the hydrophilic or hydrophobic contact situation) is demonstrated. This allows the creation of hydrophobin membranes between either aqueous, oily, or gaseous compartments. These membranes are then used to produce aqueous, oily or gaseous hydrophobin vesicles by means of the microfluidic jetting technique. The resulting lipid-free vesicles are the first example of vesicles only composed of proteins. With the insertion of functioning gramicidin pores, the foundation for employing these vesicles as a new experimental class of encapsulating platform in synthetic biology is laid.

Advanced Materials 2016 (online version: 10.1002/adma.201602888)

30 min break

BP 38.6 Wed 11:30 HÜL 386

Measurements of lateral diffusion of phospholipids in the artificial cell membrane using diamond nanomagnetometry — ●FARIDA SHAGIEVA, YA WANG, ZHIQIN CHU, ANDREA ZAPPE, FELIPE FAVARO DE OLIVEIRA, ANDREJ DENISENKO, AMIT FINKLER, and JÖRG WRACHTRUP — 3rd Institute of Physics, University of Stuttgart, Stuttgart, Germany

Nuclear magnetic resonance (NMR) spectroscopy is serving as a powerful tool in physics and life sciences, but is limited by macroscopic sample quantities (several micrometers). Most recently, the shallow nitrogen vacancy centres underneath the surface of diamond chip started to be used to perform nanoscale NMR imaging and spectroscopy of nuclear species under ambient conditions [1]. These multifunctional quantum sensors provide the noninvasive methods to not only get the chemical composition of the molecules but also study the system dynamics in the nanoscopic volume above the diamond surface. The incredibly small size of the detection volume allows to study the membrane structure around each biomolecule individually.

Here we demonstrate the measurements of lateral diffusion of phos-

pholipids in artificial vesicles modelling cell membranes on the top of diamond nanopillars through the correlation spectroscopy protocol. Pillar-shaped photonic structures hosting such NV centers enables not only significantly increase the photon flux in comparison to the bulk diamond, but also provide NMR measurements inside the vesicles.

[1] T. Staudacher, F. Shi, S. Pezzagna et al., *Science* 339, 561 (2013).

BP 38.7 Wed 11:45 HÜL 386

Rupturing the hemi-fission intermediate in membrane fission: roles of tension and dynamin's conformational changes —

•GUOJIE ZHANG and MARCUS MÜLLER — Institute for Theoretical Physics, Georg-August University, Göttingen, Germany

Membrane fission is a fundamental process in cell, involved in intracellular trafficking, virus infection, etc. It is a collective phenomenon mediated by proteins (mainly dynamin), in which an initially continuous membrane breaks into two topologically independent membranes. So far, however, its underlying molecular mechanism, especially on the specific role of dynamin in fission, is only incompletely understood. Recent experimental and simulation studies concluded that dynamin-mediated fission proceeds via the formation and rupture of a metastable hemi-fission intermediate by dynamin's conformational changes. The latter is a thermally activated process but the transition state is unknown. Here, we employ computer simulation of coarse-grained models of membrane and dynamin, combined with enhanced sampling techniques, to explore: (a) pathways, free-energy barriers, and the concomitant transition states during the rupture of a protein-free hemi-fission state under tension; (b) dynamin's conformational changes, which could lower the free-energy barriers of rupturing the hemi-fission and thus complete membrane fission.

BP 38.8 Wed 12:00 HÜL 386

High-speed single particle tracking on giant unilamellar vesicles — SUSANN SPINDLER, •MARTIN KALLER, and VAHID SANDOGHDAR — Max Planck Institute for the Science of Light, Erlangen, Germany

Interferometric scattering detection microscopy (iSCAT) is a powerful method for single particle tracking (SPT) experiments. Recently, we reported on the use of iSCAT for visualizing the diffusion of gold nanoparticles (GNPs) as small as 5nm attached to lipids in model membranes with nanometer lateral precision and at up to 1 MHz frame rate [1]. Here, we demonstrate one of the unique capabilities of iSCAT, namely high axial resolution in tracking the displacement of a nanoparticle and present three-dimensional trajectories of GNP-labeled lipids and unlabeled virus-like particles diffusing on a giant unilamellar vesicle (GUV) membrane. We discuss the differences in the observed diffusion behaviour in this system and compare them to our previous studies in supported bilayers [2].

[1] S. Spindler, J. Ehrig, K. König, T. Nowak, M. Piliarik, H. E. Stein, R. W. Taylor, E. Garanger, S. Lecommandoux, I. D. Alves, V. Sandoghdar, *J. Phys. D: Appl. Phys.* 49 (2016) [2] C.-L. Hsieh, S. Spindler, J. Ehrig, V. Sandoghdar, *J. Phys. Chem. B* 118 (2014).

BP 38.9 Wed 12:15 HÜL 386

Solid-supported DMPC multilayers containing cholesterol at high hydrostatic pressure — •GÖRAN SURMEIER, MICHAEL PAULUS, PAUL SALMEN, YURY FOROV, SUSANNE DOGAN, LUKAS TEPER, BENEDIKT NOWAK, METIN TOLAN, and JULIA NASE — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany

A phospholipid bilayer is the basic component of cell membranes, which separates the intracellular and extracellular region. Bilayers undergo pressure- and temperature-induced phase transitions. However, they need their high flexibility, which is given in the liquid phase, to fulfill their biological functionalities. Real membranes are highly complex systems that are interstratified by cholesterol and proteins. Adding cholesterol shifts the phase boundaries of phospholipid bilayers. While these phase transitions were already studied in bulk solutions in de-

tail, the behavior of solid-supported membranes at high hydrostatic pressure is widely unknown.

We present an in-situ high pressure X-ray reflectometry study on the structure of solid supported DMPC bi- and multilayers containing cholesterol in different concentrations. The reflectivities were measured at the solid-liquid interface between silicon and an aqueous buffer solution in a high pressure cell employing pressures up to a maximum of 5000 bar. We observed a decrease of the critical pressure and an expansion of the transition area of the liquid-gel phase transition with increasing cholesterol concentrations at 37°C and were able to determine the cholesterol concentration-dependent behavior of the compressibility of gel phase membranes at 20°C.

BP 38.10 Wed 12:30 HÜL 386

Molecular Dynamics Simulations Elucidate the Tight Cohesion between Glycolipid Membranes — MATEJ KANDUC^{1,2},

ALEXANDER SCHLAICH², ALEX DE VRIES³, JULIETTE JOUHET⁴, ERIC MARÉCHAL⁴, BRUNO DEMÉ⁵, ROLAND NETZ², and •EMANUEL SCHNECK⁶ — ¹Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin (Germany) — ²Freie Universität Berlin (Germany) — ³University of Groningen (The Netherlands) — ⁴CEA Grenoble (France) — ⁵Institut Laue-Langevin, Grenoble (France) — ⁶Max Planck Institute of Colloids and Interfaces, Potsdam (Germany)

Membrane systems that naturally occur as densely packed membrane stacks contain high amounts of glycolipids whose saccharide headgroups display multiple small electric dipoles in the form of hydroxyl groups. Experimentally the hydration repulsion between glycolipid membranes is of much shorter range than that between phospholipids whose headgroups carry single large electric dipole due to the zwitterionic charge distribution. Using solvent-explicit Molecular Dynamics simulations and accounting for the water chemical potential, we quantitatively reproduce the experimentally observed, different pressure-versus-distance curves of membrane stacks composed of phospholipids and of the glycolipid digalactosyldiacylglycerol (DGDG). We show that the short-ranged water uptake into the glycolipid membranes is solely driven by the hydrogen-bond balance involved in non-ideal water/sugar mixing. Water structuring effects and lipid configurational perturbations, responsible for the more long-ranged repulsion between phospholipid membranes, are inoperative for the glycolipids.

BP 38.11 Wed 12:45 HÜL 386

DNA-oligomers as model linkers for membrane adhesion — •MOHAMMAD KAMAL¹, FRANCK THIBAUDAU¹, ANA-SUNČANA SMITH², and KHEYA SENGUPTA¹ — ¹Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Aix - Marseille Université-CNRS UMR 7325, Campus de Luminy, Case 913, 13288 Marseille Cedex 9, France — ²PULS Group, Department of Physics and Cluster of Excellence: EAM, Friedrich-Alexander University Erlangen-Nuremberg, Erlangen, Germany

In the last decade, DNA-linkers have been extensively used as selective glue to tune inter-colloidal interactions with the aim of creating new meta-materials which exploit the versatility of DNA. Here we take a similar approach to use the power of DNA origami to test ideas in the context of model membrane adhesion. We use Reflection Interference Contrast Microscopy (RICM) to quantify the interaction between the membrane of a giant unilamellar vesicle and a supported lipid bilayer employing short DNA sequences as linkers. The linker-length was varied independently of its binding affinity. The linker flexibility was also varied by using either single (ss) or double stranded (ds) DNA. For ds-DNA, the separation (d) between the two interacting membranes is smaller than or equal to the linker length. For corresponding ss-DNA, d is always smaller. The linker-length influences the adhesion strength only at low concentrations, and for a given length, ds-DNA is a more efficient binder than ss-DNA. We also explore the possibility of adhesion induced phase separation using binary-mixtures of linkers. The results are interpreted in terms of a thermodynamic model.

BP 39: Optogenetics for the Cytoskeleton - Focus Session organized by Ulrich Schwarz

Time: Wednesday 9:30–12:30

Location: SCH A251

BP 39.1 Wed 9:30 SCH A251

Synthetic reconstitution of morphogenetic processes in naïve embryonic tissues — EMILIANO IZQUIERDO and ●STEFANO DE RENZIS — EMBL-Heidelberg, Germany

Morphogenesis of multicellular organisms is characterized by changes in cell and tissue behaviours that occur at specific space and time in a coordinated manner. This stereotypic and genetically encoded spatiotemporal organization makes it difficult to determine the extent to which individual cell behaviour drive morphological remodelling. In my talk, I will present a novel optogenetic-based synthetic approach that allowed us to reconstitute complex morphogenetic processes in naïve *Drosophila* embryonic tissues independent of any pre-determined physical and biochemical conditions or other tissue-scale properties that accompany endogenous morphogenetic processes.

BP 39.2 Wed 10:00 SCH A251

Collective dynamics determine selection and regulation of leaders during epithelial wound healing — ●MEDHAVI VISHWAKARMA, TAMAL DAS, and JOACHIM P. SPATZ — Department New Materials and Biosciences, Max-Planck-Institute for Intelligent Systems, Stuttgart

Collective migration involves coordinated movement of several cells, and influences many biological processes including embryogenesis, wound healing, and cancer metastasis. The prevalent view on collective cell migration, especially in the context of epithelial cells during wound healing, assumes a hierarchical leader-follower organization and belittles the contribution of follower cells in choosing or regulating the leaders. Here, we report and analyse distinct phases of collective migration during wound closure and demonstrate how collective dynamics influence selection and regulation of leader cells in these phases. We found that in the preparatory phase, before the initiation of migration (Phase 0), the selection of leader cells at the epithelial wound margin is largely governed by dynamic heterogeneity of the followers in the monolayer. Long before the prospective leaders actually start displaying their phenotypic peculiarities, cells behind them manifest stochastic augmentations in the traction forces and monolayer stresses, and display large perimeter-to-area ratio indicating a local unjamming. Strikingly, the length scale of this collective dynamics matches with the distance between two emerging leaders. Furthermore, it is also possible to control the leader cell formation by introducing followers with high contractile forces at the back. For that, we used an optogenetic technique involving a photo-excitable form of RhoA to transiently increase the RhoA activation and hence the cellular traction stresses. Upon photoactivation of RhoA in the followers, we could spatially bias the formation of leaders at the interface. As the migration progresses from the phase 1 to the phase 2, the number of followers per leader is limited by formation of new leaders at the margin and this limit is again set by the length scale of cell-cell force transmission. Any perturbations in mechanical forces that modifies the force correlation lengths and hence the collective dynamics of the system, invariably enforces a change in the number of followers per leader thereby modifying the time required to transit from one phase to the other. Together, these findings provide a novel insight into formation and regulation of leader cells, and indicate integrative leader-follower interactions during wound closure.

BP 39.3 Wed 10:15 SCH A251

Optogenetic switches to control cellular actin dynamics — ●ROBERT GROSSE — University of Marburg

Actin dynamics is essential for cellular functions such as adhesion, motility and spatial organization. The Rho-GTPase effector proteins of the formin family are tightly regulated through autoinhibitory interactions. Formins are potent actin assembly factors that can nucleate and elongate linear actin filaments for multiple cellular functions including transcriptional control. Here we discuss tools and approaches to rapidly and reversibly modulate actin assembly by light by targeting Rho-GTPases, formins and beyond at the plasma membrane as well as in the somatic cell nucleus.

BP 39.4 Wed 10:45 SCH A251

Optogenetic manipulation of membrane signaling and cytoskeletal dynamics in the social amoeba *Dictyostelium discoideum* — ●SVEN FLEMMING, KIRSTEN SACHSE, and CARSTEN

BETA — University Potsdam, Department of Physics and Astronomy, Potsdam, Germany

Motile cells such as macrophages, mesenchymal stem cells, or cancer cells show complex spatiotemporal pattern formation in the actin cytoskeleton. These patterns can be influenced by external cues such as chemoattractant signals, which lead to directed movement but can also occur without an external stimulus, for example as self-sustained actin oscillations or waves. We use the social amoeba *Dictyostelium discoideum* as a model organism to elucidate how different components of the signaling pathways contribute to these dynamics. To this end, we establish an optogenetic approach to recruit downstream targets of cAMP signaling — agonists as well as antagonists of actin polymerization — to distinct areas of the plasma membrane. We will show to what extent these downstream targets affect the actin dynamics in the targeted regions and will use successful constructs for the mechanistic characterization of dynamic actin structures. Ultimately, our approach will allow us to manipulate and control the formation of complex spatiotemporal actin patterns in the cell cortex.

15 min break

Invited Talk

BP 39.5 Wed 11:15 SCH A251

Navigating the cytoskeleton: new tools to dissect and direct intracellular transport — ●LUKAS KAPITEIN — Utrecht University

Cellular organization depends on the cytoskeleton, a mechanical network of biopolymers that controls cell shape and strength, as well as on motor proteins that can move over these biopolymers to deliver cargo to specific subcellular compartments. Nevertheless, the precise mechanisms that control cytoskeletal organization, the function and dynamics of different motor proteins, and the precise functions of subcellular positioning are still poorly understood. In my lecture, I will highlight novel light-based technologies that enable addressing these questions with unprecedented precision. First of all, we successfully engineered a system to control the transport and positioning of intracellular components with light through the controlled recruitment of specific motor proteins. This allows us to directly explore the intracellular activity of motor proteins and the functional consequences of organelle mislocalization. In addition, we have engineered novel probes and methodology for the super-resolution imaging of the cytoskeleton. These approaches allow us to better resolve cytoskeletal organization in dense cellular compartments, such as the axons and dendrites of neurons. Together, these technologies hold great promises for exploring cellular organization and dynamics in health and disease.

BP 39.6 Wed 11:45 SCH A251

Controlling and modelling contractility in adherent cells

— ●DIMITRI PROBST¹, CHRISTOPH A. BRAND¹, MARCO LINKE¹, PATRICK W. OAKES², ELIZABETH WAGNER³, MICHAEL GLOTZER³, MARGARET L. GARDEL², and ULRICH S. SCHWARZ¹ — ¹Institute for Theoretical Physics & BioQuant, Heidelberg University, Germany — ²Institute for Biophysical Dynamics, James Franck Institute and the Department of Physics, University of Chicago, USA — ³Department of Molecular Genetics and Cell Biology, University of Chicago, USA

Cellular contractility is known to be controlled by a small GTPase called RhoA, whose active form promotes both actin polymerization and myosin II motor activity. For example, a global increase of active RhoA in adherent tissue cells leads to the formation of focal adhesions and stress fibers. However, how localized RhoA signals translate into cell-level responses is not well understood. Here we address this question through experiments and modelling using an optogenetic approach. Local activation of RhoA stimulates local contraction that is quickly propagated over the whole cell through the stress fibers. It also drives F-actin and myosin towards the region of heightened RhoA. Surprisingly, the flow reverses direction when local RhoA activation stops. We explain our experimental findings with a viscoelastic physical model that demonstrates that stress fibers are elastic-like structures. We show that the elasticity of the stress fibers is preserved even at time scales exceeding turnover of constituent proteins. Our model furthermore allows to identify the repair molecule zyxin as a key regulator of stress fiber mechanics, as they become fluid-like in its absence.

BP 39.7 Wed 12:00 SCH A251

Towards in vivo optomechanical control of actomyosin —
 ●STEPHAN GRILL — BIOTEC, Technische Universität Dresden

In the nematode *Caenorhabditis elegans*, actomyosin-based active ten-

sion and active torque generation drive morphogenetic processes such as cell polarization and left/right symmetry breaking. I will report on our ongoing activities towards perturbing and remote-controlling active tension and active torque by light.

BP 40: Colloids and Complex Fluids II (Joint Session CPP/BP/DY)

Time: Wednesday 10:15–13:00

Location: ZEU 260

Invited Talk

BP 40.1 Wed 10:15 ZEU 260

Computer simulations of colloidal systems under flow —
 ●ARASH NIKOUBASHMAN — Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz, Germany

Colloidal systems under flow are ubiquitous in nature and technology, whether it is the transport of proteins and enzymes in biological systems or the flow of surfactants in enhanced oil recovery. Such microrheological systems are also highly intriguing from a purely scientific point of view due to the intricate interplay between the solute and solvent particles. To better understand the physical properties of these complex systems and to assist the design of microfluidic devices, we performed extensive simulations of both rigid and soft colloidal particles under flow. This computational approach allows for systematic control over the system parameters while also providing microscopic insight. In this presentation, selected systems will be discussed to give an overview of the possibilities and challenges in this field. For example, microfluidic channels can be used to distinguish polymers based on their topology, such as linear, dendritic or ring-shaped macromolecules. Furthermore, non-linear flow effects such as inertia or viscoelasticity can be exploited to control the lateral motion of dispersed particles. Flow can also be used to enhance the growth as well as the breakup of colloidal aggregates, depending on the applied flow strength.

BP 40.2 Wed 10:45 ZEU 260

A temporarily arrested state in protein solutions —
 ●STEFANO DA VELA¹, FAJUN ZHANG¹, CHRISTIAN EXNER¹, JOHANNES MÖLLER², ZHENDONG FU³, and FRANK SCHREIBER¹ —
¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — ²ESRF, Grenoble, France — ³JCNS, Garching, Germany

The interplay of liquid-liquid phase separation (LLPS) with the glass transition is a possible route to the formation of arrested states in colloidal and protein systems. LLPS requires attractive interactions, the microscopic details of which set the temperature dependence of the LLPS phase boundary. We report the kinetics of phase separation and arrest for two protein systems: γ -globulin in the presence of PEG 1000, featuring upper critical solution temperature behavior, and bovine serum albumin in the presence of Y(III), featuring lower critical solution temperature behavior. For both systems, the time evolution of the characteristic length is followed during phase separation by Ultra Small Angle X-ray Scattering (USAXS) and Very Small Angle Neutron Scattering (VSANS). This time evolution corresponds to classical LLPS proceeding by spinodal decomposition for shallow quenches in the two-phase region, and to arrested LLPS for deep enough quenches [1]. For intermediate quenches, we report evidence of an unusual three-stage coarsening process. In this case, a temporary arrest of the kinetics is found, which is overcome at later times. We interpret the finding in the light of simulations and experimental results on colloidal systems.

[1] Da Vela et al. *Soft Matter*, 2016, 12, 9334 - 9341

BP 40.3 Wed 11:00 ZEU 260

Demixing and clustering in a binary system of long-ranged capillary interactions — ●MALTE LÜTJE, JOHANNES BLEIBEL, and MARTIN OETTEL — Institut für Angewandte Physik, Universität Tübingen, Deutschland

We consider a binary system of micron-sized spherical colloidal particles trapped at a fluid interface, which induces long-ranged capillary interactions. If one species has positive and one has negative buoyancy, colloids of the same species attract while different species repel. This leads to the demixing of initially uniform densities, and ultimately to the formation of close-packed clusters for each species. Demixing competes with the clustering of each species.

We present static phase diagrams for the system. Brownian Dynamics simulation results illustrate the evolution from a homogeneous state to the demixed and clustered states. The system has unusual phase separation dynamics: The timescales of demixing and clustering can

be different, yielding an intermediate stage with halo-like structures.

BP 40.4 Wed 11:15 ZEU 260

Poisson-Boltzmann study of the effective electrostatic interaction between colloids at an electrolyte interface — ●ARGHYA MAJEE^{1,2}, MARKUS BIER^{1,2}, and S. DIETRICH^{1,2} — ¹Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569, Stuttgart — ²IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart

The effective electrostatic interaction between a pair of colloids, located close to each other at an electrolyte interface, will be discussed by employing the full, nonlinear Poisson-Boltzmann (PB) theory within classical density functional theory. Using a simplified yet appropriate model, all contributions to the effective interaction are obtained exactly, albeit numerically. The comparison between our results [1] and those obtained within linearized PB theory [2] reveals that the latter overestimates these contributions significantly at short inter-particle separations. Whereas the surface contributions to the linear and the nonlinear PB results differ only quantitatively, the line contributions show qualitative differences at short separations. Moreover, a dependence of the line contribution on the solvation properties of the two adjacent fluids is found, which is absent within the linear theory. Our results are expected to enrich the understanding of effective interfacial interactions between colloids.

References:

[1] A. Majee, M. Bier, and S. Dietrich, *J. Chem. Phys.* **145**, 064707 (2016). [2] A. Majee, M. Bier, and S. Dietrich, *J. Chem. Phys.* **140**, 164906 (2014).

15 min break

BP 40.5 Wed 11:45 ZEU 260

Entropic Interactions between Dendrimers and Impenetrable Surfaces — ●RON DOCKHORN^{1,2}, STEPHAN MESCHEDER³, MARTIN WENGENMAYR^{1,2}, and JENS-UWE SOMMER^{1,2} — ¹Leibniz Institute of Polymer Research Dresden, D-01069 Dresden, Germany — ²Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — ³Institute for Physics, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany

Monte Carlo simulations are performed to investigate depletion effects on dendrimers using the bond fluctuation model. Two different situations are investigated: The interaction between a single dendrimer against a hard wall and the interaction between two dendrimers. The simulations of the dendrimers are performed with implicit solvent as well as in a linear polymer matrix. The free energy landscape along the particular reaction coordinate is determined by Umbrella Sampling (WHAM algorithm) and compared to a mean-field approach. Both systems immersed in a polymer matrix show entropic attraction (depletion forces) depending on the length of the surrounding linear chains. Additionally, a spontaneous conformational change and rapid mixing caused by the strong interaction in the two dendrimers' system can be noticed. These findings are aimed to understand the agglomeration and the coagulation processes of hyperbranched structures in drug-delivery systems in medical applications.

BP 40.6 Wed 12:00 ZEU 260

Liquid-state theory of the interactions between colloids mediated by attractive reversibly adsorbed polymers. — ●A.I. CHERVANYOV — Institute for Nano- and Microfluidics, TU Darmstadt

By making use of the liquid state theory, we analytically study the effect of attractive polymer-colloid (P-C) and polymer-polymer (P-P) interactions on the effective forces acting between colloids immersed in a polymer system. The performed theoretical analysis has no restrictions with respect to the polymer density and relative sizes of the colloids and polymers. The polymer mediated (PM) potential acting

between fillers is shown [1,2] to significantly depend on the strength and range of the P-P and P-C interactions. In the nano-particle limit, where the colloid radius is much smaller than the polymer gyration radius, the presence of attractive P-P interactions causes significant, but only quantitative changes to the PM potential. In the opposite limit of relatively large colloids, the P-P interactions revert the sign of the total effective force acting between colloids so that this force becomes attractive at sufficiently large polymer densities. The effect of the C-P interactions on the PM potential is found to be most pronounced in the case of large polymer densities and small colloid-to-polymer size ratios. The dependence of the second virial coefficient of the effective PM potential on the polymer density is discussed in detail, revealing several novel features of the PM forces caused by the presence of attractive P-P and P-C interactions.

[1] A.I. Chervanyov, *Soft Matter* 11,1038-1053 (2015).

[2] A.I. Chervanyov, *J. Chem. Phys.* 141, 244902(2014).

BP 40.7 Wed 12:15 ZEU 260

Determining helicity modulus in systems with orientational order from microscopic properties through Zwanzig-Mori formalism — ●JOHANNES HÄRING and MATTHIAS FUCHS — FB Physik, Universität Konstanz, 78457 Konstanz, Germany

Up to now, we have studied crystals with point disorder and applied the theory to crystals of soft core particles, so-called cluster crystals [1]. Now, systems with orientational order like nematic liquid crystals are considered. With the Zwanzig-Mori formalism it is possible to calculate the helicity modulus for all temperatures in the ordered phase, even near the critical point.

The Zwanzig-Mori formalism is a way to treat many-body systems systematically. Projection Operators are used to focus on the dominant variables of the system and their correlation functions. Simulations of the three dimensional XY model are done to test the accuracy of the approach. The XY model consists of particles with one orientational degree of freedom which are fixed on a lattice.

It is known from the Mermin-Wagner theorem that two dimensional systems show no conventional long range order, i.e have vanishing order parameters. That leads to problems in calculating the helicity modulus. We discuss how it is still possible to obtain a solution.

[1] J. M. Häring, C. Walz, G. Szamel, and M. Fuchs, *Phys. Rev. B* 92, 184103 (2015)

BP 40.8 Wed 12:30 ZEU 260

Clusters in dipolar fluids — ●MICHELA RONTI¹, ALEXEY O. IVANOV², LORENZO ROVIGATTI³, JOSE M. TAVARES⁴, FRANCESCO SCIORTINO⁵, and SOFIA S. KANTOROVICH^{1,2} — ¹Computational Physics, University of Vienna, Sensengasse 8, 1090 Vienna, Austria — ²Ural Federal University, 3 Ural Federal University, Lenin av. 51, Ekaterinburg, 620000, Russia — ³Rudolf Peierls Centre for Theoretical Physics, University of Oxford, 1 Keble Road, Oxford, OX1 4 NP, United Kingdom — ⁴Instituto Superior de Engenharia de Lisboa-ISEL, Rua Conselheiro Emidio Navarro 1, 1950-062 Lisboa, Portugal — ⁵University of Rome La Sapienza, Piazzale Aldo Moro 2, I-00185, Roma, Italy

We describe the self-assembly in magnetic nanocolloids by using a dipolar hard sphere (DHS) model. The phase diagram of this system at low temperature remains debatable regardless the expected simplicity of the model. At low temperature DHS particles self-assemble into complex structures, with primary structures composed by rings and chains. The latter form the building blocks for further aggregation. To elucidate the formation of branched structures analytically, we need to calculate accurately partition functions of various clusters. For that we introduce grand-canonical single cluster Monte Carlo simulations.

BP 40.9 Wed 12:45 ZEU 260

Ferromagnetic phases in colloidal suspensions — ●GRIGORI ZARUBIN^{1,2} and MARKUS BIER^{1,2} — ¹Max Planck Institute Int. Sys. — ²University of Stuttgart, Germany

A ferromagnetic phase of anisotropic particles suspended in a nematic liquid crystal (NLC) was predicted as early as 1970 [1]. A recent experimental realization [2] confirmed that a dilute suspension of magnetic platelets in NLC forms ferromagnetic phase which is susceptible to weak magnetic fields. In this work we describe such a suspension of plate-like particles using density functional theory. The influence of the NLC is taken into account implicitly through the introduction of the effective elastic interaction between platelets. Following approach of Lev and Tomchuk [3], the effective potential was derived under the assumption of weak anchoring of the NLC at the surface of the platelets. An ordered phase was identified with help of the orientational distribution function, and the dependence of the ferromagnetic phase on the strength of the magnetic and the elastic coupling was studied.

References: [1] F. Brochard and P.G. de Gennes, *J. Physique* 31, 691 (1970). [2] A. Mertelj, D. Lisjak, M. Drofenik and M. Copic, *Nature* 504, 237 (2013). [3] B.I. Lev and P.M. Tomchuk, *Phys. Rev. E* 59, 1 (1998).

BP 41: Active Matter I (Joint Session DY/BP/CPP)

Time: Wednesday 15:00–19:00

Location: HÜL 186

BP 41.1 Wed 15:00 HÜL 186

Flocking ferromagnetic particles — ●ANDREAS KAISER, ALEXEY SNEZHKO, and IGOR S. ARANSON — Materials Science Division, Argonne National Laboratory, 9700 South Cass Ave, Argonne, Illinois 60439, USA

Suspensions of microswimmers, show fascinating collective behaviours like clustering, flocking and turbulence [1]. Here, we demonstrate the discovery of ferromagnetic flocking colloids. The self-propulsion is an outcome of the spontaneous rotation of a ferromagnetic colloidal sphere in a vertical alternating (AC) magnetic field [2]. Depending on the frequency of this magnetic field, a sequence of transitions can be observed: from gas-like motion of individual particles to the onset of flocking and global rotation followed by a reentrant flocking and gas-like state for increasing frequency [3]. We also emphasize a subtle role of rotational noise: While the low-frequency flocking appears to be noise-insensitive, the reentrant flocking happens to be noise-activated. Moreover, we uncover a new relation between collective motion and synchronisation.

[1] T. Vicsek, A. Zafeiris, *Physics Reports* 517, 71 (2012)

[2] G. Kokot, D. Piet, G.M. Whitesides, I.S. Aranson, A. Snezhko, *Scientific Reports* 5, 9528 (2015)

[3] A. Kaiser, A. Snezhko, I.S. Aranson, *Science Advances* (submitted)

BP 41.2 Wed 15:15 HÜL 186

Unexpected enhancement of rotational dynamics of self-propelled particles in a colloidal glass — ●CELIA LOZANO^{1,2}, JUAN RUBEN GOMEZ-SOLANO¹, and

CLEMENS BECHINGER^{1,2} — ^{1,2} Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

It has been recently demonstrated that the glass transition of dense colloidal suspensions is progressively shifted by increasing activity of embedded self-propelled particles (SPP) [1]. However, it is not clear yet how the dynamics of such SPP becomes affected by the surrounding glassy environment. We experimentally investigate the active motion of spherical Janus particles within a cage created by a binary mixture of colloidal particles. We observe a dramatic enhancement of the rotational diffusion of active particles with increasing particle velocity and the density, in a similar fashion as SPP in semi-dilute polymer solutions [2]. This experimental approach allows us to measure, in parallel, the temporal evolution of the active particle and the passive colloidal suspension. Our findings suggest that these effects originate from the coupling between the thermal fluctuations of the particle and the surrounding heterogeneities, which displays large relaxation times of several seconds.

[1] Ni, R., Stuart, M. A. C. & Dijkstra, M. *Nature communications* 4, 2704 (2013). [2] Gomez-Solano, J. R., Blokhuis, A. & Bechinger, C. *Phys. Rev. Lett.* 116, 138301 (2016).

BP 41.3 Wed 15:30 HÜL 186

Motility-Induced Phase-Separation of Microswimmers: Hydrodynamics and Phase-Equilibria — ●JOHANNES BLASCHKE and HOLGER STARK — Institut für Theoretische Physik, Technische Uni-

versität Berlin, Hardenberg Str. 36, 10623 Berlin, Germany

Active motion of microorganisms and artificial microswimmers is relevant both to real world applications as well as for posing fundamental questions in non-equilibrium statistical physics. Microswimmers are often modelled as active Brownian particles, neglecting hydrodynamic interactions between them. However, real microswimmers, such as ciliated microorganisms, catalytic Janus particles, or active emulsion droplets, employ propulsion mechanisms reliant on hydrodynamics. Therefore, we use multi-particle collision dynamics to explore the influence of hydrodynamics on the collective behavior of spherical microswimmers in quasi-two-dimensional geometry [1].

A striking feature of the collective motion of microswimmers is that for sufficiently strong self-propulsion they phase-separate into dense clusters coexisting with a low-density gas phase. Here we examine the influence of hydrodynamic interactions on this motility-induced phase separation. The most striking difference with the phase diagram of active Brownian particles is that a larger mean density results in a lower density of the coexisting dilute phase, which is a clear signature of hydrodynamics. Furthermore, we find that pushers or pullers suppress phase separation by increasing the critical Péclet number.

[1] J. Blaschke, M. Maurer, K. Menon, A. Zöttl, and H. Stark, *Soft Matter* (2016), DOI:10.1039/C6SM02042A.

BP 41.4 Wed 15:45 HÜL 186

Synthetic Janus microswimmers moving under confinement in viscoelastic media — ●JUAN RUBEN GOMEZ SOLANO¹, MAHSA SAHEBDIVANI¹, and CLEMENS BECHINGER^{1,2} — ¹2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — ²Max-Planck-Institut fuer Intelligente Systeme, Heisenbergstrasse 3, 70569 Stuttgart, Germany

The motion of many natural microswimmers, e.g. bacteria and spermatozoa, commonly takes place in viscoelastic media and under confinement close to solid walls. Recent experiments demonstrate that active colloids in Newtonian liquids can be hydrodynamically and phoretically trapped or guided by solid walls depending on the surrounding flow field and on the geometry of the confinement [1-3]. In our work, using spherical Janus microswimmers activated by light in a semidilute polymer solution [4], we experimentally investigate how viscoelasticity affects the motion of such self-propelled particles when approaching or leaving a flat wall. Unlike self-propulsion in Newtonian fluids, we find a strong particle-wall repulsion induced by the surrounding viscoelastic liquid over large distances from the wall. We show that this phenomenon has dramatic consequences for the particle translational and rotational dynamics in more complex confined geometries, as well as for collective motion in crowded environments.

[1] G. Volpe et al., *Soft Matter* 7, 8810 (2011). [2] D. Takagi et al., *Soft Matter* 10, 1784 (2014). [3] J. Simmchen, *Nat. Comm.* 7, 10598 (2016). [4] J. R. Gomez-Solano, A. Blokhuis, and C. Bechinger, *Phys. Rev. Lett.* 116, 138301 (2016).

BP 41.5 Wed 16:00 HÜL 186

Dynamics of microswimmer molecules — SONJA BABEL, NIKLAS KÜCHLER, HARTMUT LÖWEN, and ●ANDREAS M. MENZEL — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

In recent years, the dynamical properties of individual microswimmers have been investigated intensively. The same applies for their collective dynamical behavior in dilute and dense suspensions. Here we address an intermediate level. We study the dynamics of compound objects of coupled swimmers that we term “microswimmer molecules” [1,2].

First, we address three spherical magnetic microswimmers connected by elastic springs to a straight object [1]. The magnetic interactions support the straight arrangement. However, with increasing active drive, hydrodynamic interactions destabilize the straight shape. Technically, this occurs via a subcritical Hopf bifurcation. The oscillatory feature of this bifurcation is connected to a cork-screw-like motion of the molecule.

Second, we consider an active microswimmer coupled by elastic springs to one or more passive swimmers [2]. The dynamics of this type of molecule in an external planar swirl flow is investigated, while hydrodynamic interactions are neglected to lowest order. Because of the finite extension and deformability of these molecules, interesting dynamical features arise. They comprise an expulsion from or undertow into the swirl, rotations of the deformed trajectories, and changes in the sense of the trajectory rotations.

[1] Babel et al., *EPL (Europhys. Lett.)* **113**, 58003 (2016).

[2] Küchler et al., *Phys. Rev. E* **93**, 022610 (2016).

BP 41.6 Wed 16:15 HÜL 186

Microscopic derivation of the hydrodynamics of active-Brownian-particle suspensions — STEFANO STEFFENONI¹, ●GIANMARIA FALASCO², and KLAUS KROY² — ¹Max planck for the mathematics in the science, leipzig — ²Institute for theoretical physics, leipzig

We derive the hydrodynamic equations of motion for a fluid of active particles described by under-damped Langevin equations that reduce to the Active-Brownian-Particle model, in the overdamped limit. The contraction into the hydrodynamic description is performed by locally averaging the particle dynamics with the non-equilibrium many-particle probability density, whose formal expression is found in the physically relevant limit of high-friction through a multiple-time-scale analysis. This approach permits to identify the conditions under which self-propulsion can be subsumed into the fluid stress tensor and thus to define systematically and unambiguously the local pressure and surface tension of the active fluid.

15 min. break

BP 41.7 Wed 16:45 HÜL 186

Determination of the phase behavior and the critical point in systems of active particles in depletants — ●JONATHAN TAMMO SIEBERT¹, BENJAMIN TREFZ^{1,2}, THOMAS SPECK¹, KURT BINDER¹, and PETER VIRNAU¹ — ¹Department of Physics, Johannes Gutenberg University of Mainz, D-55128 Mainz, Germany — ²Graduate School Materials Science in Mainz, D-55128 Mainz, Germany

We study a modified, active variant of the well-known Asakura-Oosawa model for colloid-polymer mixtures. Activity is introduced as Vicsek-like self-propulsion. This system already undergoes phase separation in case of zero propulsion. In the driven case, the binodal lines are shifted towards lower densities.

Building on earlier results for the binodal line, we completed the phase diagram by determination of the critical point, using a subsystem-block-density distribution analysis. In addition to understanding critical phenomena in this specific system far from equilibrium, the proposed method can serve as a recipe to find critical points and the associated exponents for other types of active particles.

BP 41.8 Wed 17:00 HÜL 186

Clustering of nematic active particles in low Reynolds number Navier-Stokes flow — ●REBEKKA BREIER, CRISTIAN C. LALESCU, DEVIN WAAS, MICHAEL WILCZEK, and MARCO G. MAZZA — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen

Large groups of self-propelled particles are ubiquitous in nature, from flocks of starlings and herds of wildebeests down to schools of fish and groups of bacteria or algae. Many of these creatures exist in (possibly mildly) turbulent habitats, like motile plankton in the pycnocline of the ocean. We study large systems of self-propelled, nematically aligning, hard core particles by means of molecular dynamic simulations which inhabit a turbulent environment. We investigate the active dynamics and compare the results from kinematic simulations (“synthetic turbulence”) with direct numerical simulations of the turbulent background field. We find a “sweet spot” for clustering, that is, an optimal strength of turbulence leads to very dense small-scale clusters. We explain the mechanism that induces clustering. Moreover, we investigate the effect of hard cores compared to point particles, and also give the appropriate dimensionless numbers to describe the dynamic transitions.

BP 41.9 Wed 17:15 HÜL 186

Reinforcement learning of artificial microswimmers — ●SANTIAGO MUIÑOS-LANDIN¹, KEYAN GHAZI-ZAHEDI², and FRANK CICHOS¹ — ¹Molecular Nanophotonics, University of Leipzig, Institut für Experimentale Physik I — ²Information Theory of Cognitive Systems, Max Planck Institute for Mathematics in the Sciences

Reinforcement Learning (RL) is a special area of the Machine Learning discipline which consist in the search of an optimal policy in the context of Markovian Decision Processes (MDP). Learning is based on the interaction of the system with its environment and is guided by sparse rewards. In RL a policy is a function that connects the available actions that an agent can execute with the states where this agent can be located at. MDPs were already proposed as a model for the navigation of natural microswimmers. Here we present now a method that uses this RL in order to achieve an autonomous explorative be-

havior from a self-thermophoretic microswimmer. We implement it experimentally by photon nudging to reach reinforcement learning of a symmetric microswimmer.

BP 41.10 Wed 17:30 HÜL 186

Self-propelled motion of an extra particle in a two-dimensional plasma crystal — •INGO LAUT, CHRISTOPH RÄTH, SERGEY K. ZHDANOV, VOLODYMYR NOSENKO, GREGOR E. MORFILL, and HUBERTUS M. THOMAS — Deutsches Zentrum für Luft- und Raumfahrt, Forschungsgruppe Komplexe Plasmen, 82234 Weßling, Germany

Plasma crystals consist of charged microparticles that levitate in a weakly ionized gas. In these nonequilibrium systems the particle interaction is nonreciprocal due to flowing ions. Plasma crystals were successfully used to study dynamical effects in liquids and solids at the kinetic level and have the potential to also enable the study of active particles.

Here, we analyze in simulations and theory the self-propelled motion of an “extra” particle in a two-dimensional plasma crystal. Experimental observations [1] showed that the extra particle is confined in a channel of two neighboring rows of particles and moves persistently through the crystal. We use the simple model of a pointlike ion wake charge to reproduce this intriguing effect in simulations. We show that the nonreciprocity of the particle interaction, owing to the plasma flow, is responsible for a broken symmetry of the channel that enables the self-propelled motion of the extra particle [2].

[1] C.-R. Du, V. Nosenko, S. Zhdanov, H. M. Thomas, and G. E. Morfill, *Phys. Rev. E* **89**, 021101(R) (2014)

[2] I. Laut, C. R  th, S. K. Zhdanov, V. Nosenko, G. E. Morfill, and H. M. Thomas, accepted for publication in *Phys. Rev. Lett.*

BP 41.11 Wed 17:45 H  L 186

Dynamics of model bacteria in dense polymer suspensions and networks — •ANDREAS Z  TTL and JULIA M. YEOMANS — Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK

Swimming bacteria, such as *Helicobacter pylori*, *Pseudomonas aeruginosa* and sperm cells, move through viscoelastic fluids, such as mucus, in vivo. Theoretical models for these complex fluids are typically based on continuum equations which assume a constant density of sufficiently small polymers, homogeneously embedded in a Newtonian fluid. However, real viscoelastic fluids are more structured when considered on the length scale of a microswimmer: they can consist of heterogeneously distributed, up to micrometer long, macromolecules such as mucin polymers.

Here we present results of coarse-grained hydrodynamic simulations of a flagellated bacterium swimming in explicitly modeled macromolecular polymer solutions and cross-linked networks. We find a remarkable increase in the bacterium’s swimming speed at high polymer density. We further discuss the effect of polymer properties such as length, stiffness and cross-linking. We also report the flow fields and the local polymer properties in the vicinity of the bacterium, which can be strongly influenced by its motion.

BP 41.12 Wed 18:00 H  L 186

Rheology and shear-induced dynamics of passive and active anisotropic colloids — •HENNING REINKEN and SABINE H. L. KLAPP — Institut f  r Theoretische Physik, Technische Universit  t Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate the rheology of passive and active fluids focusing on shear-induced instabilities and emerging spatiotemporal structures. Prominent examples of active matter, which is composed of self-driven units converting energy into motion on the microscopic scale, are anisotropic colloidal particles with polar or nematic interactions. Already in the passive case, these systems show very interesting rheological properties including oscillatory orientational states and shear banding [1]. Introducing activity into the system modifies the rheology and leads to additional instabilities [2].

We study the rheological properties via the Doi-Hess theory [1], a continuum theoretical approach. In this framework, the orientational order parameter is coupled to the flow via the stress tensor, which can be extended to include an active stress [2]. In particular, we focus on parameter regimes where interesting spatiotemporal structures like banded states or active turbulence [3] emerge and discuss the differences between active and passive systems.

[1] R. Lugo-Fr  as, H. Reinken, S. H. L. Klapp, *Eur. Phys. J. E* **39**: 88 (2016).

[2] M. C. Marchetti et al. *Rev. Mod. Phys.* **85**, 1143 (2013).

[3] S. Heidenreich, J. Dunkel, S. H. L. Klapp, M. B  r, *Phys. Rev. E* **94**, 020601(R) (2016).

BP 41.13 Wed 18:15 H  L 186

Effective interactions of active particles: interfacial phase behavior and swim pressure — •REN   WITTMANN, ABHINAV SHARMA, and JOSEPH BRADER — Departement f  r Physik, Universit  t Fribourg, 1700 Fribourg, Schweiz

We employ classical density functional theory to study the self-organization in active systems. Using a first-principles approach, we map the self-propulsion onto an effective pair interaction potential, which has been shown [1] to account for the motility-induced phase separation (MIPS) observed for active Brownian particles. We further introduce an effective external potential and investigate inhomogeneous situations.

Solely as a result of their activity, we predict [2] that active (Brownian) particles undergo a variety of interfacial phase transitions, e.g., wetting and capillary condensation in purely repulsive systems or drying and capillary evaporation of attractive colloids. We explain why the effective thermodynamic pressure and interfacial tension do not coincide with the mechanical results, which we recover by embedding the presented effective-potential approach within a more general (dynamical) framework. Finally, we comment on situations with a non-vanishing particle current [3].

[1] T. F. F. Farage, P. Krinninger and J. M. Brader, *Phys. Rev. E* **91**, 042310 (2015).

[2] R. Wittmann and J. M. Brader, *Europhys. Lett.* **114**, 68004 (2016).

[3] A. Sharma, R. Wittmann, J. M. Brader, arXiv:1611.03897 (2016).

BP 41.14 Wed 18:30 H  L 186

Patterns in chemically interacting microswimmers: Do they really exist? — •BENNO LIEBCHEN¹, DAVIDE MARENDUZZO¹, and MICHAEL E. CATES² — ¹SUPA, School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom — ²DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Chemotaxis is the directed motion of particles in response to a gradient in a chemical signal. It allows micro-organisms, like bacteria, to find food and to escape from toxins. Some micro-organisms can produce the species to which they respond themselves and use chemotaxis for signalling. Remarkably, artificial Janus colloids that swim by catalysing reactions in a bath naturally feature chemical interactions and thereby provide a synthetic analogue to signalling micro-organisms. While, it is well known that cases where these interactions are attractive lead to clustering and phase separation, we have recently demonstrated that the purely repulsive case does not simply stabilize the uniform phase but creates a versatile new route to pattern formation in active systems.

In this talk, I will briefly review our work on chemorepulsive pattern formation and will focus the question on how generic and realistic these patterns are for Janus colloids. Our work unveils a fundamental link between autophoresis and chemotaxis leading to a massive collapse of parameter space and generic instability criteria which we confirm using particle based simulations.

BP 41.15 Wed 18:45 H  L 186

Kinetic theory of self-propelled particles: von Mises distribution and Chapman-Enskog expansion — •R  DIGER K  RSTEN and THOMAS IHLE — Institut f  r Physik, Ernst-Moritz-Arndt Universit  t Greifswald

We consider Vicsek-type models [1] with multi-particle interactions and discrete time dynamics. Starting from the exact evolution equation for the N-particle probability distribution, an Enskog-like kinetic equation is derived. Recently, the von Mises distribution and an geometric series ansatz were proposed to treat this nonlinear integral equation [2,3]. We critically assess them for a Vicsek-model with bounded-confidence interactions. Both approaches recover the qualitative behavior of the system but the von Mises distribution causes large deviations in certain parameter regions [4]. We extend the von Mises approximation by an additional term that leads to much better agreement. The geometric series ansatz for the Fourier modes of the probability density is typically very accurate but fails for very weak noise. We therefore suggest an alternative approach – a Gaussian ansatz – for the higher modes, which is robust at all noises. Furthermore, we present a non-standard Chapman-Enskog expansion with a fast time scale. This expansion

is used to derive the macroscopic transport equations from the microscopic collision rules. We discuss the expressions for the transport coefficients, which become simple in the limit of infinite density.

- [1] Phys. Rev. Lett. 75 (1995) 1226 [2] J. Stat. Mech. (2015) P10017
[3] Phys. Rev. E 90 (2014) 063315 [4] arXiv:1611.00624

BP 42: Neurosciences

Time: Wednesday 15:00–17:30

Location: ZEU 250

Invited Talk BP 42.1 Wed 15:00 ZEU 250

Linking AMPA receptor nanoscale organization and function at excitatory synapses — •DANIEL CHOQUET — Interdisciplinary Institute for Neuroscience, CNRS, Université de Bordeaux, Bordeaux, France,

The spatio-temporal organization of neurotransmitter receptors in the postsynaptic membrane is a fundamental determinant of synaptic transmission and thus information processing by the brain. Using a combination of high resolution single molecule imaging techniques and video-microscopy, we had previously established that AMPARs are not stable in the synapse as thought initially, but undergo continuous entry and exit to and from the post-synaptic density through lateral diffusion. Using three independent super-resolution imaging methods, on both genetically tagged and endogenous receptors, we demonstrated that, in live hippocampal neurons, AMPAR are highly concentrated inside synapses into a few clusters of around seventy nanometers. AMPAR are stabilized reversibly in these domains and diffuse freely outside them. These results open the new possibility that glutamatergic synaptic transmission is controlled by the regulation at the nanometer scale of the position and composition of these highly concentrated nanodomains. This finding provides a functional support to our hypothesis that fast AMPAR surface diffusion can tune short term plasticity by allowing fast replacement of desensitized AMPAR by naïve ones during high frequency stimulation.

BP 42.2 Wed 15:30 ZEU 250

Hippocampal learning with memristive devices: device requirements for the use in recurrent networks — •NICK DIEDERICH^{1,2}, THORSTEN BARTSCH², MARTIN ZIEGLER¹, and HERMANN KOHLSTEDT¹ — ¹Technische Fakultät, Christian-Albrechts-Universität zu Kiel — ²Neurologie, Universitätsklinik Schleswig-Holstein

Memristive devices are considered as promising candidates for hardware based synapses since they fulfill important biological plasticity rules such as long-term potentiation and long-term depression. Furthermore, their low energy consumption, scalability, and rather simple device structure are especially interesting for artificial neural networks. In this talk, the opportunities of memristive devices for recurrent neural networks are presented. Those networks are in particular important structures in mammal brains. In detail, a memristive network-model of the hippocampal loop is presented which allows the realization of physiological behavior of learning. The unique behaviors and desired device characteristics of memristive devices for those network structures will be discussed.

Financial support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

BP 42.3 Wed 15:45 ZEU 250

Protocol for fluctuation analysis of ion channel currents in nonstationary conditions: application to Ca^{2+} channels — •CHRISTIAN SCHEPPACH^{1,2} and HUGH P.C. ROBINSON² — ¹Physikalisches Institut, Albert-Ludwigs-Universität Freiburg i. Br., Germany — ²Department of Physiology, Development and Neuroscience, University of Cambridge, U.K.

Fluctuation analysis is a method which allows measurement of the single channel current of ion channels even when it is too small to be resolved directly with the patch clamp technique. The method in its original form depends on stationary conditions, such that meaningful ensemble-averaging over several successive current traces can be performed. However, experimentally this is sometimes not possible, for example when the ion channel current runs down rapidly. We therefore developed a novel fluctuation analysis protocol which extracts information from individual current traces. It is based on voltage ramp stimulation, mean current fitting of individual current responses and band-pass filtering. We apply the method to Ca^{2+} channels in pyramidal neurons of layer 5 of rat neocortex, arriving at a single-

channel current of 0.07 pA (membrane potential: -20 mV; external Ca^{2+} concentration: 2 mM). We validate the accuracy of the method by analysing simulated data and compare it with another established method of dealing with ion channel rundown.

Reference: C. Scheppach & H.P.C. Robinson (arXiv, under review).

BP 42.4 Wed 16:00 ZEU 250

A circuit to mimic a bio-inspired two-alternatives decision-making experiment based on elementary motion detection — •TOM BIRKOBEN, MIRKO HANSEN, MARINA IGNATOV, MARTIN ZIEGLER, and HERMANN KOHLSTEDT — Nanoelektronik, Technische Fakultät, Christian Albrechts Universität zu Kiel, Germany

Decision-making belongs to one of the most important principles in the nervous system of living species. A decision is based on the temporally available sensory input data and previous experiences made in similar situations, i.e. related to memory and reward. In-depth studies utilizing two-alternatives saccadic eye movement tasks led to a profound understanding of neuronal information processing. Three fundamental processing stages are needed to perform this kind of tasks successfully: a neuronal representation of the sensory signal, the integration of the stimuli and the comparison of the accumulated information to a threshold for a final decision. We present an analogue electronic decision-making circuit. Our concept study includes an LED-matrix as the task screen, an array of photo diodes, a Hassenstein-Reichardt Detector based motion detection and finally a signal integration circuit based on an inhibitory coupling scheme. The biologically well motivated effects of previous experiences (memory and reward) for decision making might be effectively implemented into the circuit by memristive devices, which will be discussed in the framework of I-V characteristics and the circuit layout.

Financial Support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

15 min break

BP 42.5 Wed 16:30 ZEU 250

The temporal dimension of information coding in the brain, studied via neuroimaging in an insect model. — MARCO PAOLI¹, ANGELA ALBI¹, RENZO ANTOLINI^{1,2}, and •ALBRECHT HAASE^{1,2} — ¹Center for Mind/Brain Sciences, University of Trento, Italy — ²Department of Physics, University of Trento, Italy

We apply fast two-photon calcium imaging to study information coding in the brain of honeybees. Recording the responses of the first local neuronal network along the olfactory pathway, the antennal lobe, we investigate whether information about the odour stimulus is encoded in temporal features of the neuronal activation. Besides the spatial distribution of activation, we identified odour-specific oscillatory features modulating the slow activation curves. Furthermore, we found that the activation onset varies for different stimuli and different network nodes. By predicting test odours only from the order of network node activation, we proof that these response latencies form an odour-specific code across individuals.

BP 42.6 Wed 16:45 ZEU 250

On collision of action potentials — •CHRISTIAN FILLAFER, ANNE PAEGER, and MATTHIAS F. SCHNEIDER — Technische Universität Dortmund, Medizinische und Biologische Physik, Dortmund, Germany
It is a common incident in nature, that two waves or pulses run into each other head-on. The outcome of such an event is of special interest, because it allows conclusions about the underlying physical nature of the pulses. The present experimental study dealt with the head-on meeting of two action potentials (AP) in a single excitable plant cell (*Chara braunii* internode). The membrane potential was monitored at the two extremal regions of an excitable cell. In control experiments, an AP was excited electrically at either end of the cell cylinder. Subsequently, stimuli were applied simultaneously at both ends of the cell

in order to generate two APs that met each other head-on. When two action potentials propagated into each other, the pulses did not penetrate but annihilated ($N=14$ experiments in $n=4$ cells). It was difficult to judge whether annihilation was complete or partial. A small data set indicated that both outcomes are possible. APs in excitable plant cells did not penetrate upon meeting head-on. In the classical electrical model, this behavior is attributed to relaxation of ion channel proteins. From an acoustic point of view, annihilation is a result of nonlinear material properties of the excitable medium. The present results indicate that APs in excitable animal and plant cells are similar nonlinear phenomena. Intriguingly, other excitation waves in biology (intracellular waves, cortical spreading depression, etc.) also annihilate upon collision and thus may be fundamentally related to action potentials.

BP 42.7 Wed 17:00 ZEU 250

Patch Clamping of T cells and Neurons on Nanowire Substrates — ●JANN HARBERTS¹, AUNE KOITMÄE¹, GABRIELE LOERS², CARSTEN RONNING³, HEINER LINKE⁴, and ROBERT H. BLICK^{1,5} — ¹Institute of Nanostructures and Solid State Physics (INF), Hamburg — ²Center for Molecular Neurobiology Hamburg (ZMNH) — ³Institute for Solid State Physics, University of Jena — ⁴Solid State Physics, Lund University, Sweden — ⁵Center for Hybrid Nanostructures (CHyN), Hamburg

Nano- and micro-structured substrates achieved an increasing amount of interest in cell biology during the recent years. Chemical and physical properties of culturing substrates have a significant influence on adhesion and viability of overgrowing cells. For instance, substrates with vertically aligned nanowires (NWs) can control the outgrowth of cells depending on diameter, length and density.

Typically, such experimental studies are analyzed with staining techniques in fluorescent microscopes. For quantitative measurements of

cell characteristics, such as gating properties of ion channels, a more precise method—the patch clamp technique—is required. This technique facilitates the exact measurement of currents and voltages at the cell membrane. A potential disadvantage is the mechanical pressure on the cell during the measurement procedure, which could damage the cell, especially on NW substrates. However, conventional patch clamp setups are not designed for patch clamping on opaque substrates. We present a modified setup which meets this requirement and show successful measurements of T cells and neurons settled on NW substrates.

BP 42.8 Wed 17:15 ZEU 250

On the Mechanical Component of an Action Potential — ●MATAN MUSSEL, CHRISTIAN FILLAFER, and MATTHIAS F. SCHNEIDER — Technische Universität Dortmund, Dortmund, Germany

Action potentials (AP) in neurons are accompanied by a bi-phasic surface displacement, which is composed of swelling during depolarization and contraction during repolarization. This mechanical pulse (~ 1 – 10 nm) has not received a satisfactory explanation up to date. Herein, we present results on mechanical changes during AP propagation in excitable plant cells (internodes of *Chara Braunii*). In a native *Chara* cell, the plasma membrane is tightly pressed against the cell wall by turgor pressure (~ 6 bar). In order to directly study deformations of the cell surface, turgor pressure was reduced by osmosis until the plasma membrane detached from the cell wall. Upon excitation of an AP, the surface displaced by ~ 1 – 10 μm . This mechanical deflection (i) propagated with the same velocity as the electrical pulse (~ 10 mm/s), (ii) was reversible and (iii) in most cases of biphasic nature. We propose a mechanical model that describes these shape transformations as an interplay between the surface forces and the pressure difference across the surface. Our model captures the essence of the cell shape dynamics and makes testable predictions about the underlying mechanism.

BP 43: Cytoskeletal Filaments

Time: Wednesday 15:00–17:15

Location: HÜL 386

Invited Talk

BP 43.1 Wed 15:00 HÜL 386

Diffusive anchorage of molecular motors allows for adaptive force generation — ●STEFAN DIEZ — B CUBE, TU Dresden, Germany

Cytoskeletal motor proteins have been well characterized in vitro as single molecules or as ensembles rigidly attached to non-biological substrates. However, in cells, motors are often only loosely coupled to their cargo. Towards understanding the resulting collective transport properties we reconstituted membrane-anchored kinesin-1 gliding motility assays. We found that motor slippage in the membrane rendered the gliding velocity of the microtubules strongly dependent on the number of motors and their diffusivity in the lipid bilayer. Moreover, we investigated the force generation of kinesin-14 motors diffusively anchored with their tail domains on one microtubule while sliding another microtubule. Again, slippage significantly reduced the transport efficiency leading to a strongly reduced force production as compared to rigidly bound motors. Notably, under these conditions the motor forces were low enough to be fully balanced by the entropic forces arising from the diffusive anchorage of non-motor crosslinkers, hence allowing for the adaptive formation of persistent partial microtubule overlaps. Taken together, our results illustrate the importance of motor-cargo coupling, which provides cells with an additional means of regulating transport efficiency and force generation.

BP 43.2 Wed 15:30 HÜL 386

Structure and Dynamics of Stress fibers in adult Stem Cells — ●CARINA WOLLNIK¹, BENJAMIN ELTZNER², STEPHAN HUCKEMANN², and FLORIAN REHFELDT¹ — ¹Third-Institute of Physics - Biophysics, Georg-August University Göttingen, Germany — ²Institute for Mathematical Stochastics, Georg-August University Göttingen, Germany

Adult human mesenchymal stem cells (hMSCs) are capable of differentiation towards various cell types such as nerve, bone, and muscle precursor cells. Strikingly, substrate stiffness as physical stimulus is enough to guide hMSCs towards different lineages in the absence of additional biochemical stimuli [1]. Connecting focal adhesions throughout the cell, stress fibres generate and transmit tension [3], lack of which stops the differentiation process [1]. Characteristic stress fibre

reorganisation patterns are detected after 24 hours and used as early morphological marker [2], backed up with genetic evidence [6]. Here, we present data from massive parallel live cell imaging of mechano-guided early stem cell differentiation of RFP-Lifeact transfected hMSCs [7]. Stress fibres are traced with sophisticated tracking algorithms [4,5].

[1] A. Engler et al., Cell (2006) [2] A. Zemel et al., Nature Physics (2010) [3] E. K. Paluch et al., BMC Biology (2015) [4] B. Eltzner et al., PLoS One (2015) [5] S. Huckemann et al., Bernoulli (2016) [6] C. Wollnik et al., in preparation (2016+) [7] C. Wollnik et al., in preparation (2016+)

BP 43.3 Wed 15:45 HÜL 386

Electron Microscopy (EM) and Single Particle Analysis on Myosin — ●DARIO SACZKO-BRACK, CHRISTOPHER BATTERS, BENOIT ROGEZ, MARKUS KRÖSS, and CLAUDIA VEIGEL — LMU, Department of Cellular Physiology, Schillerstrasse 44, 80336 Munich, Germany

Myosin-IX is critically involved in structural reorganizations of the acto-myosin cytoskeleton in the lamellipodium of migrating cells and in cell polarization in morphogenesis. Using a combination of negative stain EM, single particle image processing, fluorescence spectroscopy and motility assays we discovered that myosin-IXa assembles actin filaments into highly ordered lattices with parallel actin polarity and a repeat distance of precisely 36 nm, matching the helical repeat of actin. We resolved three distinct conformations of myosin-IXa crosslinks in the absence of nucleotide. Furthermore we found that calmodulin binds to a large insert in the motor domain exclusively found in class IX myosins. This creates two coordinated actin binding sites that constrain the acto-myosin interactions which generates the lattices. These might introduce a myosin-related, force-sensing mechanism into the cytoskeleton in cell polarization and collective cell migration.

The cytoskeletal motor myosin VI is involved in many motile processes including cancer cell migration and is the only myosin shown to move towards the minus end of actin. We demonstrate that calcium is the cellular switch that induces a structural rearrangement of this motor which regulates the transition from an inactive to a cargo-binding state and controls the mechanical properties.

Batters, Brack et al. PNAS 2016

BP 43.4 Wed 16:00 HÜL 386

Lateral association and elongation of vimentin intermediate filament proteins: A time-resolved light-scattering study — ●CARLOS LOPEZ¹, OLIVA SALDANHA², KLAUS HUBER¹, and SARAH KÖSTER² — ¹Department Chemie, Universität Paderborn, 33098 Paderborn, Germany — ²Institut für Röntgenphysik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Intermediate filaments constitute one of the three protein filament systems in the cytoskeleton of metazoa. Together with actin filaments and microtubules they form a sophisticated composite network, which has been identified as a main player in cell mechanics. The assembly pathway of the cytoskeletal protein vimentin may be responsible for the mechanical properties of the emerging filaments, such as high flexibility and extensibility, and thus play a key role in cellular mechanics.

Assembly of Vimentin from its tetrameric form can be triggered by addition of a monovalent salt. A two-step assembly mechanism: lateral association and a subsequent elongational step, has been established; however, the elongational step has not been followed in solution.

We present direct in situ observation and modeling of the elongation reaction of the filaments on the relevant length (60-600nm) and time scales, using time-resolved, multiangle static and dynamic light scattering. We thus achieve sufficient spatio-temporal resolution without the need of labeling, staining, or adsorption to substrates. The mass per unit length, hydrodynamic diameter and the end-to-end elongation rate constant of the assembling filaments are evaluated as a function of added salt.

15 min break

BP 43.5 Wed 16:30 HÜL 386

Mechanisms of microtubule nucleation and size in spindles — ●FRANZISKA DECKER^{1,2}, ELISA RIECKHOFF^{1,2}, BENJAMIN DALTON^{1,2}, DAVID ORIOLA^{1,2}, and JAN BRUGUES^{1,2} — ¹Max Planck Institute for the Physics of Complex Systems — ²Max Planck Institute of Molecular Cell Biology and Genetics

The spindle is the protein machinery responsible for segregating the genetic material into the daughter cells. Microtubules, the main building blocks of the spindle, have a lifetime of 20 sec while the entire spindle remains for minutes or even up to hours. Thus, maintenance of the spindle requires constant creation of new microtubules through microtubule nucleation. Here, we used laser ablation to measure the minus ends of monopolar spindles in *Xenopus laevis* egg extract as a proxy to microtubule nucleation. We found that microtubule dependent microtubule nucleation explains the nucleation profile and microtubule density in these structures, with the amount of nucleators activated in chromosomes setting the number of microtubules in spindles. This nucleation mechanism could account for the scaling of spindles with cell volume as observed in early embryogenesis or spindles encapsulated in extract, and provides an alternative prediction to previous models based on microtubule dynamics. To test whether microtubule dynamics or microtubule nucleation are responsible for the scaling of spindles, we performed measurements of microtubule dynamics and nucleation during the early rounds of cell division in Zebrafish embryos.

BP 43.6 Wed 16:45 HÜL 386

Overlapping microtubules establish a microenvironment enabling the autoregulation of molecular motors — ●MARCUS BRAUN^{1,2}, ZDENEK LANSKY^{1,2,3}, AGATA SZUBA^{1,2}, FRIEDRICH W. SCHWARZ², ANNIRUDDHA MITRA^{1,2}, MENGFEI GAO^{1,2}, ANNEMARIE LÜDECKE^{1,2}, PIETER REIN TEN WOLDE⁴, and STEFAN DIEZ^{1,2} — ¹B CUBE, TU Dresden, Arnoldstraße 18, 01307 Dresden, Germany — ²MPI-CBG, Pfotenhauerstraße 108, 01307 Dresden, Germany — ³CAS, BIOCEV, Prumyslova 595, Vestec 25250, Czech Republic — ⁴AMOLF, Science Park 104, 1098 XG Amsterdam, the Netherlands

Collective action of molecular motors is required for the remodeling of microtubule networks underpinning essential cellular processes, such as cell division. Among these motors are microtubule-crosslinking motors, which slide microtubules along each other. However, additional regulatory proteins are thought to be necessary to establish stable overlaps between the sliding microtubules and to prevent the breakdown of the networks. Here, we show in vitro that human kinesin-14 HSET motors - as they slide overlapping microtubules apart - collectively detect the decrease in overlap length and slow down the sliding in an autoregulatory manner, leading to the formation of stable overlaps. Slowdown is quantitatively explained by the dependence of HSET sliding on the local HSET density in the overlap and the generation of an entropic force antagonizing the sliding. We argue that overlapping filaments, when crosslinked by proteins sensitive to their spatial arrangement, establish envelope-free compartments constituting distinct microenvironments that can locally catalyze biochemical processes.

BP 43.7 Wed 17:00 HÜL 386

Microtubule pivoting and minus end directed motors drive the formation of the mitotic spindle — ●IVANA BAN¹, MARCEL PRELOGOVIĆ¹, LORA WINTERS², ANA MILAS³, IVA TOLIC^{2,3}, and NENAD PAVIN¹ — ¹Faculty of science, University of Zagreb, Croatia — ²Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — ³Division of Molecular Biology, Ruder Bošković Institute, Zagreb, Croatia

During mitosis, the genetic material is divided into two equal parts by the spindle. This complex micro-machine is made of chromosomes, microtubules (MTs) and a variety of accessory proteins. In the fission yeast *Schizosaccharomyces pombe*, the mitotic spindle is a bundle of MTs emanating from two spindle pole bodies, whose formation is mediated by motor proteins. A key question is what are the physical principles underlying the formation of a mitotic spindle. In this work, we combine theory and experiment to describe how angular motion of MTs and forces exerted by motor proteins lead to spindle formation. In our model, MTs explore their environment by performing angular movement around the spindle poles, until two MTs come into close proximity, allowing motor proteins accumulate in the overlap region. In the case of minus end directed motors, this leads to formation of antiparallel bundles. We experimentally observed random angular motion of MTs as well as accumulation of Cut7 motor proteins in the overlap region, followed by antiparallel bundle formation. In conclusion, these results provide an explanation for how the angular Brownian motion and motor proteins drive the formation of a stable mitotic spindle.

BP 44: Biomaterials and Biopolymers (Joint Session BP/CPP)

Time: Wednesday 15:00–17:15

Location: SCH A251

BP 44.1 Wed 15:00 SCH A251

The microstructural function of the tendon-bone insertion — ●LEONE ROSSETTI¹, LARA A. KUNTZ^{1,2}, ELENA KUNOLD³, JONATHAN SCHOCK¹, KEI W. MÜLLER⁴, HEINRICH GRABMAYR¹, JOSEF STOLBERG-STOLBERG⁵, FRANZ PFEIFFER¹, STEPHAN A. SIEBER³, RAINER BURGMART², and ANDREAS R. BAUSCH¹ — ¹Physik Department, TU München, D-85748 Garching, Germany — ²Klinik für Orthopaedie und Sportorthopaedie, Klinikum rechts der Isar, TU München, D-81675 München, Germany — ³CIPSM, Department of Chemistry, TU München, D-85747 Garching, Germany — ⁴Institute for Computational Mechanics, TU München, D-85748 Garching, Germany — ⁵University Hospital Münster, D-48149 Münster, Germany

The exceptional mechanical properties of the connection of tendon to bone rely on an intricate interplay of its biomolecular composition,

microstructure and micromechanics. Here we identify that the Achilles tendon insertion is characterized by a stress reducing mechanism within an interfacial zone of 500 micrometres, with a distinct fiber organisation and biomolecular composition. Proteomic analysis detects enrichment in the interface region that are predominantly involved in cartilage and skeletal development as well as proteoglycan metabolism. Micromechanical testing coupled with multiscale confocal microscopy identifies a heterogeneous mechanical response in the interface area, endowing the enthesis with a graded response to strains acting from different angles. The presented mechanisms mark a guideline for further biomimetic strategies to rationally design hard-soft interfaces.

BP 44.2 Wed 15:15 SCH A251

Exposure of leukocytes and hematopoietic stem cells to

graphene quantum dots — ●STEFAN FASBENDER¹, SONJA ALLANI¹, CHRISTIAN WIMMENAUER¹, PATRICK CADEDDU², KATHARINA RABA³, JOHANNES FISCHER³, BEKIR BULAT⁴, CLAUD SEIDEL⁴, THOMAS HEINZEL¹, and RAINER HAAS² — ¹Heinrich-Heine-Universität Düsseldorf, Institut für experimentelle Physik der kondensierten Materie — ²Universitätsklinikum Düsseldorf, Klinik für Hämatologie — ³Universitätsklinikum Düsseldorf, Institut für Transplantationsdiagnostik — ⁴Heinrich-Heine-Universität Düsseldorf, Institut für Molekulare Physikalische Chemie

Fluorescent graphene quantum dots (GQDs) are prepared by the method of Wu et. al [1] via hydrothermal treatment of citric acid and dicyandiamide with subsequent dialysis to obtain a pure GQD solution. The obtained aqueous solution is analyzed with fluorescence spectroscopy, UV-vis, XPS and AFM. Human leukocytes and hematopoietic stem cells are exposed to two different concentrations of GQDs for various times and the uptake dynamic is determined using flow cytometry. A higher uptake is observed into cells with phagocytotic properties. The number of incorporated GQDs is estimated by comparing the fluorescence of cells with GQDs and without GQDs. A permeability constant for the various cell types is calculated and the effect of the GQDs on the viability of the cells is assessed with the XTT viability assay.

[1] Wu et al., *Nanoscale*, 2014, 6, 3868

BP 44.3 Wed 15:30 SCH A251

Guanidinium Salts Can both Cause and Prevent the Hydrophobic Collapse of Biomacromolecules — ●JAN HEYDA^{1,2}, HALIL OKUR³, JOACHIM DZUBIELLA^{2,4}, PAVEL JUNGWIRTH⁵, and PAUL CREMER^{3,6} — ¹Physical Chemistry Department, UCT Prague, Czech Republic — ²Institut für Weiche Materie und Funktionale Materialien, HZB Berlin, Germany — ³Chemistry Department, Penn. State University, Pennsylvania, USA — ⁴Institut für Physik, HU Berlin, Germany — ⁵Institute of Organic Chemistry and Biochemistry, CAS, Prague, Czech Republic — ⁶Biochemistry and Molecular Biology Department, Penn. State University, Pennsylvania, USA

A combination of experimental methods with theory and simulations were performed to probe the mechanisms by which guanidinium (Gnd^+) salts influence the stability of the collapsed vs. uncollapsed state of an elastin-like polypeptide (ELP). The Gnd^+ action was found highly dependent upon its counteranion, resulting in three distinct physical regimes. (1) Well-hydrated Gnd_2SO_4 salt was depleted from the ELP/water interface and was found to stabilize the collapsed state of the macromolecule. (2) Salts (e.g. GndSCN), which interacted very strongly with the polymer, stabilized the collapsed state at low salt concentrations, when both ions were found to be enriched in the collapsed state of the polymer. The collapsed state is stabilized due to crosslinking of the polymer chains. At higher salt concentrations, the same strong salt-polymer interaction results in stabilization of the uncollapsed state. (3) GndCl interacted in an intermediate fashion favored the uncollapsed state at all salt concentrations.

BP 44.4 Wed 15:45 SCH A251

Altering Synthetic Semiflexible DNA Nanotube Networks by Tunable Cross-linking — ●MARTIN GLASER^{1,2}, PAUL MOLLENKOPF^{1,2}, CHRISTIN MÖSER², CARSTEN SCHULDT^{1,2}, JÖRG SCHNAUSS^{1,2}, JOSEF KÄS¹, and DAVID SMITH² — ¹Faculty of Physics and Earth Sciences, Institute of Experimental Physics I, Leipzig University, Germany — ²Fraunhofer Institute for Cell Therapy and Immunology IZI, DNA Nanodevices Group, Germany

The mechanical properties of complex soft matter have been subject to various experimental and theoretical studies. The underlying constituents often cannot be modeled in the classical physical frame of flexible polymers or rigid rods. Polymers in the semiflexible regime, where the finite bending stiffness leads to a non-trivial mechanical contribution, are a highly interesting subclass and can be found in the cytoskeleton of living cells. A natural occurring model system for such polymers is the protein actin. However, experimental studies of actin networks to validate existing theories, are limited since the persistence length cannot be altered. Here, we establish a tunable system of cross-linked, synthetically DNA nanotubes to overcome this limitation. We present first results of the impact tunable cross-linking has on the well-characterized entangled DNA nanotube networks. These studies enable investigations of the impact of a crucial parameter of semiflexible polymers, namely the persistence length, on emerging network properties. Also, the study will allow a deeper insight into the underlying mechanics of biomaterials, such as hydrogels, which are extensively used for in vitro as well as in vivo applications.

BP 44.5 Wed 16:00 SCH A251

Ion and Molecule Transport in Surface Modified Nanopores - a NMR Study — ●SARAH SCHNEIDER and MICHAEL VOGEL — TU Darmstadt Solid State Physics, Darmstadt, Germany

We analyze ion and molecule transport in surface modified nanopores. It is part of a project that aims to develop a new generation of nanosensors by combining biological and synthetic nanopores. While being highly selective and sensitive, biological ion channels lack the robustness for technological applications. Contrarily silica pores are well-proven in industrial and clinical environments, but possess inferior capabilities, e.g. no selectivity. A hybrid system would combine the favorable properties of both fields.

To optimize such pores, it is of strong interest to understand the influence of this confinement on the ion and molecule transport inside. Such confined dynamics depend on the pore geometry and the guest-host interactions determined by the properties of the inner surfaces.

We vary these parameters systematically, in particular by peptide functionalization of the silica surfaces and study their effects on the dynamics by NMR. This includes various techniques aiming at local dynamics. SFG NMR is applied to measure self-diffusion coefficients of aqueous salt solutions in bulk and nanopore confinement. The experimental setups include ^1H and ^2H NMR to selectively investigate water dynamics as well as ^7Li and ^{23}Na NMR to analyze the diffusion of various ionic species. We find a slowdown of dynamics in confinement. The extent of the effect and the relation between short- and long-range dynamics substantially depends on the confinement properties.

15 min break

BP 44.6 Wed 16:30 SCH A251

Model-independent measurements of ATP diffusion in PEG-DA hydrogels with various mesh sizes — ●GÜNTER MAJER¹ and ALEXANDER SOUTHAN² — ¹MPI für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, Germany — ²Institut für Grenzflächen-verfahrenstechnik und Plasmatechnologie IGVP, Universität Stuttgart, Nobelstraße 12, 70569 Stuttgart, Germany

Hydrogels are semi-solid polymer networks formed by cross-linked hydrophilic polymer chains, with mesh sizes that can be tailored by varying the concentration and/or the molecular mass of the polymers. Well-defined hydrogels are ideal materials for various applications including drug delivery, transport of nutrients, or devices to separate small molecules chromatographically. In this context, a fundamental understanding of the diffusion processes of solutes in hydrogels with different mesh sizes is important. A powerful tool to determine the diffusion coefficients of solutes directly, i.e. without the need of a fluorescent label and independent of any diffusion-model assumptions, is pulsed field gradient nuclear magnetic resonance (PFG-NMR). In this work, polyethylene glycol diacrylate (PEG-DA)-based hydrogels with mesh sizes ranging from 1.35 to 3.70 nm were prepared using polymers with molecular masses between 700 and 8000 g/mol and concentrations of up to 30%. The diffusion coefficients of adenosine triphosphate (ATP) in these hydrogels were studied by PFG-NMR. The correlation between the mesh sizes and the diffusion coefficients is analyzed and discussed.

BP 44.7 Wed 16:45 SCH A251

Stress-induced long-range ordering in spider silk — ●JOHANNES WAGNER and FRAUKE GRÄTER — Heidelberg Institute for Theoretical Studies, Heidelberg, Germany

A range of composite or semi-crystalline materials consist of particles or crystallites embedded randomly in a much softer phase. Emergence of long-range order of these particles within the softer matrix could result in lowering the mechanical energy of the system upon stretching, in consistence with the well-known coalescence of defects in materials. Using small-angle neutron scattering (SANS) and finite element (FE) models we show the presence of such stress-induced ordering in spider silk fibers. Both methods show striking quantitative agreement of the position, shift and intensity increase of the long period upon stretching. We demonstrate that this mesoscopic ordering does not originate from strain-induced crystallization at the atomistic scale, and instead arises from a non-affine deformation that enhances density fluctuations of the two phases along the direction of stress. Our results suggest long-range ordering as a wide-spread phenomenon that can be exploited for tuning the mechanical properties of many hybrid materials with stiff and soft phases.

BP 44.8 Wed 17:00 SCH A251

Tuning coiled coils mechanically and thermodynamically by histidine-metal coordination — •ISABELL TUNN, KERSTIN G. BLANK, and MATTHEW J. HARRINGTON — Max Planck Institute of Colloids and Interfaces, Science Park Potsdam Golm, 14424 Potsdam

Coiled coils serve as structural motifs in proteins with mechanical function, such as myosin or α -keratin. In the field of bioinspired materials, naturally occurring and synthetic coiled coils with high binding specificity have become versatile material building blocks, which are used as crosslinkers for hydrogels with applications in cell culture and tissue engineering. Very little is currently understood about the mechanical properties of coiled coils. Yet, this information is critical for controlling and tuning bulk properties of coiled coil-based materials.

In order to generate mechanically tunable coiled-coil based materials, metal coordination sites were engineered into a well-characterized heterodimeric coiled coil. Protein-metal coordination bonds are strong, non-covalent interactions mediated by amino acid ligands. Here, two histidine residues were introduced at the coiled coil termini with the goal of stabilizing helical turns. Histidine-metal coordination increased the stability of the coiled coil mechanically and thermodynamically, as demonstrated by AFM single molecule force spectroscopy and CD spectroscopy. We conclude that increasing the stability of single helical turns via metal binding directly affects the overall stability of the coiled coil, providing the potential for generating mechanically tunable biomimetic polymers. Furthermore, these results also provide crucial information about the failure mechanism of coiled coils under load.

BP 45: Annual General Meeting of the BP Division (BP Mitgliederversammlung)

Time: Wednesday 18:30–19:30

Location: HÜL 386

Discussion

BP 46: Active Matter II (Joint Session DY/BP/CPP)

Time: Thursday 9:30–13:00

Location: HÜL 186

Invited Talk

BP 46.1 Thu 9:30 HÜL 186

Rolling, rolling, rolling – a new self-propulsion mechanism — •FALKO ZIEBERT^{1,2} and IGOR KULIC² — ¹Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany — ²Institut Charles Sadron UPR22-CNRS, 67034 Strasbourg Cedex 2, France

We describe a generic mechanism that induces an instability towards rolling motion of a rod along a heated plate. The mechanism, relying on geometric planar confinement, can be explained by an effective model combining elasticity of a rod with thermal advection-diffusion. We exemplify the versatility of the effect by investigating self-propellers, as well as simple motors and energy storage devices, both experimentally and theoretically.

BP 46.2 Thu 10:00 HÜL 186

Cluster Formation and Deformation of Spherical Circle Swimmers Dispersed on a Monolayer — •GUO-JUN LIAO and SABINE H. L. KLAPP — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

Inspired by recent experimental developments in manufacturing "active" colloidal particles with unusual, e.g. curved, modes of motion (such as form-anisotropic particles [1] or decorated metallodielectric Janus spheres [2]), as well as by the proceeding of a theoretical study on the collective behavior of curved polymers with circular paths [3], we computationally investigate models of spherical particles in which the colloids dispersed on a monolayer feel not only a propelling force, but also a propelling torque. In the absence of propulsion torque (without circular motion), we find clustering of "conventional" self-propelled disks, in accordance with Ref. [4]. We show that the motility-induced cluster formation is enhanced by polar interaction, and cumulatively hindered by increasing the propulsion angular velocity ω_0 . Different from the model of curved polymers [3], in which the occurrence of stable vortices is attributed to the shape anisotropy, our generic model of isotropic "active" spheres also form clockwise vortices as ω_0 approaches the rotational diffusion coefficient D_r .

- [1] F. Kümmel et al., Phys. Rev. Lett. **110**, 198302 (2013)
- [2] S. Gangwal et al., Phys. Rev. Lett. **100**, 058302 (2008)
- [3] J. Denk et al., Phys. Rev. Lett. **116**, 178301 (2016)
- [4] J. Bialke et al., EPL **103**, 30008 (2013)

BP 46.3 Thu 10:15 HÜL 186

Effect of the orientational relaxation on the collective motion of patterns formed by self-propelled particles. — •ALEXANDER CHERVANYOV¹, HECTOR GOMEZ², and UWE THIELE¹ — ¹Institut für Theoretische Physik, WWU Münster, Germany — ²Universidade da Coruna, A Coruna, Spain

We investigate the collective behavior of self-propelled particles (SPPs) undergoing competitive processes of pattern formation and rotational

relaxation of their self-propulsion velocities. As a main result of this study, we quantitatively explain [1] transitions between different steady states of the SPPs caused by the intricate interplay among the involved effects of pattern formation, orientational order, and coupling between the SPP density and orientation fields. Based on rigorous analytical and numerical calculations, we prove that the rate of the orientational relaxation of the SPP velocity field is the main factor determining the steady states of the SPP system. Further, we determine the exact boundaries between domains in the parameter plane that delineate qualitatively different resting and moving states. In addition, we analytically calculate the collective velocity of the SPPs and show that it perfectly agrees with our numerical results. Our results can be effectively used to identify the regimes of collective behavior of SPPs in living systems in relevance to the domains of dominance of the above described effects of the self-propulsion, pattern formation and orientational relaxation of SPPs.

[1] A.I. Chervanyov, H. Gomez, U. Thiele, EPL **115**, 68001 (2016).

BP 46.4 Thu 10:30 HÜL 186

Statistical features of active turbulence — •MARTIN JAMES and MICHAEL WILCZEK — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Dense bacterial suspensions display rich dynamical features including turbulence-like behavior. Recent studies have shown that such turbulent dynamics of active fluids can be modeled by a generalized Navier-Stokes equation (Wensink et al., PNAS 2012). The statistical features of active turbulence, however, differ significantly from classical hydrodynamic turbulence (see, e.g., Bratanov et al., PNAS 2015). We further explore the statistical features of this active turbulence model both, numerically and analytically. In particular, we focus on scale-dependent statistics to characterize deviations from Gaussianity and the occurrence of extreme events. Moreover, we investigate the transport properties of active flow by using Lagrangian tracer techniques. Our results provide insight into mixing of microbial suspensions due to turbulent dynamics.

BP 46.5 Thu 10:45 HÜL 186

Large scale vortex-patterns in dense suspensions of microswimmers — •SEBASTIAN HEIDENREICH¹, JÖRN DUNKEL², SABINE H. L. KLAPP³, and MARKUS BÄR¹ — ¹Physikalisch-Technische Bundesanstalt — ²Massachusetts Institute of Technology — ³Technische Universität Berlin

In this talk we consider a prominent examples of an active biological fluid - dense suspension of swimming bacteria (e. g. *Bacillus subtilis*). For dense suspensions of bacterial swimmers, we have proposed a simple phenomenological model that predicts regular and turbulent vortex lattices and reproduces recent experimental findings of mesoscale turbulence in two- and three-dimensional suspensions of *Bacillus subtilis* in a quantitative manner [1]. A continuum model that couples

the orientation of the swimmers with the surrounding velocity field was derived from stochastic equations of motions for individual active swimmers for a realistic hydrodynamical model of swimmers in a fluid [2]. This model contains the simple phenomenological model used in [1] as a special case. Furthermore, the continuum model enables us to understand the mechanism and properties of pattern formation in microswimmer suspensions and relate the physical parameters characterizing the individual swimmers and their interaction to the coefficients for continuum model equations.

[1] Dunkel, S. Heidenreich, K. Drescher, H. H. Wensink, M. Bär & R. E. Goldstein *Phys. Rev. Lett.* 110; *New. J. Phys.* (2013).

[2] S. Heidenreich, J. Dunkel, S. L. Klapp, and M. Bär (2016). *Phys. Rev. E*, 93

BP 46.6 Thu 11:00 HÜL 186

Collective Effects of Active Particles at Fluid-Fluid Interfaces. — ●IRINA KISTNER, PAOLO MALGARETTI, MIHAIL NICOLAE POPESCU, and SIEGFRIED DIETRICH — Max-Planck-Institut fuer Intelligente Systeme, Stuttgart, Germany

Micrometer sized particles capable of self-induced motility are of high interest for various applications in medicine, sensing and environmental science. Recent works report of different types of collective motion such as clustering, swarming or fluid-solid phase separation. Moreover different phenomena may arise when active particles are bounded or reside in the proximity of a fluid-fluid interface [1], [2].

The model system we are investigating consists of two or more chemically active, spherical colloidal particles located close to a fluid-fluid interface. Due to the Marangoni stresses self-induced at the interface, the particles experience a repulsive long-ranged effective force field under harmonic confinement. We show that this effective interaction results in a crystal-like pattern formation of collectively rotating particles and define a gas-crystal phase separation governed by the Marangoni force constant.

[1] A. Dominguez, P. Malgaretti, M. N. Popescu, and S. Dietrich: Effective interaction between active colloids and fluid interfaces induced by Marangoni flows, *Phys. Rev. Lett.* 117, 079902 (2016)

[2] A. Dominguez, P. Malgaretti, M. N. Popescu, and S. Dietrich: Collective dynamics of chemically active particles trapped at a fluid interface, *Soft Matter*, 12, 8398-8406 (2016)

15 min. break

BP 46.7 Thu 11:30 HÜL 186

Mechanical Instabilities in Active Systems — ●CHRISTOPH A. WEBER and LAKSHMINARAYANAN MAHADEVAN — Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA

Active stress can affect the stability of biological systems and drive macroscopic changes of matter on very short time scales that cannot be explained by the liquid-like transport of the constituents. Examples are contracting active gels or the compaction of cells in tissues. For these systems the solid-like response to active stress is the key to understand the physics underlying the change of matter. Here we study a generic framework to describe mixtures composed of an active solid and a passive liquid phase. We find that such a mixture is unstable for large enough activity and can demix into regions mostly consisting of solid or fluid, respectively. The instability leads to the formation of disintegrated patches of a length scales which arises from the competition between the shear transport in the solid phase versus the solid-liquid momentum transfer. This mechanical instability might be relevant for many very dense active systems where liquid-like particle transport is mostly jammed.

BP 46.8 Thu 11:45 HÜL 186

Defect dynamics in topological active matter — ●AXEL VOIGT and FRANCESCO ALAIMO — Institute für Wissenschaftliches rechnen, TU Dresden

If active systems are confined on curved surfaces, topological constraints strongly influence the emerging spatiotemporal patterns. Using these topological constraints to guide collective cell behavior might be a key in morphogenesis and active nematic films on surfaces have been proposed as a promising road to engineer synthetic materials that mimic living organisms. Recent experiments consider an active nematic film of microtubules and molecular motors encapsulated within a lipid vesicle. As in passive systems the mathematical Poincaré-Hopf theorem forces topological defects to be present in the nematic film.

On a spherical vesicles this leads to an equilibrium defect configuration with four $+1/2$ disclinations arranged as a tetrahedron. In active systems unbalanced stresses drive this configuration out of equilibrium. But in contrast to planar active nematics with continuous creation and annihilation of defects the creation of additional defect pairs can be suppressed on curved surfaces. This led to the discovery of a tunable periodic state that oscillates between the tetrahedral and a planar defect configuration. We confirm this finding by computer simulations. For non-constant Gaussian curvature constraints local geometric properties can be used to control defect dynamics. We are concerned with a systematic investigation of the impact of such constraints on the emergence of complex patterns and oscillations.

BP 46.9 Thu 12:00 HÜL 186

Dancing disclinations in living fluids — ●AMIN DOOSTMOHAMMADI, TYLER SHENDRUK, KRISTIAN THIJSEN, and JULIA YEOMANS — University of Oxford

The spontaneous emergence of collective flows is a generic property of active fluids and often leads to chaotic flow patterns characterised by swirls, jets, and topological disclinations in their orientation field. However, the ability to achieve structured flows and ordered disclinations is of particular importance in the design and control of active systems. By confining an active nematic fluid within a channel, we find a regular motion of disclinations, in conjunction with a well defined and dynamic vortex lattice. As pairs of moving disclinations travel through the channel, they continually exchange partners producing a dynamic ordered state, reminiscent of Ceilidh dancing. We anticipate that this biomimetic ability to self-assemble organised topological disclinations and dynamically structured flow fields in engineered geometries will pave the road towards establishing new active topological microfluidic devices.

BP 46.10 Thu 12:15 HÜL 186

Effective interactions between catalytic particle and fluid-fluid interfaces — ●PAOLO MALGARETTI, MIHAIL NICOLAE POPESCU, and SIEGFRIED DIETRICH — Max Planck Institute for Intelligent Systems, Heisenbergstr. 3 70569 Stuttgart Germany

When catalytic particles, such as Janus particles, or enzymes are in the vicinity of a fluid-fluid interface, their is strongly modulated by the presence of the interface and/or by the inhomogeneity in the transport properties of the two fluid phases. Hence, the effective interaction with the interface can lead to novel dynamical regimes absent in homogeneous fluids. For example, if the by-products of the catalysis are surfactants their spatial distribution will affect the local value of the surface tension. In such a scenario, when catalytic particles approach a fluid-fluid interface a Marangoni flow will set up in response to the inhomogeneity in the surface tension induced by the byproducts of the catalysis. The onset of such a flow attracts the catalytic particle towards the interface. Interestingly the strength of such an effective attraction is strongly affected by the affinity of the byproduct to the interface as well as by the transport properties of the two fluid phases. In particular, for water-oil interfaces such an effect overwhelms other means of active transport such as self-diffusiophoresis and makes it suitable to enhance particle accumulation close to fluid-fluid interfaces. Finally I will discuss the onset of collective behavior.

BP 46.11 Thu 12:30 HÜL 186

Active crystals on the sphere — ●SIMON PRAETORIUS¹, AXEL VOIGT¹, RAPHAEL WITTKOWSKI², and HARTMUT LÖWEN³ — ¹Institute of Scientific Computing, Technische Universität Dresden, D-01062 Dresden, Germany — ²Institut für Theoretische Physik Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — ³Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany

Two-dimensional crystals on curved manifolds like a sphere exhibit nontrivial defect structures. Here we consider "active" crystals on the sphere which are composed of self-propelled particles. A coarse-grained model is proposed by unifying the Phase-Field Crystal approach with a Toner-Tu-like theory which involves a density and a polarization field on the sphere. Depending on the strength of the self-propulsion, four different dynamical modes are found: a resting crystal, a self-spinning "vortex-vortex" crystal containing two vortical poles with integer defects of the polarization, a "source-sink" crystal and a travelling/spinning lamellar. We analyze the dependence of orientational and translational defects on the activity of the crystal.

BP 46.12 Thu 12:45 HÜL 186

Green-Kubo approach to active Brownian systems — ●ABHINAV SHARMA and JOSEPH BRADER — Université de Fribourg, Rue du Musée 3, ch 1700, Fribourg

We develop an exact Green-Kubo formula relating nonequilibrium averages in systems of interacting active Brownian particles to equilibrium time-correlation functions. The method is applied to calculate the

density-dependent average swim speed, which is a key quantity entering coarse grained theories of active matter. The average swim speed is determined by integrating the equilibrium autocorrelation function of the interaction force acting on a tagged particle. We generalize our approach to a spatially and time varying activity. Analytical results are validated using Brownian dynamics simulations.

BP 47: Cell Adhesion

Time: Thursday 9:30–10:45

Location: ZEU 250

Invited Talk

BP 47.1 Thu 9:30 ZEU 250

Mechanotransduction in Collective Cell Migration — ●JOACHIM SPATZ — Max Planck Institut für Medizinische Forschung, Dept. Cellular Biophysics, Jahnstr. 29, 69120 Heidelberg

The collective movement of epithelial cells drives essential multicellular organization during various fundamental physiological processes like embryonic morphogenesis, cancer, and wound healing. Two hallmarks of collective behavior in migrating cohesive epithelial cell sheets is the emergence of so called leader cells and the communication between adjacent cells to move correlated to each other. Here we discuss these two phenomena: 1. The geometry-based cue imposed by the matrix environment like local curvature of the collective's perimeter is capable of triggering leader cell formation and promoting enhanced motility at defined positions. Cytoskeletal tension was found to be important for geometry induced leader cell formation. Together our findings suggest that high curvature leads to locally increased stress accumulation, mediated via cell-substrate interaction as well as via cytoskeleton tension. The stress accumulation in turn enhances the probability of leader cell formation as well as cell motility. 2. Within this cohesive group each individual cell correlates its movement with that of its neighbours. We investigate the distinct molecular mechanism that links intercellular forces to collective cell movements in migrating epithelia. More specifically, we identified the molecular mechanism whereby Merlin, a tumor suppressor protein and Hippo pathway regulator that functions as a mechanochemical transducer, coordinates collective migration of tens of hundreds of cells.

BP 47.2 Thu 10:00 ZEU 250

Adhesion of *Chlamydomonas* microalgae to surfaces is switchable by light — ●CHRISTIAN KREIS, MARINE LE BLAY, CHRISTINE LINNE, MARCIN MAKOWSKI, and OLIVER BÄUMCHEN — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, D-37077 Göttingen, Germany

Many microalgae live in complex confined geometries, such as soil and temporary pools, consisting of water inclusions and a plethora of surfaces. They have adapted to these habitats by developing planktonic (freely swimming) and surface-associated states. While the swimming of microalgae has been widely studied in recent years, the mechanism that triggers the adhesion to surfaces remains elusive. We performed *in vivo* force spectroscopy experiments on the unicellular biflagellated microalga *Chlamydomonas*, a prime model organism in cell- and microbiology, and discovered that the flagella-mediated adhesion to surfaces can be switched on and off by light [1]. The light-switchable adhesiveness of the flagella is a completely reversible process based on a redistribution of adhesion-promoting flagella-membrane proteins. This functionality enables the cell to regulate the transition between planktonic and surface-associated state, which possibly represents a significant biological advantage for photoactive microorganisms. Gaining control of the initiation of biofilm formation bears an immediate relevance in technological applications, including the production of biofuel as a renewable source of energy in microalgae photo-bioreactors. [1] C. Kreis, M. Le Blay, C. Linne, M. Makowski, and O. Bäümchen, in review (2016).

BP 47.3 Thu 10:15 ZEU 250

Measuring the contact area of *Staphylococcus aureus* to solid substrates using single-cell force spectroscopy — ●CHRISTIAN SPENGLER, NICOLAS THEWES, and KARIN JACOBS — Saarland University, 66123 Saarbrücken

Bacteria adhere to virtually every surface and promote the formation of - desirable or unwanted - biofilms. Therefore, in many fields, like engineering, medicine, and biology, understanding bacterial adhesion is of great interest in order to support or inhibit the formation of biofilms. Consequently, there exist different models that describe the process of bacterial adhesion. In these models, besides direct values, like adhesion force and rupture distance, also more indirect quantities, like the size of the contact area between bacterial cell and surface, play a crucial role. We present a method to measure the radius of this circular contact area for *Staphylococci* by taking advantage of the fact that the adhesion force of these cells differs strongly between surfaces with different surface energies[1]. We collect multiple force/distance curves with single-cell AFM probes at a very sharp interface between hydrophilic silicon and a hydrophobic self assembling monolayer of silanes. The measured radii of the contact area range from tens of nanometers up to 300 nm and differ strongly between individual cells. Our results also give new insights into the properties and distribution of surface molecules in the bacterial cell wall.

[1] N. Thewes et al., "Hydrophobic interaction governs unspecific adhesion of staphylococci: a single cell force spectroscopy study"; Beilstein J. Nanotechnol. 5(2014) 1501

BP 47.4 Thu 10:30 ZEU 250

Measuring Cell Dynamics at the Substrate-Interface with Surface Plasmon Resonance Microscopy — ●EVA KREYSING, HOSSEIN HASSANI, and ANDREAS OFFENHÄUSSER — ICS8/PGI8, Forschungszentrum Jülich, 52425 Jülich

In neuroelectronics the cell-electrode distance is one of the most critical parameters during cell recordings. Cardiomyocyte-like cells are among the most popular model systems because they periodically generate an action potential. This feature also leads to a cell contraction which affects the cell-electrode distance. To achieve a qualitative and quantitative characterization of the dynamics at the interface *in vitro* and label-free, we built a surface plasmon resonance microscope (SPRM). Using gold coated sapphire chips as the substrate for cell culture it is possible to excite plasmons in the gold layer due to specific illumination. The resonance frequency of the plasmons depends strongly upon the dielectric constant of the gold's environment. In turn the angle spectrum of the reflected light depends upon said resonance frequency. Due to these dependencies it is possible to deduce the cell-substrate distance. Our microscope is capable of imaging the interface in a live-imaging mode where we can observe cell dynamics qualitatively. A scanning mode uses localized surface plasmons to measure the cell-substrate distance. The resolution in z-direction lies in the nanometer range. This allows us to measure the movement of the cell membrane at each scanning point with a time resolution of 150 ms. Using this method we have been able to record the dynamics of multiple cardiomyocytes.

BP 48: Membranes and Vesicles II

Time: Thursday 9:30–13:00

Location: HÜL 386

Invited Talk

BP 48.1 Thu 9:30 HÜL 386

Shaping membranes: ENTH activity as a function of membrane tension — •CLAUDIA STEINEM¹, MARTIN GLEISNER¹, BENJAMIN KROPPE², NELLI TESKE¹, ANDREAS JANSHOFF³, and MICHAEL MEINECKE² — ¹Institute of Organic and Biomolecular Chemistry, University of Göttingen, Germany, — ²Department of Cellular Biochemistry, University of Göttingen, Germany — ³Institute of Physical Chemistry, University of Göttingen, Germany

One of the early players of the process of clathrin-mediated endocytosis is the protein epsin. The epsin N-terminal homology domain (ENTH) binds to PtdIns(4,5)P₂ resulting in tubulation as a result of membrane bending. This process is highly sensitive to the lateral membrane tension σ . By means of protruded pore-spanning membranes (PSMs, $\sigma = 2$ mN/m) and adhered giant unilamellar vesicles (GUVs, $\sigma = 0.1$ – 1 mN/m), we analyzed how ENTH binding alters membrane tension and whether membrane tubules are formed. Binding of ENTH to PtdIns(4,5)P₂-doped protruded PSMs resulted in a growth of the protrusions, which indicates a reduction of the membrane tension. Tubulation was not observed. At low membrane tension of adhered GUV, ENTH binding induced tubular structures, while at higher membrane tension, ENTH interaction only led to a flattening of the GUVs. GUV flattening was attributed to an increased surface area caused by the insertion of the ENTH helix-0 into the membrane. Our results demonstrate that ENTH is capable of reducing the lateral membrane tension, which makes membrane bending energetically less costly.

BP 48.2 Thu 10:00 HÜL 386

Optical control of membrane permeability and fluidity with synthetic photoswitchable phospholipid molecules — •STEFANIE PRITZL¹, PATRICK URBAN¹, JAMES FRANK², CARLA PERNPEINTNER¹, DIRK TRAUNER², and THEOBALD LOHMÜLLER¹ — ¹Chair for Photonics and Optoelectronics, Physics Department and CeNS, LMU Munich — ²Department of Chemistry and CiPSM, LMU Munich

Phospholipid bilayer membranes are almost impermeable for ions or small substances while individual lipids and other membrane components within the bilayer sheet display a high level of lateral mobility. In our work, we devised a strategy to control both membrane permeability and fluidity with light by using photoswitchable phospholipid molecules embedded in an artificial bilayer membrane. These photolipids contain an azobenzene group in one of the hydrocarbon chains that undergoes photoisomerization upon irradiation with blue and UV light. The effect of photoswitching on membrane properties was tested by patch-clamp measurements on free-standing lipid membranes and by fluorescence methods. We observed a fast and reversible switching of membrane currents upon light activation, while membrane fluidity and lipid diffusion could be altered by a factor of two. These results highlight a new principle for controlling membrane properties on fast time scales, which are important for applications in cell signaling and drug delivery.

BP 48.3 Thu 10:15 HÜL 386

Controlling Membrane Rigidity and Deformability of Giant Lipid Vesicles with Photoswitchable Lipid Molecules — •CHRISTIAN RÖSKE¹, CARLA PERNPEINTNER¹, JAMES FRANK², PATRICK URBAN¹, DIRK TRAUNER², and THEOBALD LOHMÜLLER¹ — ¹Chair for Photonics and Optoelectronics, Physics Department, LMU Munich — ²Department of Chemistry and CiPSM, LMU Munich

The shape and deformability of lipid vesicles is strongly depending on the mechanical properties of its bilayer membrane. Manipulating the membrane rigidity to induce membrane fluctuations or even shape transformations is usually achieved by changing the temperature, ion concentration, or molecular composition of the membrane itself. Such drastic changes of experimental parameters, however, are often non-reversible or difficult to control. Here, we demonstrate an alternative approach to manipulate membrane properties by incorporating photoswitchable lipid molecules into giant unilamellar vesicles (GUVs). The photolipids used in this study contain an azobenzene moiety that undergoes reversible photoisomerization upon illumination with UV and visible light. The immediate effect of photoswitching on membrane stiffness and deformability was characterized by using optical twee-

ers and micropipette aspiration. We observe that membrane rigidity of GUVs can be switched fast and reversibly by almost two orders of magnitude depending on the photolipid concentration and the illumination intensity. Based on these findings, we devised a mechanism to utilize photolipid membranes for storing energy and to releasing it as locally usable work, which is only controlled by light.

BP 48.4 Thu 10:30 HÜL 386

Influence of Mono- and Divalent Ions on Cardiolipin Monolayers — •RENKO KENSBOCK, HEIKO AHRENS, and CHRISTIANE A. HELM — Inst. of Physics, Greifswald University, Germany

We investigate electrostatic interactions within negatively charged cardiolipin monolayers at the air-water interface with isotherms and real-time Brewster angle microscopy (BAM). A non-monotonic dependence for the LE/LC transition surface pressure on monovalent salt concentration (NaCl, KCl, CsCl) is observed with a maximum at around 0.1 M. No specificity for monovalent cations is detectable, which points to the prevalence of electrostatics. For subphases of 0.15 M NaCl with different divalent cations, the transition surface pressure decreases upon increase of their concentration. This indicates binding of divalent cations to the monolayer and an increase in electrostatic screening. The mono- and divalent salt effects are in accordance with electrostatic model calculations accounting for the head-group interactions: an electrostatic contribution (Grahame's equation) and counter-ion binding (law of mass action) are considered. The divalent binding constant assumes a 1:1 divalent cation to cardiolipin binding and is specific for the divalent cations used.

BP 48.5 Thu 10:45 HÜL 386

Receptor distribution in supported lipid bilayer upon binding of norovirus like particle — •NAGMA PARVEEN¹, DANIEL MIDTVEDT¹, VLADIMIR ZHDANOV¹, GUSTAF RYDELL², VESA HYTONEN³, and FREDRIK HÖÖK¹ — ¹Department of Physics, Chalmers University of Technology, Gothenburg, Sweden — ²Department of Infectious Diseases, Sahlgrenska Academy, University of Gothenburg, Gothenburg, Sweden — ³BioMediTech, University of Tampere, Biokatu 6, FI-33520 Tampere, Finland

Prior to internalization and infection, virions first bind to specific receptors present on the external lipid membrane of their host cells. This process is typically dynamic and multivalent, and known to influence the receptor distribution on the cell membrane and the shape of membranes, factors that are believed to be also crucial during the internalization process. To explore this, we have used fluorescently labeled histidine-tagged virus like particles (VLP) of norovirus and followed their binding to histo-blood group antigens (HBGAs) embedded in cell-membrane mimic, i.e. supported lipid bilayer (SLB). These HBGAs, e.g. Btype1 and Htype1 are known to be natural receptors of norovirus. Interestingly, we found that in case of Btype1 the VLPs bind in small clusters (1–2 μ m) whereas the binding is homogeneous to Htype1 indicating that Btype1 forms clusters in SLB upon VLP binding. The kinetics of VLP binding and cluster growth is detected using time-lapse total internal fluorescence microscopy. The cluster formation is further supported by a competitive binding assay using inhibitory lectin.

30 min break

BP 48.6 Thu 11:30 HÜL 386

Minimum-free-energy paths in membrane fusion: Coarse-grained molecular dynamics simulations — •YULIYA SMIRNOVA and MARCUS MÜLLER — Georg August University, Institute for Theoretical Physics, Göttingen, Germany

Collective phenomena in membranes such as fusion and fission involve reorganization of many molecules. Such transformations do not occur spontaneously but require the crossing of large (compared to $k_B T$) free energy barriers. Recent advances in free-energy calculation techniques, in particular, implementation of the so-called string method in MD simulations, allow us to study membrane transformations and calculate free energies along the transformation paths without a priori knowledge of the reaction coordinate. We focus on two initial stages of fusion: (1) bringing two membranes into close apposition and (2) forming an initial lipid connection (stalk) between the two apposed

bilayers. With help of the string method, we calculated the minimum free-energy paths of stalk formation between two apposed membranes as a function of membrane separation, lipid composition, and tension. Within the range of membrane separation distances, which allow formation of at least a metastable stalk structure, the free energy-barrier is not sensitive to the separation distance, however, the excess free-energy of the stalk decreases substantially with decreasing distance. Changing lipids to more fusogenic species or introducing tension does not change the free-energy barrier significantly. On the other hand, the free-energy contribution of bringing two membranes from large to small separation distance significantly decreases for more fusogenic lipids.

BP 48.7 Thu 11:45 HÜL 386

Lipid vesicle and SNARE-mediated membrane fusion studied by small-angle X-ray scattering — ●KARLO KOMOROWSKI^{1,2}, ANALENA SALDITT¹, YIHUI XU¹, HALENUR YAVUZ², REINHARD JAHN², and TIM SALDITT¹ — ¹University of Göttingen, Institute for X-Ray Physics, Göttingen, Germany — ²Max-Planck-Institute for Biophysical Chemistry, Department of Neurobiology, Göttingen

Membrane fusion takes place in numerous physiological processes on the cellular and subcellular level as in the case of synaptic transmission. In order to release neurotransmitters into the synaptic cleft, fusion of synaptic vesicles with the presynaptic plasma membrane is mediated by the SNAREs synaptobrevin 2, syntaxin 1a and SNAP-25, initiating the merger by a zippering process of a four-helix bundle. Using mutants of synaptobrevin, a stable docking state between SNARE-liposomes can be arrested due to partial zippering of the SNARE complex. That way it is possible to overcome the short timescales in which the intermediates naturally occur. The biochemically well controlled systems are then suitable for steady state small-angle X-ray scattering (SAXS) experiments. Here we aim at the structure of the intermediates of the SNARE-mediated liposome fusion pathway, which can be partly arrested. In addition, we have performed protein-free vesicle fusion studies, aiming at an understanding of the role of inter-membrane potentials in docking and in fusion. Finally, we propose to enhance SAXS studies of vesicles by microfluidic sample environments, which allow the monitoring of different steps along the fusion pathway. In order to obtain structural parameters from the SAXS data, we make use of form and structure factor models of lipid bilayers.

BP 48.8 Thu 12:00 HÜL 386

Scattering Study on Small Unilamellar DMPC-Vesicles Incorporating the Saponin Escin — ●CARINA DARGEL¹, RAMSIA SREIJ¹, AUREL RADULESCU², and THOMAS HELLEWEG¹ — ¹Physical and Biophysical Chemistry, Bielefeld University, Germany — ²Jülich Center for Neutron Science, outstation at FRM II, Garching, Germany

1,2-Dimyristoyl-sn-glycero-3-phosphocholine (DMPC) belongs to the class of phospholipids and acts i.a. as a major membrane component. Therefore, model membranes consisting of DMPC mimic biological membranes quite well and allow to study effects of additives under different conditions, e.g. composition and temperature. Saponins are plant derived surfactants which occur among others in nuts and garlic and exhibit an amphiphilic structure built of a hydrophobic steroidal or triterpenic backbone with a varying number of hydrophilic sugar chains. The interaction of saponins with biological membranes is not yet scrutinized. Therefore in this study the effect of the pure saponin escin on small unilamellar vesicles of DMPC, prepared by extrusion, is investigated mainly by different scattering methods in dependence on the escin-amount and the temperature. An incorporation of escin above a critical amount can be deduced from the investigated parameters, namely the thermal phase transition temperature and vesicle size parameters like the radius, membrane thickness and lipid head-to-head distance within one monolayer.

BP 48.9 Thu 12:15 HÜL 386

Hydrodynamic interactions nearby elastic cell membranes — ●ABDALLAH DADDI-MOUSSA-IDER, ACHIM GUCKENBERGER, and STEPHAN GEKLE — Biofluid Simulation and Modeling, Universität

Bayreuth, Universitätsstraße 30, Bayreuth 95440, Germany

We present an analytical calculation of the hydrodynamic interaction between two spherical particles moving nearby an elastic cell whose membrane is endowed with a resistance towards shearing and bending. The theory predicts the frequency-dependent self- and pair-mobility functions up to the fifth order of the ratio between particle radius and membrane distance as well as between radius and interparticle distance. We find that the steady motion of two particles towards a planar elastic membrane possessing only shearing resistance leads to attractive interaction in contrast to the hard-wall case where the interaction is known to be repulsive. We further compute the mobility function of a particle moving perpendicular to the surface of a spherical capsule, finding that membrane curvature leads to the appearance of a prominent additional peak in the mobility caused by shear resistance. In the vanishing frequency limit, the particle mobility near a no-slip hard-sphere is recovered only when the membrane possesses a non-vanishing resistance towards shearing. Our analytical predictions are compared with boundary-integral simulations where an excellent agreement is obtained.

Reference

Daddi-Moussa-Ider, A. and Gekle, S., J. Chem. Phys., 145, 014905 (2016)

BP 48.10 Thu 12:30 HÜL 386

Optically active, self-assembled solid-state nanopores for single particle detection — ●ANDREAS SCHLEGEL, PAUL V. GWOZDZ, CHRISTIAN HEYN, WOLFGANG HANSEN, and ROBERT H. BLICK — Institute of Nanostructure and Solid State Physics and Center for Hybrid Nanostructures (CHyN), University of Hamburg, Germany

Nanopores (NPs) are crucial components for single molecule detection setups. So far, NPs are used in DC i.e. for ionic blockage current measurements. Typically those DC measurements lack parallelity for high throughput. To address this, attempts using optically active NPs have been made.

In contrast to existing solid-state NP (SNP) experiments, we present an approach to use an SNP system which is inherently self-assembled and provides scalable pore diameters. These MBE-grown III-V SNPs are contained in a GaAs membrane. Furthermore, the SNPs in our system show photoluminescence and are potentially optically active due to the quantum confined Stark effect. This will be used for DNA sequencing in the future [1].

We introduce a procedure to transfer the membranes from its wafer substrate onto a transparent polymer. The membranes shall be suspended to use the embedded SNPs in a setup which combines DC with optical read-out.

[1] P. V. Gwozdz et. al., Appl. Phys. Lett. **109**, 223103 (2016)

BP 48.11 Thu 12:45 HÜL 386

Adhesion ability of angiotensin II with model membranes — JULIA PREU¹, LOUIS TIEFENAUER², and ●THOMAS GUTBERLET³ — ¹Department of Molecular Membrane Biology, Max-Planck-Institute of Biophysics, Frankfurt, Germany — ²Laboratory of Biomolecular Research, Paul Scherrer Institut, Villigen PSI, Switzerland — ³Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Forschungszentrum Jülich GmbH, Garching, Germany

The octa-peptide angiotensin II (Ang II, (H₂N-Asp*Arg*Val*Tyr*Ile*His*Pro*Phe*COOH)) is one of the key player on blood pressure regulation in mammals. Predominantly binding to the Angiotensin type 1 and 2 receptors, the hormone is one of several peptide ligands binding to G protein coupled receptors (GPCR). The chemical nature of the amino acid sequence has an impact on the behavior in the proximity of membranes, demonstrated using different membrane model systems and biophysical methods. Applying electrochemical impedance spectroscopy and small angle x-ray scattering a detailed view on the adhesion of the peptide with model membrane surfaces was performed. The role of specific amino acids involved in the interaction with the phospholipid head group were investigated and, studying a truncated version of Ang II, Ang (1-7), the key role of the C-terminal phenylalanine was proven.

BP 49: Physics of the Genesis of Life - Focus Session organized by Moritz Kreysing and Dieter Braun

Time: Thursday 9:30–13:00

Location: SCH A251

Invited Talk

BP 49.1 Thu 9:30 SCH A251

The Origin of Cellular Life — ●JACK W SZOSTAK — Dept. of Molecular Biology, Massachusetts General Hospital, Boston, MA 02115 USA

The earliest living cells must have had very simple structures in order to emerge spontaneously from the chemistry and physics of the early earth. We are attempting to synthesize such simple artificial cells in order to discover plausible pathways for the transition from chemistry to biology. Very primitive cells may have consisted of a self-replicating nucleic acid genome, encapsulated by a self-replicating cell membrane. We have described robust pathways for the coupled growth and division of primitive cell membranes composed of fatty acids, which were likely to have been available prebiotically. However, no process for the replication of a nucleic acid genome, independent of evolved enzymatic machinery, has yet been described. I will discuss our recent progress towards the realization of an efficient and accurate system for the chemical replication of RNA. I will also discuss physical constraints on the replication of RNA, and the implications of these constraints for efforts to deduce potential environments that could have nurtured the beginnings of life.

BP 49.2 Thu 10:00 SCH A251

Exploring the emergence of function in microfluidic droplets — ●REBECCA TURK MACLEOD¹, ANDREW GRIFFITHS², and LEROY CRONIN¹ — ¹University of Glasgow, Glasgow, UK — ²ESPCI, Paris, France

Metabolism-first theories on the origin of life suggest that there may have been prebiotic systems capable of propagation and Darwinian evolution that were not dependent on nucleotide-based replication. We are testing this idea by observing proposed prebiotic reactions compartmentalized in protocell analogues. Using microfluidics, we generate water-in-oil emulsions that contain prebiotic reactants and/or products, and subsequently observe the behavior of the droplets as a function of their chemistry. Compartmentalized carbohydrate products of the formose reaction affect the osmotic pressure of the droplets, thus driving the droplets to grow at the expense of formaldehyde-containing neighbors. Furthermore, a minority population of efficient formose reaction droplets (those with rates enhanced by reaction products) grow at the expense of less-efficient formose droplets.

This phenomenon of growth correlated with chemical complexity may present a means of selection for metabolizing protocells. Accordingly, we are utilizing the automated chemo-robotic tools developed by the Cronin lab to test the progress and evolution of other prebiotic chemistries compartmentalized in water-in-oil emulsions.

BP 49.3 Thu 10:15 SCH A251

Robustness in supramolecular assemblies far-from-equilibrium — ●JOB BOEKHOVEN, MARTA TENA-SOLSONA, BENEDIKT RIESS, and RAPHAEL GRÖTSCH — TUM, Chemistry Department, Garching, Germany

We will describe supramolecular assemblies that can only exist far-from-equilibrium driven by a chemical reaction network. As a result of their dissipative nature these assemblies are intrinsically unstable and can only be sustained by constant consumption of energy. We found that these assemblies can exert feedback on the reaction network that drives their own formation or degradation. This feedback can increase the robustness of the assemblies, and thus increase the survival time of the structures, compared to assemblies without this feedback. With this minimalist approach, we aim to study how typically life-like features, like robustness, oscillatory behavior and self-replication can emerge from simple, non-biological components.

BP 49.4 Thu 10:30 SCH A251

Could dividing active droplets provide a model for protocells? — ●RABEA SEYBOLDT¹, DAVID ZWICKER^{1,2}, CHRISTOPH A. WEBER^{1,2}, ANTHONY A. HYMAN³, and FRANK JÜLICHER¹ — ¹Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ²School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA — ³Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

Macromolecular aggregation and phase separation into droplets has been proposed as a mechanism to organize chemical reactions that could have been a key precursors at the origins of the first living cells. However, it remains unclear how early protocells could have proliferated and divided. Deformed droplets usually relax towards a spherical shape and do not easily divide. Our theoretical study shows that in the presence of chemical reactions that produce droplet material, a chemically active droplet may undergo a shape instability and subsequently divide into two daughter droplets, which may then grow and divide again. We also find that when considering the effects of hydrodynamics which tend to stabilize spherical droplets, the shape instability can still occur for sufficiently small droplets. Our work suggests that chemically active droplets that divide and propagate could serve as a model for prebiotic protocells.

BP 49.5 Thu 10:45 SCH A251

Thermally driven DNA phase transitions and protein expression — ●CHRISTOF B. MAST¹, MARA L. HEINLEIN¹, MATTHIAS MORASCH¹, NOEL YEH MARTIN², SHEREF MANSY², HANNES MUTSCHLER³, and DIETER BRAUN¹ — ¹LMU Munich, Amalienstrasse 54, 80799 München, Germany — ²University of Trento, Via Sommarive 9, 38123 Povo TN, Italy — ³Max Planck Institute of Biochemistry, Am Klopferspitz 18, 82152 Martinsried, Germany

Energy fluxes are the driving forces that push complex systems out of equilibrium into the living state. While modern organisms predominantly use chemical energy fluxes, we argue that the fundamental flux of heat energy across water filled pores was essential to jump start life four billion years ago: A thermal gradient drives thermal fluid convection and thermophoresis of bio-molecules, resulting in their massive and length selective accumulation. We demonstrate that this process is also selective for sequence and chirality which is essential for the emergence of the first functional, homochiral polymers. Starting from nanomolar concentrations of short and unbound single stranded DNA with a length of 36 bases, thermal trapping cooperatively increases their local concentration and length by hybridization, ultimately leading to the formation of a DNA hydrogel. Single mutations in sequence as well as strands of different chirality are spatially separated and therefore locally amplified during the hydrogel phase transition. We also show that thermal traps are compatible and enhance cell free protein expression, possibly mimicking a later stage during the origin of life.

15 min break

BP 49.6 Thu 11:15 SCH A251

Eutectic phase of water-ice as medium for the early RNA world — ●HANNES MUTSCHLER¹ and PHIL HOLLIGER² — ¹Max Planck Institute for Biochemistry, Martinsried, Germany — ²MRC Laboratory of Molecular Biology, Cambridge, UK

There is strong evidence for a primordial biology, in which RNA was the central biomolecule responsible information storage and catalysis. One of the key questions of this "RNA world" hypothesis is: Which environment might have been sufficiently benign to allow formation and evolution of inherently instable RNA molecules creating ever more complex catalysts including self-replicating ribozymes? We investigate the crowding environment of the eutectic phase of water-ice as a potential medium hosting the early RNA world. We found that eutectic conditions allow derivatives of primitive, naturally occurring ribozymes to efficiently catalyse entropically disfavoured RNA polymerisation and ligation reactions using only very weakly activated but credible building blocks as substrate. We also find that cyclic freeze-thaw cycling is a potent driver of RNA assembly and critical to unlocking the full functional potential of short RNA ligase modules through an unanticipated RNA chaperone effect.

BP 49.7 Thu 11:30 SCH A251

Temperature gradients assemble RNA rich protocells — ●JUAN M. IGLESIAS ARTOLA and MORITZ KREYSING — Max Planck Institute of Cell Biology and Genetics, Dresden, Germany

We now know that the several components of life (i.e. peptides, nucleic acids and lipids) were plausibly available at an early stage of Earth's

history [1]. However, concentration and selection of these biomolecules still eludes a fulfilling answer. In general, how could scarce functional biomolecules find each other in order to build in complexity? Temperature gradients as available at hydrothermal vent pores, and elsewhere, have already been shown to be a suitable setting to address these questions. These environments have previously been shown to accumulate nucleic acids and exert a selective pressure on sequence length, promoting molecular complexity [2]. Here we show that by using such an out of equilibrium environment we are able to form protocells from a dilute solution of peptides and functional RNA, and that these microdroplets are able to sustain RNA enzymatic activity. The observation that these temperature gradients also enhance micro-droplet formation opens a new set of possibilities. Within protocells even higher concentrations are possible, as known to be important for ribozyme activity. Moreover, these liquid micro-droplets could be the basis for competitive growth and selection at the protocellular level.

[1]. P. B. H. Patel, et al. *Nat. Chem* 7, (2015) [2] M. Kreysing, et al. *Nat. Chem* 7, 203 (2015) [3] T. Z. Jia, et al. *Nat. Chem* 8, 915 (2016)

BP 49.8 Thu 11:45 SCH A251

ATP as a Biological Hydrotrope — ●AVINASH PATEL¹, LILIANA MALINOVSKA¹, SIMON ALBERTI¹, YAMUNA KRISHNAN², and ANTHONY A HYMAN¹ — ¹Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany — ²Department of Chemistry and Grossman Institute for Neuroscience, Quantitative Biology and Human Behavior, University of Chicago, Illinois-60637

Hydrotropes are small molecules that solubilize hydrophobic molecules in aqueous solutions. Typically, hydrotropes are amphiphilic molecules and differ from classical surfactants in that they have low cooperativity of aggregation and work at molar concentrations. We discovered that ATP has properties of a biological hydrotrope. It can both prevent the formation of and dissolve previously formed protein aggregates. This chemical property is manifested at physiological concentrations between 5 to 10 millimolar. Therefore, in addition to being an energy source for biological reactions, for which micromolar concentrations are sufficient, we propose millimolar concentrations of ATP may act as a biological hydrotrope, preventing proteins from aggregating. This may in part explain why ATP is maintained in such high concentrations in cells. During origin of life, we hypothesize the role of ATP as a biological hydrotrope might have been an advantage for its selection by enzymes as an energy source.

BP 49.9 Thu 12:00 SCH A251

Origin of a folded repeat protein from an intrinsically disordered ancestor — ●HONGBO ZHU, EDGARDO SEPULVEDA, MARCUS D HARTMANN, MANJUNATHA KOGENARU, REINHARD ALBRECHT, JÖRG MARTIN, and ANDREI N LUPAS — Max Planck Institute for Developmental Biology, Tuebingen, Germany

Life today depends entirely on proteins as catalysts, but this activity is dependent on the formation of defined three-dimensional structures (folding). As only few randomly synthesized polypeptide chains have a folded structure, folding was clearly a major obstacle in the evolution of DNA-protein-based lifeforms from simpler precursor forms. We have proposed that folded proteins resulted from the increasing complexity of a preselected, ancestral set of peptides, which supported RNA-based life and required the RNA to assume their active conformation. A dominant mechanism to increase complexity is repetition and we have attempted to recreate experimentally the path from an unstructured precursor to a folded protein by amplification. Specifically we used a fragment of the putatively ancient ribosomal protein S20 (RPS20), which is only structured in the context of the ribosomal RNA, to generate a wide-spread fold in living organisms today, the TPR fold. After computational optimization of the fragment, we obtained a native-like TPR fold with 2-5 point mutations, which were neutral in the parent organism, suggesting that they could have been sampled in the course of evolution. TPRs could thus have plausibly arisen by amplification from an ancestral peptide.

BP 49.10 Thu 12:15 SCH A251

Spontaneous emergence of chemical oscillation of oligomers in a primordial broth — ●SABRINA SCHERER¹, EVA WOLLRAB², VARUN GIRI¹, LUCA CODUTTI³, TERESA CARLOMAGNO³, and ALBRECHT OTT¹ — ¹Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — ²Laboratory of Microbial Morphogenesis and Growth, Institut Pasteur, Paris, France — ³Centre of Biomolecular Drug Research, Leibniz University, Hannover, Germany

We study the dynamics of a complex chemical system, driven by electric discharge that forms from a gas mixture of methane and ammonia in the presence of water. In the course of a running experiment, a hydrophobic organic layer emerges besides the hydrophilic aqueous phase and the gaseous phase that were initially present. The hydrophilic phase contains at least a few thousands of different molecules, primarily distributed in a range of 50 and 500Da. Using real-time mass spectrometry, we observe the spontaneous emergence and disappearance of oligomeric surfactants. Strong non-linearities are required for the observed aperiodic chemical oscillations. The phenomenon is robust against different gas compositions and concentrations, temperatures and many details of the experimental set-up. In contrast, NMR spectroscopy reveals overall high chemical variability that suggests strong non-linearities due to interdependent, sequential reaction steps. We find that oxidation, or doping with small amounts of an active broth can trigger the production of the oligomers. We suggest that surface active molecules perform phase transfer catalysis in the oil/water mixture and self-organize to a spontaneously emerging autocatalytic network.

BP 49.11 Thu 12:30 SCH A251

Divergent prebiotic synthesis of ribonucleotides — ●MATTHEW POWNER — UCL, London, UK

RNA is a leading candidate for the original informational biopolymer of life, however a common prebiotic pathways to both purine and pyrimidine ribonucleotides remain elusive. We recently described a prebiotically plausible synthesis of pyrimidine ribonucleotides, but both purine and pyrimidine nucleotides must be synthesised together to access an information rich biopolymer. A divergent strategy to synthesise pyrimidine and 8-oxo-purine ribonucleotides from prebiotic precursors will demonstrate for the first time generational parity between 8-oxo-purine and pyrimidine heterocycles, allowing stepwise synthesis with regiospecific, stereoselective glycosidation and simultaneous phosphorylation with stereochemical inversion to furnish the β -ribo-stereochemistry found in the biological nucleic acids.

BP 49.12 Thu 12:45 SCH A251

Driving the system out of equilibrium - a key to understand the formamide-based model of the origin of life — ●JUDIT ŠPONER — Institute of Biophysics, Academy of Sciences of the Czech Republic, Královopolská 135, 612 65 Brno, Czech Republic

Thermodynamic stability of prebiotic building blocks is generally considered to be one of the decisive factors controlling their accumulation in the prebiotic pool. On the other hand higher stability means lower reactivity. How to challenge this apparent paradox in prebiotic chemistry? A simple formamide-based origin model[1], I am going to outline in my talk, provides a tentative answer to this question. This model is based on a strongly non-equilibrium chemistry, in which the stepwise decrease of the temperature of the prebiotic environment drives those chemical transformations which could lead to more and more complex molecular entities. Thus, we suggest that each synthetic step took place at different temperatures, i.e. precursors that formed and accumulated at a higher temperature, become thermodynamically unstable and thus more reactive at a lower temperature.

[1] Šponer JE, Šponer J, Nováková O, Brabec V, Šedo O, Zdráhal Z, Costanzo G, Pino S, Saladino R, Di Mauro E. Emergence of the first catalytic oligonucleotides in a formamide-based origin scenario. *Chem. Eur. J.* 2016, 22:3572-3586 and Šponer JE, Šponer J, Di Mauro E. New evolutionary insights into the non-enzymatic origin of RNA oligomers. *Wiley Interdisciplinary Reviews: RNA* 2016: DOI: 10.1002/wrna.1400.

BP 50: Networks: From Topology to Dynamics I (Joint Session SOE/DY/BP)

Time: Thursday 9:30–13:00

Location: GÖR 226

BP 50.1 Thu 9:30 GÖR 226

Structure and dynamics of multiplex networks: beyond degree correlations — ●KAJ-KOLJA KLEINEBERG — Computational Social Science, ETH Zurich, Clausiusstrasse 50, CH-8092 Zurich, Switzerland

The organization of constituent network layers to multiplex networks has recently attracted a lot of attention. Here, we show empirical evidence for the existence of relations between the layers of real multiplex networks that go beyond degree correlations. These relations consist of correlations in hidden metric spaces that underlie the observed topology. We discuss the impact and applications of these relations for trans-layer link prediction, community detection, navigation, game theory, and especially for the robustness of multiplex networks against random failures and targeted attacks. We show that these relations lead to fundamentally new behaviors, which emphasizes the importance to consider organizational principles of multiplex networks beyond degree correlations in future research.

BP 50.2 Thu 10:00 GÖR 226

Large-deviation properties of the stochastic block model — ●STEPHAN ADOLF¹, TIAGO P. PEIXOTO², and ALEXANDER K. HARTMANN¹ — ¹Institut of Physics, University of Oldenburg — ²Department of Mathematical Sciences, University of Bath

In this contribution we study the distribution of the size of the largest components for the stochastic block model. The stochastic block model is a generative model for graphs, which can be used to model social relationships [1, 2]. Suppose $N \in \mathbb{N}$ vertices which can be partitioned into at least two groups (also called blocks). For generating a graph in the stochastic block model ensemble one inserts edges between pairs of vertices with different probabilities depending on whether the vertices are in the same group or not [1]. To obtain the distribution of the size of the largest component over the full support we use a large-deviation method [3] to determine even small probabilities (like for example 10^{-100}). We compare the results to those obtained for Erdős-Rényi random graphs.

[1] A. Decelle and F. Krzakala and C. Moore and L. Zdeborová, Phys. Rev. E **84**, 066106 (2011)

[2] P.W. Holland and K.B. Laskey and S. Leinhardt, Social networks **5**, 109-137 (1983)

[3] A.K. Hartmann, Eur. Phys. J. B **84**, 627-634 (2011)

BP 50.3 Thu 10:15 GÖR 226

Improving Causal Gaussian Bayesian Network Inference using Parallel Tempering — ●PASCAL FIETH¹, GILLES MONNERET^{2,3}, ANDREA RAU³, FLORENCE JAFFRÉZIC³, ALEXANDER K. HARTMANN¹, and GREGORY NUEL² — ¹IFP, University of Oldenburg, Germany — ²LPMA, CNRS 7599, UPMC, Paris, France — ³GABI, INRA, Jouy-en-Josas, Paris, France

Gene regulatory networks describe causal relationships in biological processes like signal transduction or disease mechanisms. A considerable interest exists in supporting experimental network inference by developing computational methods to infer gene regulatory networks from available gene expression data.

To infer causality within those networks from mixed, observational and intervention, data, we make use of causal orderings and Gaussian Bayesian networks. An introduction to the necessary foundations is given. In the presented framework, for a given causal ordering, the likelihood of the model network can be maximized analytically. The space of causal orderings, growing as $n!$ for n genes, can be reliably explored via a simple Markov Chain Monte Carlo algorithm [1] for 10-20 genes only.

We show that parallel tempering helps in finding the orderings with highest maximum likelihood estimators as well as in exploring the set of alternative orderings with comparable maximum likelihood estimators for networks with > 50 genes.

[1] A. Rau, F. Jaffrézic, G. Nuel, BMC Sys. Biol., **7**(1):111 (2013)

BP 50.4 Thu 10:30 GÖR 226

Phase transition in detecting causal relationships from observational and interventional data — ●ALEXANDER K. HARTMANN¹ and GREGORY NUEL² — ¹Institut for Physics, University of Oldenburg, Germany — ²Laboratory of Probability and Stochastic Models

(LPMA), Université Pierre et Marie Curie, Paris, France

Analysing data of, e.g., gene-expression experiments, and modelling it via network-based approaches is one of the main data analysis tasks in modern science. If one is interested in modelling *correlations*, approaches like the inverse Ising model can be used, which is already algorithmically challenging. If one wants to analyse even *causal relationships*, i.e., beyond correlations, it becomes even harder.

One way out is to include interventions to the system, e.g., by knocking out genes when studying gene expression. This allows, in principle, to get a grip on the causal structure of a system. Here, we model the data using Gaussian Bayesian networks defined on directed acyclic graphs (DAGs). Our approach [1] allows for multiple interventions in each single experiment and calculating joint maximum likelihoods (MLs) for the complete network. Furthermore, we have to sample different causal orderings, which induce different DAGs. The sampling is efficient because we approximate the full ML by probabilities of orderings of triplets. This allows us to study the quality of the causality detection as a function of the fraction of interventional experiments. We observe an information phase transition between phases where the causal structure cannot be detected and where it can be detected.

[1] A. Rau, F. Jaffrézic, and G. Nuel, BMC Sys. Biol. **7**:111 (2013)

BP 50.5 Thu 10:45 GÖR 226

Surveillance for outbreak detection in livestock-trade networks — ●PHILIPP HÖVEL¹, FREDERIK SCHIRDEWAHN¹, ANDREAS KOHER¹, VITALY BELIK², HARTMUT H. K. LENTZ³, and VITTORIA COLIZZA⁴ — ¹TU Berlin — ²FU Berlin — ³Friedrich-Loeffler-Institut — ⁴INSERM Paris

We analyze a temporal network of livestock trade and present results of numerical simulations of epidemiological dynamics. The considered network is the backbone of the pig trade in Germany [1], which forms a major route of disease spreading between agricultural premises. The network is comprised of farms connected by a link, if animals are traded between them. We propose a concept for epidemic surveillance generally performed on a subset of the system due to limited resources. The goal is to identify agricultural holdings that are more likely to be infected during the early phase of an epidemic outbreak. These farms, which we call *sentinels* [2], are excellent candidates to monitor the whole network. To identify potential sentinel nodes, we determine most probable transmission routes by calculating functional clusters. These clusters are formed by nodes that have similar invasion paths. Then, we select sentinels by choosing nodes out of every cluster. We show that any epidemic outbreak can be reliably detected at an early stage by monitoring a small number of those sentinels.

[1] H. H. K. Lentz, A. Koher, P. Hövel, J. Gethmann, C. Sauter-Louis, T. Selhorst, and F. Conraths, PLoS ONE, **11**, e0155196 (2016).

[2] P. Bajardi, A. Barrat, L. Savini, V. Colizza, J. Roy. Soc. Interface **9**, 2814 (2012).

BP 50.6 Thu 11:00 GÖR 226

Outbreaks of interacting dynamics — ●FAKHTEH GHANBARNEJAD — Institut für Theoretische Physik, Technische Universität Berlin

Susceptible-Infective-Susceptible (SIS) and Susceptible-Infective-Recovered (SIR) are two successful idealized and simplified models for understanding the dynamics of infectious diseases. Nevertheless deadly records of some cases like tuberculosis during the 1918-1919 Spanish Flu and unexpected HIV cases in presence of hepatitis B and C, TB and Malaria, and vice versa, showed us that interaction between two spreading dynamics can dramatically change the epidemic dynamics. Here we investigate some microscopic mechanisms which might lead to the unexpected macroscopic outbreaks; In this work, we study spreading of two diseases: either cooperative or competitive interacting as a SIS or/and a SIR dynamics and address similarities and differences in comparison to other minimal cooperative models, i.e. SIR-SIR [1] and SIS-SIS [2]. We build up an idealized and simplified model and treat it in mean field approximations as well as stochastic agent based models. We find out in presence of cooperation an emerging region in the parameter space where the stable endemic and stable free-disease states co-exist. Interestingly this region appears differently in comparison to the SIR-SIR and SIS-SIS models. Also We track the dynamics on random generated networks; And argue how topological features can facilitate or neutralize the cooperation/competition effects.

[1] EPL 104 (2013) 50001; Nature Physics 11, 936-940 (2015); Rev. E 93, 042316. [2] arXiv:1603.09082v1.

15 min. break

BP 50.7 Thu 11:30 GÖR 226

Collective navigation of complex networks: Participatory greedy routing — ●KAJ-KOLJA KLEINEBERG and DIRK HELBING — Computational Social Science, ETH Zurich, Clausiusstrasse 50, CH-8092 Zurich, Switzerland

Many networks are used to transfer information or goods, in other words, they are navigated. The larger the network, the more difficult it is to navigate efficiently. Indeed, information routing in the Internet faces serious scalability problems due to its rapid growth, recently accelerated by the rise of the Internet of Things. Large networks like the Internet can be navigated efficiently if nodes, or agents, actively forward information based on hidden maps underlying these systems. However, in reality most agents will deny to forward messages, which has a cost, and navigation is impossible. Can we design appropriate incentives that lead to participation and global navigability? Here, we present an evolutionary game where agents share the value generated by successful delivery of information or goods. We show that global navigability can emerge, but its complete breakdown is possible as well. Furthermore, we show that the system tends to self-organize into local clusters of agents who participate in the navigation. This organizational principle can be exploited to favor the emergence of global navigability in the system.

BP 50.8 Thu 11:45 GÖR 226

Epidemic threshold in temporally-switching networks — LEO SPEIDEL¹, ●KONSTANTIN KLEMM^{2,3}, VICTOR M. EGUÍLUZ², and NAOKI MASUDA⁴ — ¹University of Oxford, UK — ²IFISC, Palma, Spain — ³Nazarbayev University, Astana, Kazakhstan — ⁴University of Bristol, UK

Data of physical contacts and face-to-face communications suggest temporally varying networks as the media on which infections take place among humans and animals. Epidemic processes on temporal networks are complicated by complexity of both network structure and temporal dimensions. We develop a theory to understand the susceptible-infected-susceptible epidemic model on arbitrary temporal networks, where each contact is used for a finite duration. We show that temporality of networks always lessens the epidemic threshold such that infections persist more easily in temporal networks than in their static counterparts [1]. The effect of temporality on the epidemic threshold, which depends on a data set, is approximately predicted by the magnitude of a commutator norm.

[1] Speidel, Klemm, Eguíluz & Masuda, New J Phys 18, 073013 (2016).

BP 50.9 Thu 12:00 GÖR 226

Correlations in sectoral value added growth in the global economic network — ●JULIAN MALUCK and REIK V. DONNER — Potsdam Institute for Climate Impact Research, Germany

Complex supply chains have resulted in increasing interconnectedness within the International Trade Network (ITN). In this context the question arises how industries adapt to changes in the demand and supply of their trading partners. We address this problem by empirically analyzing both positive and negative correlations of value added growth between industries and construct the World Economic Performance Network (WEPN). By comparing topological characteristics of the WEPN and the ITN we obtain insights into the interconnection between trade relations and correlations in economic performance. We observe that trade relations of higher orders are particularly important for assessing performance correlations on an international level. Our results contribute to a better understanding of the consequences from demand and supply changes within the ITN from a model-independent analysis.

BP 50.10 Thu 12:15 GÖR 226

Timescale of reaching stable state with relation to different ranking strategies in the stable marriage problem. — ●PIOTR NYCZKA — Jacobs University Bremen, Germany

Stable marriage problem is very well known topic. However there is still plenty of room for further investigation. In my presentation I will discuss process of reaching the stable state in the system consisting of two different types of agents.

Agents from two sets (eg. men and women) undergo random encounters and then decide whether they want to be together or not. They want to form a new couple only in the case where, as a result of this change, both of them will end up with "better" partner than actual one.

Each agent have its personal ranking list with "attractiveness" scores for potential partners of opposite sex and it's possible to make network out of these lists. In my presentation I will focus on relation between structure of this network, and timescale of process of reaching stable state. There is very strong and interesting relation between them, definitely worth of further investigation.

BP 50.11 Thu 12:30 GÖR 226

Identifying the driving processes of coupled friendship and enmity dynamics in a two-layer network model — ●MAXIMILIAN SADILEK¹ and STEFAN THURNER^{1,2,3} — ¹Section for Science of Complex Systems, Medical University of Vienna, Spitalgasse 23, A-1090, Austria — ²Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA — ³International Institute for Applied Systems Analysis, Schlossplatz 1, A-2361 Laxenburg, Austria

With the advent of social media it has become possible to study human social relations in a quantitative way. However, in most cases only data on positive relations (like friendship) are available while social balance theory states that in a social network positive and negative relations strongly depend on each other.

In the massive multiplayer online game PARDUS players can mark each other not only as friends but also as enemies, leading to a two-layer multiplex network structure.

We discuss the dynamics of friendship and enmity relations between thousands of players in PARDUS. We identify and quantify the driving processes of the associated two-layer social network formation. Well known sociological hypotheses like "The enemy of my enemy is my friend" turn out to be important building blocks of understanding the dynamics of the coupled formation of friendly and hostile interactions within a society.

BP 50.12 Thu 12:45 GÖR 226

Master Stability Functions reveal Turing Instabilities in Multi-layer Foodwebs — ANDREAS BRECHTEL², PHILIPP GRAMLICH², DANIEL RITTERSKAMP¹, BARBARA DROSSEL², and ●THILO GROSS¹ — ¹University of Bristol, UK — ²Technische Universität Darmstadt

Many systems in science and technology can be described as multilayer networks, which are known to exhibit phenomena such as catastrophic failure cascades and pattern-forming instabilities.

A particular class of multilayer networks describes systems where different interacting copies of a local network exist in different spatial locations, including for instance regulatory and metabolic networks of identical cells and interacting habitats of ecological populations.

Here, we show that such systems can be analyzed by a master stability function (MSF) approach, which reveals conditions for diffusion-driven instabilities (DDIs).

We demonstrate the methodology on the example of state-of-the-art meta-foodweb models, where it reveals diffusion-driven instabilities that lead to localized dynamics and spatial patterns.

This type of approach can be applied to a variety of systems from nature, science and engineering to aid the understanding and design of complex self-organizing systems.

BP 51: Microswimmers III (Joint Session BP/DY)

Time: Thursday 11:15–12:45

Location: ZEU 250

BP 51.1 Thu 11:15 ZEU 250

A single squirmer under gravity — ●FELIX RÜHLE and HOLGER STARK — Inst. für Theor. Physik, TU Berlin, 10623 Berlin

A simple yet versatile model for many microswimmers is the widely studied spherical squirmer [1]. In this contribution we include a gravitational force acting on a single swimmer. In experiments this setup has yielded fascinating non-equilibrium structure formation such as floating rafts formed by active emulsion droplets [2] or dancing *Volvox* algae [3]. While theoretical and numerical studies for microswimmers under gravity do exist [4,5], they usually do not account for full hydrodynamics, which need to be included in the presence of surfaces.

In our study we observe a rich phenomenology depending on gravitational strength and on squirmer type: Swimmers are caught at the wall or completely escape from its influence, or they float at a finite distance from the bottom wall, both permanently and recurrently. We reproduce and explain these findings, which we obtained in MPCD simulations, using analytical calculations, which include wall-induced linear and angular velocities in the near and far field [6].

[1] J. R. Blake, *J. Fluid Mech.* **46**, 199 (1971).

[2] C. Krüger et al., *EPJE* **39**, 64 (2016).

[3] K. Drescher et al., *Phys. Rev. Lett.* **102**, 168101 (2009).

[4] M. Enculescu and H. Stark, *Phys. Rev. Lett.* **107**, 058301 (2011);

K. Wolff, A. M. Hahn and H. Stark, *EPJE* **36**(4), 1 (2013).

[5] B. ten Hagen et al. *Nat. Comm.* **5**, 4829 (2014).

[6] J. S. Lintuvuori et al., *Soft Matter* **12**, 7959 (2016)

BP 51.2 Thu 11:30 ZEU 250

Chemotaxis in external fields: magnetotactic bacteria behavior — ●AGNESE CODUTTI¹, STEFAN KLUMPP², and DAMIEN FAIVRE¹ — ¹Max Planck Institute of Colloids and Interfaces, Research Campus Golm, 14476 Potsdam, Germany — ²Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Microswimmers such as bacteria, algae and artificial swimmers can be described with a three dimensional active brownian particle model. Here, we modify this simple model to better describe bacterial motility. First of all, different states of motion are included: the bacteria can run straight or actively change direction of motion through tumble or reverse. Second, chemotaxis is added to generate a bias towards the preferred concentration of some substance. Finally, the swimmer may be subject to external forces and torques. We show how this modified model can be applied to various scenarios, including the run and tumble chemotactic motion of *E. Coli* and the motion of magnetotactic bacteria in a magnetic field. Magnetotactic bacteria produce an intracellular chain of magnetic nanoparticles that acts like a compass and passively orients the bacterium in the external magnetic field of the earth. The orientation provides an advantage to the bacteria, since it improves chemotaxis. Therefore we explore the interaction between chemotaxis and an external magnetic field. We show that reversing is more advantageous than tumbling, when a magnetic torque is included.

BP 51.3 Thu 11:45 ZEU 250

A microscopic field theoretical approach for active systems — ●FRANCESCO ALAIMO^{1,2}, SIMON PRAETORIUS¹, and AXEL VOIGT^{1,2,3} — ¹Institut für Wissenschaftliches Rechnen, TU Dresden, Dresden, Germany — ²Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany — ³Center for Systems Biology Dresden (CSBD), Dresden, Germany

We consider a microscopic modeling approach for active systems. The approach extends the phase field crystal (PFC) model and allows us to describe generic properties of active systems within a continuum model. The approach is validated by reproducing results obtained with corresponding agent-based and microscopic phase field models. We consider binary collisions, collective motion and vortex formation. For larger numbers of particles we analyze the coarsening process in active crystals and identify giant number fluctuation in a cluster formation process.

BP 51.4 Thu 12:00 ZEU 250

Interface-Controlled Motility of Photoactive Microalgae in Confinement — ●TANYA OSTAPENKO, CHRISTIAN T. KREIS, and

OLIVER BÄUMCHEN — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

The natural habitats of many biological microorganisms include complex interfaces and varying environmental conditions. For flagellated microalgae swimming in an aqueous medium, we showed that the curvature of the compartment wall governs their motility in geometric confinement [1]. This curvature-guided motility results in long detention times towards highly curved interfaces. We determined this from the analysis of individual cell trajectories, the results of which are supported by simulations and analytics. For puller-type microswimmers, the precise nature of their flagella-surface interactions are important and remain debated to this day. We discovered that the flagella adhesiveness for photoactive microalgae can be controlled by light [2]. Here, we report on the swimming dynamics of single *Chlamydomonas* cells isolated in two-dimensional microfluidic chambers under different light conditions. We find that the cell's motility in confinement can be switched reversibly by light, which could be exploited for application in biological optical traps and wastewater decontamination. [1] T. Ostapenko, et al. (arXiv:1608.00363, 2016), [2] C. T. Kreis, et al. (in review, 2016).

BP 51.5 Thu 12:15 ZEU 250

Dynamics of spheroidal squirmers in Poiseuille flow — ●HEMALATHA ANNEPU, MARIO THEERS, GERHARD GOMPPER, and ROLAND G. WINKLER — Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, 52425 Jülich, Germany

Bacteria such as *E. coli* exhibit a remarkable rheological behavior. On the one hand, the viscosity exhibits a Newtonian plateau at low shear rates, which decreases with increasing concentration. On the other hand, the bacteria exhibit positive rheotaxis, i.e., they swim preferentially upstream next to surfaces. This points toward an intriguing interplay between the swimmer flow field with the surface. To analyze the properties of microswimmers in channel flows, we consider spheroidal squirmers with a rotlet dipole embedded in a MPC fluid and study their flow-induced structure and dynamics. The no-slip boundary condition at a surface combined with the swimmer characteristics (puller, pusher) leads to a preferential alignment parallel (pusher) or perpendicular (puller) to the wall. This applies to both, spherical as well as spheroidal squirmers as long as they are not too close to a surface and the hydrodynamics is determined by the far field. We want to shed light on the influence of near-field hydrodynamic interactions on the swimming behavior of spheroidal squirmers close to surfaces. Our simulations reveal a dependence of the swimming behavior under flow on the shape of the microswimmer. We find positive rheotaxis for spheroidal pushers in narrow channels, which disappears in the limit of zero rotlet dipole strength.

BP 51.6 Thu 12:30 ZEU 250

Interaction of 3D amoeboid swimmer with a wall — ●MOHD SUHAIL RIZVI, ALEXANDR FARUTIN, and CHAOQI MISBAH — Université Grenoble Alpes, LIPHY, CNRS, F-38000 Grenoble, France

Several micro-organisms and eukaryotic cells, including those of immune system, are known to migrate in fluids with the help of the appendages (flagella or cilia) or by deforming their body, known as amoeboid swimming. We performed a numerical study of the interaction of a three dimensional amoeboid swimmer with a plane boundary using boundary integral method. Expectedly, for purely hydrodynamic interactions, the swimmer nature is dependent on its separation and orientation relative to the wall but shows two contrasting behaviors as it either gets attracted towards the wall or moves away from it depending on its configuration. We identify the regions in the phase space associated with these two contrasting behaviors and demonstrate that the navigational motion of an amoeboid swimmer in a confined region observed in 2D also persist in 3D. In the presence of the adhesive interaction (modeled using Lennard-Jones potential) between swimmer and the wall along with hydrodynamic, the swimmer velocity demonstrates a non-monotonic relationship with the adhesion strength by demonstrating fastest migration at moderate adhesion and thus recapitulates experimental observations.

BP 52: Topological Problems in the Physics of Polymers, Biopolymers and Fibers I (Joint Focus Session CPP/BP)

Organisers: Raffaello Potestio (MPI Polymer Research, Mainz), Luca Tubiana (University of Vienna), Peter Virnau (Johannes Gutenberg Universität Mainz) and Rudolf Podgornik (University of Ljubljana)

The topological, or knotted, state of long chains influences their physical properties. Mechanical features of polymers and fibers, such as energy dissipation and tensile rupture, are known to be substantially affected by the presence and type of a knot. Entanglements have emerged as relevant players also in the realm of biophysics, as knots have been found in circular DNA as well as in proteins. In the last few decades a great effort has been put in the characterization of the properties of chains featuring a self-entangled topology. A large contribution has been provided in particular by computer simulations of knotted polymers, with a spectrum of different models and systems spanning from ideal chains to atomistic proteins and coarse-grained chromosomes. Furthermore, the advancement of experimental techniques has enabled researchers to construct, handle, and study physical knots, making possible a productive interplay between theory, computer modeling, and experimental validation. The scope of this focus session is to bring together scientists active in the multifaceted field of polymer topology, and foster the exchange of ideas among different areas. In particular, it is our aim to promote the interaction between two communities, polymer science and biophysics, that have insofar manifested a great collaborative potential.

Time: Thursday 15:00–18:00

Location: ZEU 260

Invited Talk

BP 52.1 Thu 15:00 ZEU 260

Polymers in the cell nucleus — ●MARIA BARBI, ANTONY LESAGE, and JEAN-MARC VICTOR — Laboratoire de physique Théorique de la Matière Condensée - UPMC - Paris VI - France

Understanding the genome functional architecture and its dynamics is one of the big challenges of systems biology. The three-dimensional arrangement, in the cell nucleus, of the protein-DNA assembly that constitutes chromosomes is expected to be crucial for the regulation of gene expression, hence cell differentiation and cell type setting. The rapid progress of experimental techniques begins to make it possible to explore these complex structures. I will show how, when used in connection with experimental results, polymer physics represents a powerful tool in deciphering the chromosome arrangement and dynamics.

BP 52.2 Thu 15:30 ZEU 260

Minimal surfaces on unconcatenated polymer rings in melt — ●JAN SMREK¹ and ALEXANDER GROSBERG² — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Center for Soft Matter Research and Department of Physics, New York University, New York, NY 10003, USA

In order to quantify the effect of mutual threading on conformations and dynamics of unconcatenated and unknotted rings in the melt we computationally examine their minimal surfaces. We found a linear scaling of the surface area with the ring length. Minimal surfaces allow for an unambiguous algorithmic definition of mutual threading between rings. Based on it, we found that although ring threading is very frequent, vast majority of cases correspond to very short loops. These findings explain why approximate theories which neglect threading in the description of static and dynamic properties of ring melts are so unexpectedly successful despite having no small parameter justification. We also examine threading dynamics, and identify the threading order parameter that reflects the slowdown of the ring diffusion.

BP 52.3 Thu 15:45 ZEU 260

Density effects in entangled solutions of linear and ring polymers — ●NEGAR NAHALI and ANGELO ROSA — SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste, Italy

We present here recent [1] findings from molecular dynamics computer simulations regarding the statics and dynamics of linear and circular (ring) polymer chains in entangled solutions of different densities.

While we confirm that linear chain conformations obey Gaussian statistics at all densities, rings tend to crumple becoming more and more compact as the density increases. Conversely, contact frequencies between chain monomers are shown to depend on solution density for both chain topologies.

The relaxation of chains at equilibrium is also shown to depend on topology, with ring polymers relaxing faster than their linear counterparts. Finally, we discuss the local viscoelastic properties of the

solutions by showing that the diffusion of dispersed colloid-like particles is markedly faster in the rings case [1,2].

[1] N. Nahali, A. Rosa, *Journal of Physics: Condensed Matter* 28, 065101 (2016)

[2] N. Nahali, A. Rosa, in preparation.

BP 52.4 Thu 16:00 ZEU 260

Slow diffusion of ring polymer melts originated from inter-ring threading — ●EUNSANG LEE^{1,2} and YOUNJOON JUNG¹ — ¹Department of Chemistry, Seoul National University, Seoul 08826, Korea — ²Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Halle 06120, Germany

Topological constraints of a ring, nonconcatation and unknotting, force the rings to be in a threading configuration, which is believed to be a main reason for abnormally slow diffusion observed in a melt phase. In this presentation, we provide results for the threading dynamics using molecular dynamics (MD) simulation based on a bead-spring model and Monte Carlo simulation on a kinetically constrained lattice gas model. Threading configuration between two molecules frequently observed in MD trajectories causes asymmetric dynamic state of two molecules and a set of such rules is implemented in the lattice model to describe the ring diffusion. Both models well describe long-time behavior of the ring diffusion strongly governed by a long-lasting molecular contact from threading configuration. An evidence for the glassy dynamics is also presented to support the ring melt belonging to a topological glass. From this work, we gain physical insights on the relation between molecular topology and its slow dynamics of ring polymer melts.

BP 52.5 Thu 16:15 ZEU 260

Topological Interactions in Dilute Polymer Solutions – Disentanglement of Two Single Chains — ●DIDDO DIDDENS¹, NAM-KYUNG LEE², SERGEI OBUKHOV³, JÖRG BASCHNAGEL¹, and ALBERT JOHNER¹ — ¹Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 23 Rue du Loess, 67034 Strasbourg Cedex 2, France — ²Institute of Fundamental Physics, Department of Physics, Sejong University, Seoul 05006, Korea — ³Department of Physics, University of Florida, P.O. Box 118440, Gainesville, Florida 32611-8440, United States

The non-crossing constraint of individual polymer chains is a well-known feature that explains several dynamical characteristics of dense polymer solutions or melts. However, the situation becomes less clear when dealing with an ensemble consisting of only a few long polymer chains that overlap, a scenario that is frequently encountered in *e.g.* biopolymer physics. To assess the impact of topological constraints in dilute polymer systems in a general manner, we devise a hypothetical experiment in which a long polymer chain is cleaved into two distinct halves that initially overlap, and study their subsequent disentanglement via Molecular Dynamics simulations [1]. We demonstrate that the non-crossing constraint significantly affects the separation dynam-

ics, and quantify the associated relaxation times in terms of the topological properties of the starting configuration from which the cleavage is initiated. Moreover, we rationalize our findings by analytical arguments.

[1] D. Diddens *et al.*, *ACS Macro Lett.*, **2016**, 5(6), 740-744

15 min break

Invited Talk

BP 52.6 Thu 16:45 ZEU 260

Knots as Stable Topological Order Parameter for Semiflexible Polymers — •WOLFHARD JANKE and MARTIN MARENZ — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We investigate the influence of bending stiffness on the conformational phases of a semiflexible bead-stick homopolymer and present the pseudo-phase diagram for the complete range of semiflexibility, from flexible to stiff. By varying the internal bending stiffness, the model exhibits different pseudo phases like bent, hairpin or toroidal. In particular, we find thermodynamically stable phases characterized by knots of specific topologies. The transitions into these “knotted” phases from other ordered phases are quite unusual in that they display clear phase coexistence but almost no change in the mean total energy and hence no latent heat. It will be explained how we arrive at these intriguing results by computer simulations based on a combination of the replica-exchange Monte Carlo algorithm and the multicanonical method and discussed how one can understand these effects by basic statistical physics reasoning.

M. Marenz and W. Janke, *Knots as a Topological Order Parameter for Semiflexible Polymers*, Phys. Rev. Lett. **116**, 128301 (2016).

M. Marenz and W. Janke, *Stable Knots in the Phase Diagram of Semiflexible Polymers: A Topological Order Parameter?*, J. Phys.: Conf. Ser. **750**, 012006 (2016).

BP 52.7 Thu 17:15 ZEU 260

An application of the Wang-Landau Monte Carlo method to the modeling of the thermal and mechanical behavior of knotted polymer rings in solutions — •FRANCO- FERRARI¹ and YANI ZHAO² — ¹CASA* and University of Szczecin, Szczecin, Poland — ²Centre of New Technologies, University of Warsaw, Warsaw, Poland

The subject of this seminar are the properties and behavior in solutions of single knotted polymer rings. These polymers are defined on a simple cubic lattice. Their statistical properties are investigated by computing the expectation values of a few observables, namely the specific energy, the specific heat capacity and the gyration radius. In the case in which the chain is stretched by a tensile force directed along the z-axis, the average height of the point in which the force has been applied is measured too. The averages are computed exploiting a variant of the Wang-Landau Monte Carlo method. The algorithm has been suitably accelerated and parallelized in such a way that it is possible to sample a large number (from tens to hundreds of billions) of knot conformations. Several types of knots have been considered,

including the trefoil, the figure-eight, the cinquefoil knots and many others. From the performed analysis it turns out that knotted polymer rings have a rich variety of different behaviors that can be used in order to tune the properties of polymer materials containing such knots. For instance, these polymers swell faster or slower when heated depending on the type of the knot and on the kind of interactions between the monomers. During the talk some interesting features of the stress relaxation of knotted polymer rings after the stretching force is removed will also be shown.

BP 52.8 Thu 17:30 ZEU 260

Geometry and topology of periodic filamentous structures — •MYFANWY EVANS — Mathematics Institute, TU Berlin, Berlin, Germany

High symmetry dense packings of trees and lines in the two-dimensional hyperbolic plane can be projected to triply-periodic minimal surfaces. The resulting three-dimensional structures are space-filling, symmetric and entangled structures composed of multiple networks or filaments, which challenge current characterisation techniques particularly from the perspective of entanglement. In this talk, I will discuss the construction and characterisation of these complex entangled structures alongside applications from star terpolymer self-assembly to skin swelling.

BP 52.9 Thu 17:45 ZEU 260

Three-Dimensional Nets from Hyperbolic Tilings — •BENEDIKT KOLBE — Technische Universität Berlin

A main focus of modern crystallography is to explore the systematic enumeration and construction of nets in Euclidean space. The EPINET project attempts to enumerate crystalline frameworks that arise as structures derived from hyperbolic tilings. Since hyperbolic geometry represents the most prevalent class of geometry not only in nature as a model of the geometry of minimal surfaces, but also mathematically, the use of hyperbolic surfaces to construct possible structures in 3-space is very natural. Among many others, this recipe has also led to deep results in topology from Thurston and others and is also used in modern descriptions of conformal field theory.

We focus on the study of those networks that one encounters typically in the material sciences-periodic structures. Therefore, to classify the emerging structures we employ Delaney Dress combinatorial tiling theory.

We will explain some of the mathematics and intuition involved in a new approach to enumerating the 3-dimensional structures that arise through hyperbolic tilings and give some results on the knotted networks they represent. This work is aimed at generalizing Delaney-Dress tiling theory and to develop a complexity ordering of different tilings.

The most prominent triply periodic minimal surfaces are used to illustrate the approach and provide first examples. The goal of this project is to ultimately construct systematically and order by complexity all networks that arise by decorations of hyperbolic surfaces.

BP 53: Pattern Formation (Joint Session DY/BP)

Time: Thursday 15:00–17:00

Location: ZEU 118

BP 53.1 Thu 15:00 ZEU 118

Flow Induced Instabilities in an Advected Dictyostelium Discoideum Model — •ESTEFANIA VIDAL, AZAM GHOLAMI, and EBERHARD BODENSCHATZ — Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077 Göttingen, Germany

The spirals and concentric waves of cAMP appearing during the aggregation process of the social amoeba Dictyostelium Discoideum have been widely studied as an example of pattern formation in biological systems, however in the rain forest soil, the natural environment of these amoebas, the constant rain washes away the signalling chemical, thus affecting the pattern formation. To simulate these environmental conditions, we studied numerically and theoretically a Reaction Diffusion model in the presence of a constant flow advection. The model, proposed by Martiel and Goldbeter, describes the dynamics of cAMP by taking its concentration as an activator and the ratio of active receptors in the cell membrane as inhibitor. Depending on the election of parameters this system can be in an oscillatory or an excitable state, and has successfully reproduce many of the experimentally observed

features. We show how a Dirichlet boundary condition destabilises the system, creating a continuous influx of waves upstream which grow into train waves that fill the entire system. These phenomena, which appear due to the interaction between the Flow Induced Instability and a Hopf Bifurcation provide a novel mechanism for the creation of continuous waves in Advected Reaction Diffusion systems.

BP 53.2 Thu 15:15 ZEU 118

Localized structures in the Kuramoto-Sivashinsky-Verhulst equation in context of ion-beam eroded surfaces — •CHRISTOPH KABELITZ and STEFAN JAKOB LINZ — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

Pattern formation of ion-beam eroded semiconductor surfaces has received considerable attraction because of the variety of structures (from flat, rough up to periodically arranged on large scales) being experimentally observed. Besides that, also large area localized hexagonal dot patterns have been experimentally detected [1]. Using a numerically manageable extended Kuramoto-Sivashinsky equation that mod-

els the dynamics of the surface morphology of the combined erosion and redeposition processes [2, 3], such localized hexagonal structures are identified, the existence range in the parameter space is determined and the rather involved scenarios of the creation and annihilation of these structures are classified and clarified.

[1] T. Allmers, M. Donath and G. Rangelov, J. Vac. Sci. Technol. B 24, 582 (2006). [2] C. Diddens and S. J. Linz, Europhys. Lett. 104, 17010 (2013). [3] C. Diddens and S. J. Linz, Eur. Phys. J. B 88, 190 (2015).

BP 53.3 Thu 15:30 ZEU 118

Surface instabilities in vibrating thin fluid films — ●SEBASTIAN RICHTER¹ and MICHAEL BESTEHORN² — ¹Department of Theoretical Physics, BTU, 03044, Cottbus, Germany — ²Department of Theoretical Physics, BTU, 03044, Cottbus, Germany

We investigate the spatio-temporal evolution of a thin fluid layer, which is located on a horizontal, solid substrate and is either subjected to a constant or to a time-periodic gravitational force field in normal direction. Starting with an appropriate initial state, the behavior of the liquid is simulated numerically considering both the exact problem and a long wave lubrication approximation based model obtained from the incompressible Navier-Stokes equations. The model includes inertia and viscous friction. For the case of a periodic external force, we observe the formation of time-periodic surface waves (Faraday instabilities) if the frequency and amplitude of excitation meet certain critical values. A Floquet analysis is made to determine the exact stability criteria of the linearized system. Both approaches show good agreement in the limit of a thin fluid geometry: Harmonic excitations generate patterns oscillating harmonically with the driver's frequency (ω) for low frequency ranges and subharmonically ($\omega/2$) at higher frequencies.

BP 53.4 Thu 15:45 ZEU 118

Control of competing patterns in anti-symmetrically coupled Swift-Hohenberg equations — ●MAXIMILIAN BECKER¹, SINA REICHEL², THOMAS NIEDERMAYER¹, THOMAS FRENZEL², ALEXANDER MIELKE², and MARKUS BÄR¹ — ¹Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — ²Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS), Berlin, Germany

The Swift-Hohenberg equation (SHE) provides a generic formulation for non-equilibrium pattern formation at a characteristic length scale. We present analytical and numerical investigations of two anti-symmetrically coupled 1d SHEs with cubic nonlinearities. A linear stability analysis of the homogeneous state reveals a wave instability in addition to the Turing instability of uncoupled SHEs. Weakly nonlinear analysis has been performed in the vicinity of the codimension-2-point of the Turing-wave instability, resulting in a set of coupled amplitude equations for Turing patterns and left- and right-traveling waves. In particular, these complex Ginzburg-Landau-type equations predict a mutual suppression of the amplitudes. In consequence, different patterns can coexist in distinct spatial regions, separated by localized interfaces. We identified specific control mechanisms for these interfaces which allow for global pattern selection. Extensive simulations of the underlying SHEs confirm our results.

BP 53.5 Thu 16:00 ZEU 118

Modeling collective motion and pattern formation of self-propelled rods and application to myxobacteria — ROBERT GROSSMANN^{1,2}, FERNANDO PERUANI¹, and ●MARKUS BÄR² — ¹Universite de Nice, France — ²Physikalisch-Technische Bundesanstalt, Germany

We study self-propelled particles with nematic velocity-alignment in two dimensions, which reverse their direction of motion repeatedly. The large-scale properties of these point-like self-propelled rods are analyzed within a hydrodynamic theory that can be systematically derived from the microscopic dynamics. Combining analytical methods and numerical continuation, we show that an entire family of elongated high-density regions, called bands, self-segregates spontaneously from a homogeneous background via two subcritical bifurcations. The reduction of the multi-particle system onto the dynamics of bands provides a unified framework to understand aggregation mechanisms and nonequilibrium phase separation in active systems with nematic velocity-alignment, e. g. the collective dynamics of rod-shaped, ac-

tively moving myxobacteria. R. Großmann, F. Peruani, and M. Bär, Phys. Rev. E 94, 050602 (2016).

BP 53.6 Thu 16:15 ZEU 118

Pattern formation in polymerizing actin flocks — ●THOMAS LE GOFF, BENNO LIEBCHEN, and DAVIDE MARENDUZZO — School of Physics and Astronomy, University of Edinburgh, UK

F-Actin is a polymer existing in the cytoskeleton of cells and which is involved in cell motility, cell division or cell signaling. These polymers form a network which can exhibit very interesting dynamics. Particularly, actin waves usually following formation of spots were observed experimentally [1].

We propose a simple physical model based on a minimum number of ingredients to describe the appearance of these waves : (i) treadmilling - i.e. the simultaneous growth and shrinkage at the two ends of the actin fiber, (ii) polymerisation and (iii) a nematic interaction term causing fiber alignment for large concentration of F-actin. With this simple model we obtain very rich dynamics, in particular we can observe formation of spots, spirals and waves resembling the dynamics seen experimentally. Our model also allows us to make definite predictions on the mechanism underlying wave formation in vivo.

[1] T. Bretschneider, K. Anderson, M. Ecker, A. Müller-Taubenberger, B. Schroth-Diez, H. C. Ishikawa-Ankerhold, G. Gerisch, Biophys. J. 96, 2888 (2009).

BP 53.7 Thu 16:30 ZEU 118

Size matters for Nonlinear Waves and Min Protein Patterns — ●FABIAN BERGMANN, LISA RAPP, and WALTER ZIMMERMANN — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

Self-organization is a fundamental strategy in nature. In *E. coli* bacteria, for example, self-organized pole-to-pole oscillations of the Min proteins have an important function within the cell division machinery. Such pole-to-pole oscillations in living cells behave like standing waves (SW) in very small (confined) systems. In extended in vitro experiments, Min oscillations develop into nonlinear traveling waves (TW). TW patterns are also known from many other nonequilibrium systems. But is the transition from traveling waves in extended to standing waves in strongly confined systems a specific property of the Min oscillation pattern? Or is it a generic and robust universal principle of all nonlinear traveling waves that just also applies to the Min oscillations in cells?

We address this central question by imposing strong spatial confinement to a generic model for nonlinear traveling waves. Using simulations, analytical and symmetry considerations, we conclude that traveling waves inevitably change into standing waves in sufficiently small confined systems.

BP 53.8 Thu 16:45 ZEU 118

Traveling Waves in Conserved Systems — ●LISA RAPP, FABIAN BERGMANN, MARKUS HILT, and WALTER ZIMMERMANN — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Deutschland

Nonlinear traveling waves are one of the elementary prototype patterns that occur in various systems in nature far from thermal equilibrium. So far, their behavior has mostly been investigated in systems with an unconserved order parameter. In contrast, in systems with conserved order parameter, the Hopf-bifurcation to traveling waves is nearly unexplored (except for a first approach in Ref. [1]). The effects of conservation laws, however, may play a significant role in many pattern forming systems such as the Min protein oscillations during cell division in *E. coli* bacteria.

In spatially extended conserved systems, there are two distinctly different Hopf-bifurcations from a homogeneous basic state to traveling waves. On the one hand, the transition can occur via a finite wavenumber instability, similar to convection systems. On the other hand, the basic state can also become unstable towards long wavelength modes, comparable to the non-oscillatory Cahn-Hilliard model for potential systems.

We introduce a generalized Swift-Hohenberg model for conserved systems that includes both scenarios as special cases. Exploring this model and its limiting cases, we find interesting types of coarsening behavior and spatio-temporal complexity.

[1] W. Zimmermann, Physica A **237**, 575 (1997).

BP 54: Statistical Physics of Biological Systems I (Joint Session BP/DY)

Time: Thursday 15:00–17:30

Location: ZEU 250

BP 54.1 Thu 15:00 ZEU 250

Inference of chemotactic strategies of *E. coli* and *Pseudomonas putida* using Kramers-Moyal coefficients — ●MAXIMILIAN SEYRICH¹, OLIVER POHL¹, MARIUS HINTSCHE², ZAHRA ALIREZAEI², CARSTEN BETA², and HOLGER STARK¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — ²Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam, Germany

Bacteria like *E. coli* and *Pseudomonas putida* move with alternating runs and tumbles that occur with a mean tumble rate. In the presence of gradients of a chemoattractant, they both perform chemotaxis. We set up a random-walk model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed. The dynamics include rotational Brownian motion and shot noise for the swimming direction to initiate tumbling, while thermal and shot noise together with a mean reverting drift-term analogously to an Ornstein-Uhlenbeck process governs the speed dynamics. In order to infer the parameters of our model, generalized Kramers-Moyal coefficients are calculated for our model and matched to the ones determined from experimental trajectories. In contrast to common tumbling recognition algorithms no free parameters need to be preset. We first show that our method identifies the classical bacterial chemotaxis strategy of *E. coli* and *P. putida*, i.e., the tumble rate decreases along the chemical gradient. We also find evidence that a subpopulation of *E. coli* reduces its mean tumble angle when swimming in this direction.

BP 54.2 Thu 15:15 ZEU 250

Genotypic complexity of Fisher's geometric model — SUNG-MIN HWANG¹, SU-CHAN PARK², and ●JOACHIM KRUG¹ — ¹Institute for Theoretical Physics, University of Cologne, Cologne, Germany — ²Department of Physics, The Catholic University of Korea, Bucheon, Republic of Korea

Biological evolution can be conceptualized as a dynamical process in the space of gene sequences guided by the fitness landscape, a mapping that assigns a measure of reproductive value to each genotype [1]. The relationship between genotype and fitness is generally complex, as it is mediated by the multidimensional organismic phenotype that interacts with the environment and thereby determines reproductive success. A simple mathematical framework for exploring this relationship is provided by Fisher's geometric model, which describes the phenotype as a vector in an n -dimensional Euclidean trait space with a unique optimum located at the origin [2]. Genetic mutations are encoded as random phenotypic displacements, and complex fitness landscapes arise from the projection of the discrete network of genotypes onto the continuous trait space. The talk will discuss the properties of these fitness landscapes from the viewpoint of statistical physics, focusing in particular on the exponential growth of the number of local fitness peaks as a measure of genotypic complexity.

[1] J.A.G.M. de Visser, J. Krug, Nat. Rev. Genet. 15:480 (2014).

[2] R.A. Fisher, The Genetical Theory of Natural Selection. Clarendon Press, Oxford (1930).

BP 54.3 Thu 15:30 ZEU 250

Statistical description of normalized odor representations — ●DAVID ZWICKER — Harvard University, Cambridge, USA

Natural odors comprise many molecules at different concentrations and it is unclear how such odors are discriminated by relatively few olfactory receptors. One problem is that the correlations present in natural odors cannot be removed by local computations, like center-surround inhibition in vision. Instead, the global inhibition present in the olfactory system leads to normalized odor representations, where the odor intensity is separated from its identity, encoded by the relative concentrations of the odorant molecules. This separation is useful to robustly identify odors at different intensities, but how such global inhibition influences the neural representations of odors is unclear.

In this presentation, I discuss a simple theoretical model of the olfaction system that focuses on global inhibition. The model leads to sparse odor representations and reveals two generic consequences of global inhibition: (i) odors with many molecular species are more difficult to discriminate and (ii) receptor arrays with heterogeneous sensitivities perform badly. Comparing these predictions to experiments will help us to understand the role of global inhibition in shaping nor-

malized odor representations.

BP 54.4 Thu 15:45 ZEU 250

Magnetosensing with ion channels and the origin of anomalous gating kinetics — ●IGOR GOYCHUK — Institute for Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam-Golm, Germany

It was earlier proposed by J. Kirschvink *et al.* that magnetosensitive ion channels can be involved in sensing weak magnetic fields by various animals, with a magnetic nanoparticle coupled to a gate of an ion channel and serving as sensor. I consider a generalization of this hypothesis, where a magnetic nanorod made of several magnetosomes is elastically coupled to a cluster of ion channels [1]. Magnetic nanorod reorients in viscoelastic cytosol following a Generalized Langevin equation dynamics and a gating spring instability leads to bistable open-shut dynamics in such a hypothetical magnetosensory complex. Is the proposed mechanism feasible for realistic parameters? It is shown that YES, and interestingly enough the open-shut dynamics can exhibit both stretched-exponential and power law features in the residence time distributions. Beyond this particular context of magnetosensing, viscoelasticity of the medium in which the sensory part of ion channel moves is proposed as a generic mechanism to explain the origin of anomalous gating kinetics observed in several naturally occurring ion channels.

[1] I. Goychuk, Phys. Rev. E **92**, 042711 (2015).

BP 54.5 Thu 16:00 ZEU 250

Quorum sensing in stochastic many-particle models of microbial populations — ●JOHANNES KNEBEL¹, MATTHIAS BAUER², MATTHIAS LECHNER¹, PETER PICKL¹, and ERWIN FREY¹ — ¹Ludwigs-Maximilians University, Munich — ²Max Planck Institute for Intelligent Systems, Tuebingen

Autoinducers are small signaling molecules that mediate intercellular communication in microbial populations and trigger coordinated gene expression via "quorum sensing". Elucidating the mechanisms that control autoinducer production is pertinent to understanding collective microbial behaviors such as virulence and bioluminescence. Recent experiments indicate that autoinducers can be heterogeneously produced in clonal populations. Here we ask how phenotypic heterogeneity is established and how the autoinducer concentration in the population is regulated at the same time. In our conceptual model, cells synthesize and excrete autoinducers, and replicate and adapt in this environment. The model reveals that heterogeneous autoinducer production is facilitated by the coupling of ecological and evolutionary dynamics through quorum sensing. To capture the emergent dynamics, we derived a macroscopic mean-field equation from the microscopic stochastic many-particle process in the spirit of the kinetic theory in statistical physics. This mean-field equation reduces to the continuous replicator equation when quorum sensing is absent and, notably, admits bimodal stationary distributions when quorum sensing is present. Our analysis explains phenotypic heterogeneity through quorum sensing and the observed phase transitions to homogeneity.

BP 54.6 Thu 16:15 ZEU 250

Dynamics of population fronts in the presence of finite-sized heterogeneities — ●WOLFRAM MÖBIUS^{1,3}, KIM M. J. ALARDS¹, FRANCESCA TESSER¹, ROBERTO BENZI², DAVID R. NELSON³, and FEDERICO TOSCHI¹ — ¹Technische Universiteit Eindhoven, Eindhoven, The Netherlands — ²Universita' di Roma "Tor Vergata" and INFN, Rome, Italy — ³Harvard University, Cambridge, MA, USA

Populations spread on surfaces through the combined effect of dispersal and population growth on a wide range of length and time scales, yet the effect of heterogeneous environments on this spreading process is not well understood. We here investigate the effect of finite-sized features which affect dispersal or growth of the population locally. With an individual-based simulation we investigate the effect of individual features on the population front and identify a regime within which a local front speed is sufficient to predict the resulting front. Using least-time arguments we are able to describe the front dynamics for individual features and characterize how width and length of the features determine front shape at long times. These findings combined

with numerical solutions of the Eikonal equation allow us to characterize the resulting effective front speed for dilute to dense random sets of features. The results advance our understanding of population and other fronts in two-dimensional irregular environments.

BP 54.7 Thu 16:30 ZEU 250

Universality in the clonal dynamics in developing tissues — ●STEFFEN RULANDS^{1,2}, SAMIRA CHABAB³, FABIENNE LESCROART³, CEDRIC BLANPAIN³, and BENJAMIN DAVID SIMONS¹ — ¹University of Cambridge, Cambridge, United Kingdom — ²MPI-PKS, Dresden, Germany — ³Université libre de Bruxelles, Brussels, Belgium

Lineage tracing studies based on transgenic animal models have led to advances in our understanding of cellular identity, hierarchy and function. They provide insights into the development, maintenance and regeneration of tissues, and factors leading to dysregulation in diseased states. However, large-scale cell rearrangements, particularly in growing tissues may render the retrospective analysis of lineages highly problematic. Drawing on studies of heart development, we show how such effects may lead to the emergence of universal scaling distributions. By mapping the problem of clonal evolution onto the theory of aerosols, we elucidate the origin and range of possible scaling behaviors. In generalizing our studies to other tissue types and contexts, we show how the identification of universal scaling dependences allows biological information on cell fate behavior to be distilled.

BP 54.8 Thu 16:45 ZEU 250

Incorporating sleep regulation and thalamocortical interactions in a cortical meanfield model — ●MICHAEL SCHELLENBERGER COSTA¹, ARNE WEIGENAND¹, HONG-VIET V. NGO², LISA MARSHALL³, JAN BORN², THOMAS MARTINETZ¹, and JENS CHRISTIAN CLAUSSEN^{4,1} — ¹INB, U Lübeck — ²Med. Psych. and Behav. Neurobiol., U Tübingen — ³Neuroendocrinology, U Lübeck — ⁴Comp. Syst. Biol., Jacobs University Bremen

Few models accurately reproduce the complex rhythms of the thalamocortical system, as well as the dynamical patterns of sleep regulation. Here, we build upon previous work on a meanfield (neural mass) model of the sleeping cortex [1] and investigate the effect of neuromodulators on the dynamics of the cortex and the corresponding transition between wakefulness and the sleep stages [2]. We show that our simplified model generates essential features of human EEG over a full day. This approach builds a bridge between sleep regulatory models and EEG generating neural mass models. Based on model [1], we also suggest a new interpretation of the mechanisms responsible for the generation of KCs and SOs [3]. A KC corresponds to a single excursion along the homoclinic orbit, while SOs are noise-driven oscillations around a stable focus. The model generates both time series and spectra that strikingly resemble real EEG data and points out differences between the stages of natural sleep.

[1] A. Weigenand et al., PloS Comp Biol (2014) [2] M. Schellenberger Costa et al., J. Comp. Neurosci. (2016) [3] M. Schellenberger Costa et al., PloS Comp Biol (2016)

BP 54.9 Thu 17:00 ZEU 250

Modeling the spread of West Nile Virus in Germany — ●SUMAN BHOWMICK¹, PHILIPP LORENZ², PHILIPP HÖVEL², and HARTMUT H. K. LENTZ¹ — ¹Institute of Epidemiology, Friedrich-Loeffler-Institute, Südufer 10, 17493 Greifswald — ²Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

West Nile virus (WNV) is an arthropod-borne virus (arbovirus) spreading in transmission cycle between mosquitoes and birds. In addition, horses and human are also the victims of WNV, being infected by blood feeding mosquitoes. In our current endeavour, a dynamic model has been devised to decipher the intricacy of the spreading dynamics of the West Nile virus.

The model which is of SEIR (susceptible-exposed-infected-removed) type, comprises of 19 compartments. In this model, we tried to couple the terrestrial and aqueous stages of mosquitoes through a single ODE, for the simplicity. In addition to the local spreading dynamics, spatial spread through aerial movement (diffusion) and bird migration shall be included in the model.

As results, we will present solutions of the local infection model as well as an analytical expression for the basic reproduction number R_0 . The seasonal and environmental impacts are also taken into the considerations. The associated map of the basic reproduction number R_0 will be investigated further along with the ODE coupled with network.

BP 54.10 Thu 17:15 ZEU 250

Burst-Noise induced bifurcations in the Schlögl-Model — ●JOHANNES FALK, MARC MENDLER, and BARBARA DROSSEL — TU Darmstadt, Germany

We investigate the influence of intrinsic noise on stable states of a one-dimensional dynamical system that shows in its deterministic version a saddle-node bifurcation between monostable and bistable behaviour. The system is a modified version of the Schlögl model, which is a chemical reaction system with only one type of molecule. The strength of the intrinsic noise is varied without changing the deterministic description by introducing bursts in the autocatalytic production step. We study the transitions between monostable and bistable behavior in this system by evaluating the number of maxima of the stationary probability distribution. We find that changing the size of bursts can destroy and even induce saddle-node bifurcations. This means that a bursty production of molecules can qualitatively change the dynamics of a chemical reaction system even when the deterministic description remains unchanged.

BP 55: Cell Migration and Contraction

Time: Thursday 15:00–17:15

Location: HÜL 386

Invited Talk

BP 55.1 Thu 15:00 HÜL 386

Network heterogeneity regulates steering in actin-based motility — ●LAURENT BLANCHON — CytoMorphoLab, Biosciences & Biotechnology Institute GRENOBLE, FRANCE

The growth of branched actin networks powers cell-edge protrusions and motility. These dynamic structures are characterized by a heterogeneous actin density, which yields to a tunable cellular response. We studied how actin organization controls both the rate and the steering during lamellipodium growth. We used a high-resolution surface structuration assay combined with modeling approach to describe the growth of a reconstituted lamellipodium. We demonstrated that local monomer depletion at the site of active assembly negatively impacts the network growth rate. At the same time, network architecture tunes the protrusion efficiency, and regulates the rate of growth. One consequence of this interdependence between monomer depletion and network architecture effects is the ability of heterogeneous network to impose steering during motility. We established therefore the general principles on how the cell can modulate the rate and the direction of protrusion locally by varying both density and architecture of its actin network.

BP 55.2 Thu 15:30 HÜL 386

Collective cell migration on soft substrates — ●ANDRIY GOYCHUK and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität, München, Deutschland

The extracellular matrix surrounding cells strongly influences their migratory behavior. This includes the decrease of cell proliferation with the substrate stiffness. To better understand this phenomenon, we study a modified Cellular Potts Model on a deformable hexagonal lattice. The cell polarization and cytoskeletal remodeling is simulated by a coarse-grained routine on a sub-cellular level. We show that cells exhibit a fast and persistent motion in the higher range of substrate stiffness, unlike in the lower range. In the intermediate regime, the cells show more complex behavior and move in groups.

BP 55.3 Thu 15:45 HÜL 386

Time-Resolved Measurement of Highly Dynamic Force Evolution in Small Cells — ●JANA HANKE¹, DIMITRI PROBST², ULRICH S. SCHWARZ², and SARAH KÖSTER¹ — ¹Institute of X-Ray Physics, University of Göttingen, Göttingen, Germany — ²Institute for Theoretical Physics and BioQuant, Heidelberg University, Heidelberg, Germany

Force generation is an important aspect in numerous essential biolog-

ical processes like rigidity sensing, spreading and motility. Measuring such forces as they are exerted on the cellular environment at high spatial resolution and in a time-resolved manner remains a challenge. Here we optimise traction force microscopy on soft elastic substrates for measurements of human blood platelets, which generate comparatively high traction forces although they are the smallest cells in the human body. By tracking force evolution over 30 minutes, we characterise the cells' highly dynamic force development on substrates of 19 to 83 kPa stiffness. Independent of the stiffness, we find three distinct behaviours in individual cells, namely platelets reaching a force plateau, as well as a relaxing or oscillatory behaviour after initial contraction. The average initial contraction velocity, however, is dependent of the stiffness as it increases with increasing stiffness.

BP 55.4 Thu 16:00 HÜL 386

Combined MEA- and SICM-based measurements of the cardiomyocyte contractile behavior — ●STEFAN SIMEONOV and TILMAN E. SCHÄFFER — Institute of Applied Physics, University of Tübingen, Germany

We present a novel experimental setup that combines microelectrode array (MEA) based electrical recording with scanning ion conductance microscopy (SICM). MEAs are used for non-invasive, in-vitro measurements of extracellular electrophysiological signals generated by live cells. SICM is a non-invasive scanning probe technique for imaging sample topography with sub-micrometer spatial resolution. We used this combined setup to investigate beating cardiac cells (HL-1 cell line), which exhibit both electrophysiological activity and morphological dynamics. We mapped the height of a beating cell as a function of time with sub-cellular spatial and millisecond temporal resolution. Synchronizing the SICM data with the simultaneously recorded extracellular field potential from the MEA allowed us to reconstruct the time-resolved 3D topography during the contraction and relaxation cycle of the cell. Furthermore, we investigated the effect of blebbistatin, a myosin II motor protein inhibitor, on the contractile behavior of beating cells. The contraction amplitude decreases over time until the cells stop contracting entirely despite the ongoing generation of unaltered extracellular field potential.

15 min break

BP 55.5 Thu 16:30 HÜL 386

Variability, order and myosin II acceleration of cortical dynamics of motile amoeboid cells — HSIN-FANG HSU¹, EBERHARD BODENSCHATZ¹, ALEXEI KREHKOV¹, CHRISTIAN WESTENDORF¹, AZAM GHOLAMI¹, ALAIN PUMIR², ●MARCO TARANTOLA¹, and CARSTEN BETA³ — ¹MPI-DS, Am Fassberg 17, D-37077 Göttingen — ²Laboratoire de Physique, Univ Lyon, ENS, CNRS, F-69342 Lyon — ³Institute of Physics and Astronomy, Univ Potsdam, D-14476 Potsdam

Chemotactic motion of cells relies on membrane protrusions driven by the polymerization and depolymerization of actin. Here we show that the response of the actin system of *Dictyostelium discoideum* (D.d.) to a receptor stimulus is subject to a threshold value that varies strongly from cell-to-cell. Above threshold, we observe pronounced variability in response amplitudes. Polymerization time, however, is almost constant over the entire range of response amplitudes, while depolymerization time increases with increasing amplitude. We show that cell-to-cell variability in the response amplitude correlates with the amount of Arp2/3, a protein that enhances actin polymerization. An-

other key player governing dynamics of the actin network is the motor protein myosin II. Upon chemotactic stimulation, myosin II is first released from the cell cortex but then relocates to the cortical region with actin filaments. Using Poincaré mapping, we analyze the detailed dynamical interplay of actin, myosin II and the cell area. Cells lacking myosin II show a deceleration of cortical actin recovery after stimulation, suggesting the important role of myosin II in setting the response time.

BP 55.6 Thu 16:45 HÜL 386

Transport of micro-cargo by amoeboid cells — ●OLIVER NAGEL, MANUEL FREY, VALENTIN LEPRO, MATTHIAS GERHARD, and CARSTEN BETA — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

The directed transport and positioning of micron-sized objects in complex confined geometries is difficult to achieve and often relies on laborious techniques, such as magnetic or optical tweezers, or microsurgery. Here, we propose an alternative approach based on the idea to harness motile amoeboid cells as trucks that transport micro-cargo to desired locations. We show that cells of the social amoeba *Dictyostelium discoideum* can transport micro-particles with a wide range of different sizes. The cells can be guided by gradients of the chemoattractant cAMP, which can be established with the help of classical gradient chambers or through photo-chemical release from a caged precursor. We compare the motile properties of amoeboid cells with and without cargo. To analyze the limits of cell-driven micro-transport in more detail, we measure the pulling forces applied to a micron-sized bead by a *Dictyostelium* cell with the help of an optical trap. Furthermore, we demonstrate that not only small objects can be transported in this way, but also larger objects that exceed the size of individual cells by more than an order of magnitude can be moved in a collective effort by aggregates of many cells.

BP 55.7 Thu 17:00 HÜL 386

Cell-Type Specific Mechano-Sensing altered by Blebbistatin — ●GALINA KUDRYASHEVA and FLORIAN REHFELDT — III. Physikalisches Institut Friedrich-Hund-Platz 1 37077 Göttingen Germany

Cells sense the stiffness of their surrounding with contractile actomyosin stress fibers through focal adhesions and react to such physical stimuli by altering their bio-chemical pathways. Especially striking is the mechano-guided differentiation of human mesenchymal stem cells (hMSCs) [Engler et al. Cell (2006)]. While the entire differentiation process can take several days up to weeks, the structure and dynamics of stress fibers can be used as an early morphological marker and theoretically modelled using classical mechanics with an active spring model [Zemel et al. Nat. Phys. (2010)]. We use this approach and the theoretical model to analyze the mechanical cell-matrix interactions of hMSCs and several types of differentiated cells. Using immunofluorescence we visualized stress fibers and analyzed the cytoskeletal morphology [Eltzner et al. PLoS One (2015)] of cells cultured on elastic substrates (E from 1 kPa to 130 kPa). Analyzing cell area and cytoskeletal order parameter S we could assign an effective cellular stiffness that shows distinct differences during the differentiation process and for different cell types. Our experiments show that the mechanical susceptibility is cell type specific and dependent on actomyosin contractility. Interestingly, addition of the non-muscle myosin II (NMM II) inhibitor blebbistatin alters cellular mechano-sensitivity by facilitating cell spreading on soft substrates through relaxing the cellular actomyosin cortex, but not on stiff substrates.

BP 56: Protein Structure and Dynamics

Time: Thursday 15:00–17:30

Location: SCH A251

Invited Talk

BP 56.1 Thu 15:00 SCH A251

Biophysical Studies of Amyloid Formation and Its Inhibition — ●SHEENA RADFORD — The University of Leeds

Amyloid formation involves the polymerisation of proteins and peptides into polymers with a cross-beta fold. How amyloid formation causes disease, and identifying the culprit species involved, remain a significant challenge. This results from the complexity of the aggregation process and the fact that amyloid assembly is initiated by non-native states of proteins that are partially folded or intrinsically disordered. Structure determination is thus difficult, and identifying the interacting surfaces in these transiently formed and dynamic ensembles is challenging. In this lecture I will describe our recent attempts to discover new insights into how proteins aggregate into amyloid and how to prevent cellular dysfunction caused by amyloid assembly/disassembly mechanisms using a number of different strategies. Specifically, I will show how we have used different biophysical and biochemical approaches to map the nature of the earliest protein-protein interactions in amyloid assembly and to re-assess the potential role(s) of fibrils in disease. Finally, using a novel screen developed with *E. coli*, we have been able to discover new highly potent inhibitors of aggregation for some of the most highly aggregating protein sequences known.

BP 56.2 Thu 15:30 SCH A251

Molecular mechanisms of substrate binding proteins in ABC transporters — MARIJN DE BOER, FLORENCE HUSADA, KOSTAS TASSIS, YUSRAN MUTHAHARI, GIORGOS GOURIDIS, and ●THORBEN CORDES — Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747AG Groningen, The Netherlands

ATP-binding cassette (ABC) transporters mediate unidirectional active transport of diverse substrates across membranes using ATP hydrolysis. During import in prokaryotes, specialized substrate binding proteins or domains (SBDs) at first capture a substrate for delivery to the translocator domain and subsequent transport. Different SBDs show a high structural conservation but only little sequence similarity. Their fold consists of two rigid α/β domains, which form the binding cavity, and that are connected by a (flexible) hinge. We here test the hypothesis, whether there is a relationship between the SBD hinge structure and conformational dynamics of the SBDs based on the fact that the hinge bends during the conformational transition from open unliganded to closed liganded state. For this we use single-molecule Förster resonance energy transfer (smFRET) that allows to elucidate the conformational states and dynamics of SBDs directly and with this to understand their mechanistic role for transport.[1-3]

[1] G. Gouridis et al., *Nature Structural & Molecular Biology* 22 (2015) 57-64. [2] F. Husada et al., *Biochemical Society Transactions* 43 (2015) 1041-1047. [3] J. H. M. van der Velde et al., *Nature Communications* 7:10144 (2016).

BP 56.3 Thu 15:45 SCH A251

Time-resolved observation of allosteric communication in PDZ2 domain — ●GERHARD STOCK, SEBASTIAN BUCHENBERG, and FLORIAN SITTEL — Institute of Physics, Albert Ludwigs University, Freiburg

A local perturbation of a protein may lead to functional changes at some distal site. A well-established example are PDZ domains which show an allosteric transition upon binding to a peptide ligand. Recently Hamm and coworkers (PNAS 2013) presented a time-resolved study of this transition. Using well-defined photopreparation and structure-sensitive infrared probing, they showed that the conformational rearrangement of PDZ2 occurs in a highly nonexponential manner on various timescales from pico- to microseconds.

Here we present extensive (in total 0.4 ms) nonequilibrium molecular dynamics simulations (all atom/explicit solvent) of Hamm's experiment, which allow us to monitor protein allosteric communication in real time. Along these lines, we address the following issues: What are the timescales of the transition and is there a hierarchy of processes? Is allosteric communication in PDZ2 dominated by enthalpic or entropic effects? Can the process be described as directed motion (domino picture), a simple barrier crossing, or rather via a diffusive heterogeneous transition path ensemble? Is allostery connected to the protein's pathways of energy transport? What's the role of the solvent? Does the

long-range conformational rearrangement due to ligand binding occur via population-shift or induced-fit mechanism?

BP 56.4 Thu 16:00 SCH A251

Elucidation of light-induced structural changes of aureochrome by small-angle X-ray scattering — ●SASKIA BANISTER, ELENA HERMAN, THOMAS HELLWEG, and TILMAN KOTTKE — Bielefeld University, Germany

Aureochromes function as blue-light-regulated transcription factors in algae. Their basic region leucine zipper (bZIP) effector domain binds DNA with a specific sequence while a light-, oxygen-, or voltage-sensitive (LOV) domain acts as the C-terminal sensor. Due to this unusual arrangement of sensor and effector, aureochromes are interesting for studying their mechanism and for the engineering of new synthetic optogenetic tools.

We are applying small-angle X-ray scattering (SAXS) to resolve the solution structure of the full-length receptor and the monomeric LOV domain. However, SAXS on photoreceptors is challenging. First, dark conditions need to be absolutely strict to avoid conversion of the highly sensitive receptor. Second, the analysis under illumination needs to ensure full conversion. Therefore we are establishing SAXS experiments under rigorous control of light and simultaneous UV/Vis monitoring on an in-house setup. First results from SAXS measurements on LOV under true dark conditions are presented. Experiments on the full-length aureochrome are currently pursued.

Banerjee, A., Herman, E., Serif, M., Maestre-Reyna, M., Hepp, S., Pokorny, R., Kroth, P. G., Essen, L.-O., Kottke, T. (2016), *Nucleic Acids Res.* 44(12), 5957-5970.

Herman, E., Kottke, T. (2015), *Biochemistry* 54, 1484-1492.

BP 56.5 Thu 16:15 SCH A251

Barrier crossing in the presence of long memory - a global analysis — ●JULIAN KAPPLER, JAN O. DALDROP, FLORIAN N. BRÜNIG, and ROLAND R. NETZ — Freie Universität Berlin, Germany

Rate theories are a widely used and important means for predicting meso- and macroscopic time scales from microscopic dynamics. The present rate theories for non-Markovian microscopic dynamics, i.e. in the presence of memory effects, are quite complicated to implement and have not been studied systematically for dynamics with long memory time. In our contribution, we present a global analysis of barrier crossing rates based on simulations of the massive Langevin equation with exponential memory. We extract the scaling behavior of the rates for long memory, indicate limits of current rate theories, and additionally provide a heuristic formula to calculate accurate rates quickly and easily.

BP 56.6 Thu 16:30 SCH A251

Color tuning of visual rhodopsins: a quantitative explanation by electrostatic calculations — ●FLORIMOND COLLETTE, FRANK MÜH, and THOMAS RINGER — Institut für Theoretische Physik, Johannes Kepler University Linz, Altenberger Strasse 69, 4040 Linz, Austria

Rhodopsins are biological pigment-protein complexes found in photoreceptor cells of the retina. Comparing the results of two quantum chemical/electrostatic calculation methods, that have been applied successfully to reveal the functional states of BLUF photoreceptors [1] and photosystem II antenna protein CP29 [2], we have estimated absorption shifts of the retinal chromophore for a series of site-directed mutants. Our results are in excellent agreement with recent experimental studies [3] and strongly suggest that the spectral sensitivity in animal rhodopsins is dominated by electrostatic tuning.

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

[2] F. Müh et al., *Phys. Chem. Chem. Phys.* 16, 11848 (2014).

[3] W. Wang et al., *Science* 338, 1340 (2012).

BP 56.7 Thu 16:45 SCH A251

The dynamics and flexibility of penicillin binding proteins: a combined computational/experimental approach to tackle antimicrobial resistance (AMR) — ●JASMINE L. DESMOND¹, PIERDOMENICO BELLINI², CHRISTOPHER DOWSON², P. MARK RODGER³, and RUDO A. ROEMER¹ — ¹Department of Physics,

University of Warwick, UK. — ²School of Life Sciences, University of Warwick, UK. — ³Department of Chemistry, University of Warwick, UK.

700,000 people die each year from drug-resistant infections, a figure that — if action is not taken — is estimated to increase to 10 million by 2050. The drug penicillin targets essential cell wall biosynthetic enzymes that still remain attractive targets for new efforts in drug discovery. Elucidating protein dynamics and flexibility is key to understanding the selective interactions of proteins with a drug as it docks. In spite of the success of x-ray crystallography in the determination of rigid protein structures, the experimental technique is unable to provide insight into the dynamics of proteins. Such information can, however, be elucidated using molecular modelling. Important protein conformational changes often occur on microsecond-millisecond timescales and are difficult to access using traditional modelling techniques, such as molecular dynamics (MD). Here, we present the results of computationally inexpensive, geometric simulations of protein motion for a range of penicillin binding proteins. There is a focus on differences in motion between: (1) inactive and active proteins and (2) proteins with and without bound drug molecules.

BP 56.8 Thu 17:00 SCH A251

Femtosecond Time-Resolved Dynamics in Myoglobin observed with an XFEL — ●HENRIKE M. MÜLLER-WERKMEISTER^{1,2}, HELEN M. GINN³, ANLING KUO⁴, ANTOINE SARRACINI², HELEN DUYVESTYEN³, SASCHA W. EPP¹, DARREN SHERRELL⁵, SHIGEKI OWADA⁶, OLIVIER PARE-LABROSSE², SAEED OGHBAEY², JESSICA BESAW², YOSHIKI KUMAGAI⁷, KENSUKE TONO⁶, YINPENG ZHONG¹, KOJI MOTOMURA⁷, BRYAN T. EGER², ALEXANDER MARX¹, ARWEN R. PEARSON⁸, ROBIN L. OWEN⁵, KIYOSHI UEDA⁷, DAVID I. STUART^{3,5}, OLIVER P. ERNST⁴, and R. J. DWAYNE MILLER^{1,2} — ¹Max-Planck-Institute for Structure and Dynamics of Matter, Ham-

burg, Germany — ²Departments of Chemistry and Physics, University of Toronto, Canada — ³University of Oxford, United Kingdom — ⁴Department of Biochemistry, University of Toronto, Canada — ⁵Diamond Light Source, Didcot, United Kingdom — ⁶SACLA, RIKEN Spring-8 Center, Hyogo, Japan — ⁷Tohoku University, Sendai, Japan — ⁸Hamburg University, The Hamburg Center for Ultrafast Imaging, Germany

Here we present recent results from femtosecond time-resolved serial crystallography experiments performed at the X-Ray free electron laser SACLA. We have studied the ligand dissociation in Myoglobin in the time window between 0 fs and 2 ps under functionally relevant conditions, that is, at low laser excitation conditions to prevent spurious artefacts introduced by multi photon processes. The results provide an unprecedented insight into the ultrafast structural changes right after the ligand dissociation.

BP 56.9 Thu 17:15 SCH A251

A rigid core amplifies the binding affinity of multivalent ligands — ●SUSANNE LIESE and ROLAND R. NETZ — Department of Physics, Free University Berlin, Arnimallee 14, 14195 Berlin, Germany
Multivalent interaction achieves strong, yet reversible binding through the simultaneous formation of multiple, identical bonds. The strength of multivalent binding is determined by the interplay between gain in binding enthalpy and entropic loss due to the reduction of conformational and rotational degrees of freedom upon ligand binding. We compare the binding affinities of rigid and flexible multivalent ligands. While flexible polymer based scaffolds are unsuitable to design high affinity multivalent ligands, rigid ligands with a stiff core that is similar in size to the receptor, amplify the binding affinity by several orders of magnitude. The general design principles, which we derive, might be of great importance to improve rational multivalent ligand design.

BP 57: Networks: From Topology to Dynamics II (Joint Session DY/BP/SOE)

Time: Thursday 15:00–16:15

Location: ZEU 147

BP 57.1 Thu 15:00 ZEU 147

Response Patterns for Fluctuations in Complex Flow Networks — ●XIAOZHU ZHANG¹, SARAH HALLERBERG^{1,2}, MORITZ MORITZ MATTHIAE³, DIRK WITTHAUT^{3,4}, and MARC TIMME^{1,5} — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen — ²Faculty for Engineering and Computer Science, Hamburg University of Applied Science, 20099 Hamburg — ³Institute for Energy and Climate Research - Systems Analysis and Technology Evaluation (IEK-STE), Forschungszentrum Jülich, 52428 Jülich — ⁴Institute for Theoretical Physics, University of Cologne, 50937 Köln — ⁵Department of Physics, Technical University of Darmstadt, 64289 Darmstadt

Dynamic collective phenomena prevail in networked systems across physics, biology and engineering. How external signals generate distributed responses patterns in such systems fundamentally underlies their function, yet is far from fully understood. Here we analyze the collective response patterns of oscillatory networks to fluctuating input signals. For an arbitrary network topology, we analytically find distinct response patterns to fall into three distinct frequency regimes: homogeneous responses across the network at low frequencies, topology-dependent resonances at intermediate frequencies and are frequency-dependent, localized responses at high frequencies. These results render regime-specific implications for real-world network design and control, in particular for transport and supply networks, e.g. electric power grids.

BP 57.2 Thu 15:15 ZEU 147

Control of chimeras in small networks — IRYNA OMELCHENKO¹, OLEH OMEL'CHENKO², ANNA ZAKHAROVA¹, MATTHIAS WOLFRUM², and ●ECKEHARD SCHÖLL¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — ²Weierstrass Institute, Mohrenstraße 39, 10117 Berlin, Germany

We propose a control scheme which can stabilize and fix the position of chimera states in small networks [1]. Chimeras consist of coexisting domains of spatially coherent and incoherent dynamics in systems of nonlocally coupled identical oscillators. Chimera states are generally

difficult to observe in small networks due to their short lifetime and erratic drifting of the spatial position of the incoherent domain. The control scheme, like a tweezer, might be useful in experiments, where usually only small networks can be realized.

[1] I. Omelchenko, O. E. Omel'chenko, A. Zakharova, M. Wolfrum, and E. Schöll, Phys. Rev. Lett. **116**, 114101 (2016).

BP 57.3 Thu 15:30 ZEU 147

Scaling Laws in Spatial Network Formation — ●NORA MÖLKENTHIN^{1,2} and MARC TIMME^{1,2} — ¹Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — ²Institute for Nonlinear Dynamics, Faculty of Physics, University of Göttingen, 37077 Göttingen, Germany

Geometric constraints strongly impact the formation of networked systems. Examples range from amino acid chains folding to proteins structures to rearranging particle aggregates. The dynamical self-organization of the interaction network in such systems is far from fully understood. Here, we analyze a class of spatial network formation processes by introducing a mapping from geometric to graph-theoretic constraints. Combining stochastic and mean field analyses yields an algebraic scaling law for the extent (graph diameter) of the resulting networks with system size, in contrast to logarithmic scaling known for networks without constraints. Intriguingly, the exponent falls between that of self-avoiding random walks and that of space filling arrangements, consistent with experimentally observed scaling (of the spatial radius of gyration) for protein tertiary structures.

BP 57.4 Thu 15:45 ZEU 147

Boolean network analysis reveals interaction networks among low-abundance species in the human gut microbiome — ●JENS CHRISTIAN CLAUSSEN¹, JURGITA SKIECEVICIENE², JUN WANG³, PHILIPP RAUSCH^{6,5}, TOM H. KARLSEN⁴, WOLFGANG LIEB⁵, JOHN F. BAINES^{5,6}, ANDRE FRANKE⁵, and MARC-THORSTEN HÜTT³ — ¹Computational Systems Biology, Jacobs University Bremen — ²U Kaunas — ³KU Leuven — ⁴U Oslo — ⁵UKSH, U Kiel — ⁶MPI Plön
Microbiome compositions in clinical context gained recent interest. Most analyses infer interactions among highly abundant species. The large number of low-abundance species has received less attention.

Here we present a novel analysis method based on Boolean operations applied to microbial co-occurrence patterns. We calibrate our approach with simulated data based on a dynamical Boolean network model from which we interpret the statistics of attractor states as a theoretical proxy for microbiome composition. We show that for given fractions of synergistic and competitive interactions in the model our Boolean abundance analysis can reliably detect these interactions. In our human gut microbiome dataset, we find a large number of highly significant synergistic interactions among these low-abundance species, forming a connected network, and a few isolated competitive interactions.

BP 57.5 Thu 16:00 ZEU 147

Complex Contagion and Coordinated Response in Animal Groups — ●WINNIE POEL^{1,6}, BRYAN DANIELS³, COLIN TWOMEY², IAIN COUZIN^{4,5}, and PAWEŁ ROMANCZUK^{1,6} — ¹Inst. of Theor. Biol., Dept. of Biol., Humboldt Universität zu Berlin — ²Dept. of Ecology and Evolutionary Biol., Princeton University, Princeton, US — ³ASU-

SFI Center for Biosocial Complex Systems, Arizona State University, US — ⁴Dept. of Collective Behaviour, MPI for Ornithology, Konstanz, Germany — ⁵Dept. of Biology, University of Konstanz, Germany — ⁶Bernstein Center for Computational Neuroscience Berlin, Germany

Our work focuses on the underlying communication network in animal swarms that enables coordinated movement and collective information processing in large groups while taking into account the limited attention and cognitive ability of each individual. Here, we study the influence of network structure on processes of behavioral complex contagion in fish groups. Specifically, we investigate the spreading of startling behavior in golden shiners on empirically inferred networks built on their individual visual perception of neighbors [1]. Using a simple adapted SIR model [2] we aim to uncover how the spatial configuration of a swarm (and thus its visual interaction network) aid to amplify or dampen out the information sent out by a certain individual.

[1] Rosenthal, S., et al., PNAS 112.15 (2015): 4690-4695

[2] Dodds, P., et al., J. Theor. Biol. 232.4 (2005): 587-604

BP 58: DNA & RNA

Time: Friday 9:30–10:45

Location: ZEU 250

BP 58.1 Fri 9:30 ZEU 250

Interactions between a short DNA oligonucleotide and urea in the light of Kirkwood-Buff theory: a Molecular Dynamics simulation study — ●EWA ANNA OPRZESKA-ZINGREBE and JENS SMIAŁEK — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

In nature, a wide range of biological processes, such as transcription termination or intermolecular binding, is dependent on the formation of specific DNA secondary and tertiary structures. These structures can be both stabilized or destabilized by the osmolytes, coexisting with the nucleic acids in the cellular environment. In our study, we investigate a simple 7-nucleotide DNA hairpin with the sequence d(GCGAAGC) in the presence of varying concentrations of urea.

The interaction between DNA and urea in unbiased molecular dynamics simulations has been analysed according to Kirkwood-Buff theory. We implemented the local/bulk partitioning model, complemented by the analysis of preferential hydration and preferential interaction coefficients, to get insight into the distribution of the cosolute in the vicinity of the DNA oligonucleotide. The free energy landscape of unfolding has been approached via Metadynamics upon the addition of a bias potential. This study allows us to get a more comprehensive understanding of the stability of the DNA structures in the presence of urea.

BP 58.2 Fri 9:45 ZEU 250

Dynamic Organization of Bacterial Chromosome by SMC Condensin — ●CHRISTIAAN ADRIANUS MIERMANS and CHASE BROEDERSZ — Arnold-Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians Universität München

The bacterial chromosome is highly structured across a wide range of length-scales, extending up to the full length of the genome. Recent Hi-C experiments provide evidence for anomalously high contacts between opposite pairs of DNA loci – millions of basepairs apart – on the left and right chromosome arms. These striking long-range contacts in Hi-C contact maps have been attributed to a variety of nucleoid-associated proteins, including the highly conserved ATPase SMC condensin. Although the microscopic structure of these ATPases has been mapped in detail, how SMC condensins are able to effect these long-range chromosomal contacts in living cells remains an open question. We present a minimal model for the physical mechanisms for the large-scale DNA organization by SMC condensin. Our simulations indicate that condensin is not able to generate long-range DNA-DNA contacts under equilibrium conditions. In contrast, the inclusion of non-equilibrium dynamics in our model for condensin-DNA interactions gives rise to robust long-range chromosomal contacts. Taken together, our model suggests a novel mechanism for how protein-DNA interactions can dynamically drive chromosome organization in bacteria.

BP 58.3 Fri 10:00 ZEU 250

Chromosomal Organization by an Interplay of Loop Extrusion and Compartment Interaction — ●JOHANNES NÜEBLER, GEOFFREY FUDENBERG, MAXIM IMAKAEV, CAROLYN LU, ANTON

GOLOBORODKO, NEZAR ABDENNUR, and LEONID MIRNY — Institute for Medical Engineering and Science, Massachusetts Institute of Technology (MIT), Cambridge, MA 02139, USA

The chromatin fiber in eukaryotic nuclei is far from being simply a confined but otherwise randomly arranged polymer. Rather, it shows a high degree of spatial organization on all length scales, from nucleosomes up to segregated chromosome territories. On intermediate scales, chromosome conformation capture techniques have revealed two ubiquitous modes of organization: an alternating compartment structure, where each type preferentially associates with other loci of its type, and topologically associating domains (TADs) with increased association within each domain but not across boundaries. The mechanisms behind this organization are only beginning to emerge. While a block-copolymer model is a natural starting point for the compartment structure, TADs may be more consistent with the active mechanism of loop extrusion. We review how this can explain in a unified way such diverse phenomena as TADs, DNA loops and mitotic compaction and segregation. We study in particular the interplay of active loop extrusion and a block-copolymer. We discuss consistency with recent experiments that interfere with the loading of the proposed loop extrusion factor cohesin.

BP 58.4 Fri 10:15 ZEU 250

A macromolecular crowding study of RNA folding and activity: polymer pore size matters! — ●RICHARD BÖRNER¹, ERICA FIORINI¹, MICHAEL KOVERMANN², and ROLAND K.O. SIGEL¹ — ¹Department of Chemistry, University Zürich, Zürich, Switzerland — ²Department of Chemistry, University Konstanz, Konstanz, Germany

Ribozymes are catalytic RNAs requiring a high magnesium(II) concentration to show folding and function in vitro (1,2). In contrast, in vivo conditions are characterized by a highly crowded cellular environment and much lower ion concentration. Molecular crowding agents are used to mimic the cellular crowding. However, particular physical/chemical properties explaining the crowders influence are poorly understood. In this study, we gain new insights on how polymer properties like viscosity, pore size etc. influence the activity and folding of a group II intron RNA (3,4). We combined bulk activity assays, smFRET experiments and NMR screening PEG volume fraction (%) and molecular weight (MW) and unveiled an optimal pore size in terms of the catalytic activity.

(1) Börner R, Kowanko D, Guisett-Miserach H, Schaffer MF, Sigel RKO. (2016) Coord. Chem. Rev. 327-328:123-142. (2) Steiner M, Karunatilaka KS, Sigel RKO, Rueda D. Proc. Natl. Acad. Sci. U.S.A. (2008) 105:13853. (3) Fiorini E, Börner R, Sigel RKO. (2015) Chimia. 69(4):207. (4) Fiorini E, Paudel B, Börner R, Rueda D, Sigel RKO. (2016) submitted.

BP 58.5 Fri 10:30 ZEU 250

Organization of Nucleotides in Different Environments: Implications for the Formation of First RNA under Prebiotic Conditions — ●SEBASTIAN HIMBERT^{1,2} and MAIKEL RHEINSTÄDTER¹ — ¹Department of Physics and Astronomy, McMaster

University, Hamilton, ON, Canada — ²Department of Experimental Physics, Saarland University, Saarbrücken, Germany

How nucleic acids first assembled and then incorporated into the earliest forms of cellular life 4 billion years ago remains a fundamental question of biology. There has been no obvious way for RNA-like molecules to be produced and then encapsulated in cellular compartments in the absence of enzymes and metabolism. To support the hypothesis that environmental conditions in the neighbourhood of volcanic hydrothermal springs could act to organize monomeric nucleotides through various noncovalent interactions and chemical reac-

tions in the prebiotic era, we investigated 5'-adenosine monophosphate (AMP) and 5'-uridine monophosphate (UMP) molecules captured in different matrices that have been proposed to promote polymerization [1]. Two nucleotides signals were observed in our X-ray diffraction experiments, one corresponding to a nearest neighbour distance of around 4.6 Å attributed to nucleotides that form a disordered, glassy structure. A second, smaller distance of 3.45 Å agrees well with the distance between stacked base pairs in the RNA backbone, and was assigned to the formation of pre-polymers, i.e., the organization of nucleotides into stacks of about 10 monomers. [1] S. Himbert et. al., Scientific Reports, 6, 31285 (2016).

BP 59: Multi-Cellular-Systems

Time: Friday 9:30–11:00

Location: HÜL 386

Invited Talk

BP 59.1 Fri 9:30 HÜL 386

Spatially-resolved transcriptomics and single-cell lineage tracing — ●JAN PHILIPP JUNKER — Berlin Institute for Medical Systems Biology, MDC Berlin, Germany

Tissues and organs are complex mixtures of many different cell types, each of which is defined by a characteristic set of expressed genes. Systematic analysis of tissue architecture hence requires approaches that analyze gene expression on the single cell level. Recent progress in single-cell RNA sequencing now enables gene expression analysis of single cells on the level of the whole transcriptome, an important advance over microscopy-based methods that are typically limited to studying just one or a few genes at a time. However, information about the spatial position and lineage history of cells, which can be obtained by microscopy, is lost in sequencing experiments. Here, we present tomoseq, a method that combines traditional histological techniques with low-input RNA sequencing and mathematical image reconstruction to generate a high-resolution genome-wide 3D atlas of gene expression in the zebrafish embryo at three developmental stages. Importantly, our technique allows searching for genes that are expressed in specific spatial patterns without manual image annotation. Furthermore, we introduce scartrace, a strategy for massively parallel clonal analysis in the zebrafish based on CRISPR/Cas9 technology. We exploit the fact that Cas9-induced generation of double-strand breaks leads to formation of short insertions or deletions (genetic scars), which are variable in their length and position. We demonstrate that these genetic scars are ideal cellular barcodes for lineage analysis.

BP 59.2 Fri 10:00 HÜL 386

How cell division timing leads to robust development in *Caenorhabditis elegans* — ●ROLF FICKENTSCHER, PHILIPP STRUNTZ, and MATTHIAS WEISS — Experimental Physics 1, University of Bayreuth, Universitätsstr. 30, 95444 Bayreuth

Embryogenesis of the small nematode *Caenorhabditis elegans* is a remarkably robust and reproducible, but still poorly understood self-organization phenomenon. Here, we show that the coupling of cellular volumes and cell cycle times in combination with a mechanically guided arrangement process is key for a fail-safe embryogenesis of *C. elegans*.

In particular, we have monitored cell trajectories and cellular volumes in *C. elegans* embryos over several hours at different ambient temperatures by means of a custom-made lightsheet microscope. Embryonic cell trajectories are accurately described by a simple mechanical framework, i.e. cells migrate to and adopt positions of least mechanical constraints within the confining eggshell [1]. Our experimental data also revealed an anticorrelation of cell volumes and cell cycle durations, with significant differences between somatic and germline cells. This observation can be rationalized via a simple model that invokes a limiting molecular component supporting cell division, e.g. nuclear pore complexes. Integrating this aspect into the aforementioned mechanical framework, we observed that the different scaling of the germline precursor lineage is crucial for a robust cellular arrangement process during early embryogenesis [2].

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

[2] R. Fickentscher, P. Struntz & M. Weiss, *PRL* **117** (2016)

BP 59.3 Fri 10:15 HÜL 386

Dynamic pattern scaling as a critical point of self-organized growth control — ●STEFFEN WERNER^{1,2}, DANIEL AGUILAR-HIDALGO¹, ORTRUD WARTLICK³, MARCOS GONZÁLEZ-GAITÁN⁴, FRANK JÜLICHER¹, and BENJAMIN M. FRIEDRICH² — ¹MPI for the

Physics of Complex Systems, Dresden, Germany — ²cfaed, TU Dresden, Dresden, Germany — ³MRC Laboratory for Molecular Cell Biology, University College London, UK — ⁴Department of Biochemistry, University of Geneva, Geneva, Switzerland

We present a theoretical framework of self-organized growth control, inspired by the mutual interplay of pattern formation and growth in developing organisms. There, signaling molecules instruct tissue growth, while in turn growth changes the spatial concentration profiles of the molecules, e.g. by convection and dilution. By studying this feedback loop between chemical pattern formation and growth dynamics, we identify a critical point that corresponds to perfect proportionate pattern scaling and homogeneously growing domains.

We apply our theory to two biological models systems, the wing and the eye of the fruit fly *Drosophila melanogaster*. Despite their different developmental dynamics, our theoretical framework can quantitatively explain patterning and growth in both systems, including proportionate scaling of chemical patterns with tissue size. This observation suggests that the biological system is tuned close to criticality, in order to generate pattern scaling and homogeneous growth.

BP 59.4 Fri 10:30 HÜL 386

Active T1 transitions in the developing wing imaginal disc — ●MARKO POPOVIC¹, NATALIE DYE², GUILLAUME SALBREUX³, SUZANNE EATON², and FRANK JÜLICHER¹ — ¹Max Planck Institute for Physics of Complex Systems — ²Max Planck Institute of Molecular Cell Biology and Genetics — ³Francis Crick Institute

The adult wing of the fruit fly develops from a precursor tissue called imaginal disk. We study the wing pouch region of the wing imaginal disk, a single layer epithelium from which the adult wing blade forms. Observing the two-dimensional network of cells in the wing pouch projected on a plane reveals a radially symmetric pattern of elongated cell shapes. Peripheral cells have larger apical area and are more elongated tangentially than central ones. How does this cell shape pattern emerge and how is it related to mechanical forces in the tissue?

We study this process in third instar larval wing disks growing in culture over 13 hours. We track individual cells in time and space and identify different cellular processes: divisions, extrusions and neighbor exchanges. We calculate contributions of these cellular processes to the tissue shape changes. We use a hydrodynamic theory to relate tissue stresses to tissue deformations and cell shape changes [Etournay et al. eLife e07090; Etournay et al. eLife e14334; Merkel et al., arXiv:1607.00357; Popovic et al., arXiv:1607.03304].

We find that the tangential elongation of cell shapes increases over time in the cultured discs. We further find that active radially oriented T1 transitions contribute to tissue shape change. We solve the hydrodynamic equations for a radially symmetric tissue to investigate how active T1 transitions can influence mechanical stresses in the tissue.

BP 59.5 Fri 10:45 HÜL 386

How demixing and crowding behavior influence the invasive potential of composite tumor-like systems — ●PAUL HEINE, JÜRGEN LIPPOLDT, STEFFEN GROSSER, and LINDA OSWALD — Soft Matter Physics, University of Leipzig, Germany

The progression of cancer invasion is regulated through microenvironmental properties and their transformation for example in compartment penetration but critically also by the tumor composition itself. The heterogeneity of this system gives rise to an interesting phenomenon termed the jamming transition, a switch from a fluid-like unjammed

cell layer to an almost solid-like state.

While not entirely understood, recent studies have revealed that single-cell properties like contractility, cortical tension, adhesion and motility influence this transition and have an profound impact on the cell layer behavior in a crowded environment. During the epithelial-mesenchymal transition a plethora of mechanical and biochemical changes lead to a drastic shift in cell polarity, shape, cell-cell adhesion, migratory and invasive properties.

Our investigation of mixed systems of metastatic and benign cells exposed a demixing process of the two cell types and vastly different crowding performance. While epithelial cells form a dense sheet of caged cells, the mesenchymal-like cells compose seemingly uncaged pools within the layer. This makes this a particularly fascinating system to study due to its bifurcational nature, which could allow for a transition between fluid and solid cell layer and vice versa.

BP 60: Physics of Parasites - Joint Focus Session (BP/DY) organized by Holger Stark

Time: Friday 9:30–12:15

Location: SCH A251

Invited Talk

BP 60.1 Fri 9:30 SCH A251

Spontaneous curvature and membrane curling for malaria-infected erythrocytes — ●MANOUK ABKARIAN^{1,2}, OCTAVIO ALBARRAN ARRIAGADA², GLADYS MASSIERA², CYRIL CLAUDET^{1,2}, ANDREW CALLAN JONES², VLADIMIR LORMAN², and CATHERINE BRAUN BRETON³ — ¹Centre de Biochimie Structurale, Montpellier, France — ²Laboratoire Charles Coulomb, Montpellier, France — ³Dynamique des Interactions Membranaires Normales et Pathologiques, Montpellier, France

The culminating step of the intra-erythrocytic development of *P. falciparum*, the causative agent of malaria, is the spectacular release of multiple invasive merozoites upon rupture and curling of the infected erythrocyte membrane in a split second. We rationalized curling egression by the acquisition of a high (negative) natural curvature c_0 by the iEM, at a moment during parasite development. In this presentation, we will discuss our current investigation on curling both experimentally and theoretically. In particular, we will show with recent data that c_0 is acquired several hours before maturation, by inducing a metastable curled and opened pore state in the iEM. I will discuss such stability using a more sophisticated model of the iEM taking into account its axisymmetry, the pore line tension and the iEM shear elasticity. Our model captures such a metastability and predicts the dynamics during egress when considering the internal and external viscous dissipations of the iEM. In particular, our approach underlines the importance of the membrane viscous flow thanks to the study of macroscopic elastic naturally curved ribbons.

BP 60.2 Fri 10:00 SCH A251

Shape and adhesiveness of malaria-infected red blood cells — ANIL KUMAR DASANNA, MARCO LINKE, MAILIN WALDECKER, CHRISTINE LANSCHKE, SIRIKAMOL SRISMITH, MAREK CYRKLAF, CECILIA P. SANCHEZ, MICHAEL LANZER, and ●ULRICH S. SCHWARZ — Heidelberg University

An infection of a red blood cell by the malaria parasite takes approximately 48 hours and during this time, the host cell is completely remodelled by the parasite. In particular, the parasite induces an adhesive structure on the host cell surface that keeps the infected red blood cell (iRBC) in the vasculature for a longer time and thus avoids clearance by the spleen. At the end of the infectious cycle, the iRBC ruptures and around 20 new parasites are released into the blood stream. Using fluorescence microscopy and image processing, we have found experimentally that during this process, the surface area of the iRBC is relatively constant, while the volume increases by 60 percent due to increased osmotic pressure, leading to a final reduced volume of 1 and thus to a spherical shape. This shape transition becomes apparent at the schizont stage (40 hours after infection). Using flow chamber experiments, we show that at the same time, the movement of iRBC under flow on endothelial monolayers changes from flipping to rolling adhesion. Using adhesive dynamics simulations, we systematically predict the effect of the adhesive structure on the rolling adhesion of schizont-stage iRBC, in good agreement with our experimental results.

BP 60.3 Fri 10:30 SCH A251

Deadly microswimmers - how trypanosomes move in blood and navigate in the tsetse fly — SARAH SCHUSTER, TIM KRÜGER, and ●MARKUS ENGSTLER — Department of Cell and Developmental Biology, Biocenter, University of Würzburg, Würzburg, Germany

Trypanosomes are flagellate microswimmers and causative agents of deadly human diseases. The parasites swim freely in the blood and tissue fluids of their mammalian hosts, where they employ hydrodynamic drag to escape immune destruction. We found that different

trypanosomes species reveal distinct motion patterns, which allows adaptations to diverse infection niches. Cell motility is essential for trypanosome survival, not only in the mammal, but also in the transmitting insect, the blood sucking tsetse fly. Within the tsetse, the parasites pass through different microenvironments and undergo several developmental transitions. This involves crossing various barriers and confined surroundings, concurrent with major morphological changes. This lecture introduces the trypanosome microswimmer system and focuses on the tsetse fly stages. Light sheet fluorescence microscopy is presented as a powerful tool for the 3D analysis of geometries within the tsetse fly's digestive tract. High spatio-temporal resolution microscopic analyses reveal how the different forms of trypanosomes exploit obstacles and borders for navigation in a complex environment. Transitions between solitary swimming and swarming mark the 30 days long journey of the trypanosomes through the fly. The parasites' behaviours range from self-avoidance to collective motion. We suggest that the trypanosome system is well suited for addressing some fundamental questions related to active motion in the world of low Reynolds numbers.

15 min break

BP 60.4 Fri 11:15 SCH A251

An *in silico* model for the African trypanosome — ●HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The African trypanosome is the causative agent of the sleeping sickness and there is tremendous interest in understanding all aspects of how it moves forward and how it interacts with its environment. This includes the blood flow in blood vessels and passing the brain-blood barrier. Therefore, in the past years we have developed an *in silico* model for the African trypanosome, which fairly well captures its swimming motion [1-3]. The trypanosome has a conventional eukaryotic flagellum attached to its body. When a bending wave runs along the flagellum, the whole body deforms and is able to swim in the liquid environment, which we model with a particle-based solver of the Stokes equations called multi-particle collision dynamics.

With the help of the *in silico* model, we are able to demonstrate that the helical attachment of the flagellum optimizes the swimming speed [3], which helps the trypanosome to dispose of antibodies. We also simulate different morphotypes that occur during the parasite's development in the tsetse fly [3]. Finally, we address swimming in confinement and demonstrate that nearby channel walls or obstacles help the trypanosome to move forward.

[1] S. B. Babu and H. Stark, New J. Phys. **14**, 085012 (2012).

[2] N. Heddergott *et al.*, PLoS Pathogen **8**, e1003023 (2012).

[3] D. Alizadehrad, T. Krüger, M. Engstler, and H. Stark, PLoS Comput. Biol. **11**, e1003967 (2015).

BP 60.5 Fri 11:45 SCH A251

The development of a novel malaria diagnostic device — ●AGNES ORBAN¹, ADAM BUTYKAI¹, PETRA MOLNAR¹, MARIA PUKANCSIK¹, TIVADAR ZELLES², STEPHAN KARL³, and ISTVAN KEZSMARKI¹ — ¹Dept. of Physics, Budapest Uni. of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, HU — ²Dept. of Oral Biology, Semmelweis University, 1089 Budapest, HU — ³Infection and Immunity Division, Walter and Eliza Hall Institute of Medical Research, Parkville, Victoria, AU

Although malaria is the most threatening parasitic disease worldwide and a global health issue, the current standard for its detection still remains the microscopic observation of stained blood smears. A novel

cost-effective, automated, yet sensitive diagnostic method is needed for malaria detection both as an in-field instrument and as a laboratory tool for malaria researchers.

Our group aims to design such a device based on the detection of the magnetically induced linear dichroism of the malaria pigment crystals (hemozoin) by replacing the conventional polarization-modulation detection scheme with a rotating magnetic field. This concept enables a very high sensitivity detection of both synthetic and natural malaria pigment crystals as tested on suspensions of synthetic hemozoin; on hemozoin produced by *in vitro* *Plasmodium falciparum* cultures and on *in vivo* mouse models and human samples.

My brief introduction into the technological background will be followed by the presentations of the test results by my colleagues.

BP 60.6 Fri 12:00 SCH A251

Pre-clinical testing of a novel malaria diagnostic device — •PETRA MOLNAR¹, AGNES ORBAN¹, ADAM BUTYKAI¹, MARIA PUKANCSIK¹, ISTVAN KEZSMARKI¹, TIVADAR ZELLES², ISTVAN KUCSERA³, JETSUMON PRACHUMSRI⁴, and STEPHAN KARL⁵ — ¹Dept of Physics, Budapest Uni. of Technology and Economics and

MTA-BME Lendület Magneto-optical Spectroscopy Research Group, 1111 Budapest, HU — ²Dept of Oral Biology, Semmelweis Uni., 1089 Budapest, HU — ³National Center for Epidemiology, 1097 Budapest, HU — ⁴Mahidol Vivax Research Center (MVRC) of Mahidol Uni., Bangkok, TH — ⁵Infection and Immunity Division, Walter and Eliza Hall Institute of Medical Research, Parkville, Victoria, AU

We have developed a compact and inexpensive rotating-crystal magneto-optical diagnostic (RMOD) device based on the detection of hemozoin crystals, a metabolic byproduct of all *Plasmodium* species. The first step of the in-field validation had been carried out in Thailand. To assess the diagnostic performance of the RMOD technique, 50 field-collected frozen human blood samples were measured at the MVRC. The RMOD method was also tested in collaboration with Dr. Stephan Karl, using field samples (n≈800) previously collected from symptomatic children prior to treatment and following combination therapies at Modilon Hospital in Papua New Guinea. These samples, well characterized by light microscopy and quantitative PCR, have offered an ideal opportunity to i) assess the diagnostic capability of the RMOD method and ii) study the hemozoin clearance kinetics in patient samples.

BP 61: Topological Problems in the Physics of Polymers, Biopolymers and Fibers II (Joint Focus Session CPP/BP)

Time: Friday 10:15–13:00

Location: ZEU 222

BP 61.1 Fri 10:15 ZEU 222

Mechanical properties of entwined knotted/unknotted DNA loops — •SAEED NAJAFI and RAFFAELLO POTESIO — MPIP, Mainz, Germany

Self-entanglement and knotting can play a crucial role in the mechanical and functional properties of bio-polymers such as DNA and RNA strands and fibers. By means of computer simulations of model DNA systems, we demonstrate that the crossing pattern of a braid of entwined DNA rings has a large impact on its structural and dynamical properties. In particular, we identify under which conditions the braid crossing pattern enforces a positive and stronger correlation between the entangled rings.

BP 61.2 Fri 10:30 ZEU 222

Entropic interactions between two knots on a semiflexible polymer — •STEFANIE STALTER, DAVID RICHARD, JONATHAN SIEBERT, and PETER VIRNAU — Institut für Physik, JGU Mainz Staudingerweg 7, 55128 Mainz

Two knots on a string can either be separated or intertwined and may even pass through each other. On the microscopic scale such transitions may occur spontaneously driven by thermal fluctuations and can be associated with a topological free energy barrier. In this manuscript we study the respective location of a trefoil (3_1) and a figure-of-eight (4_1) knot on a semiflexible polymer, which is parameterized to model dsDNA in physiological conditions. Two cases are considered: First, end monomers are grafted to two confining walls of varying distance. Free energy profiles and transition barriers are then compared to a subset of free chains, which contain exactly one 3_1 and one 4_1 knot. For the latter we observe a small preference to form an intertwined state, which can be associated with an effective entropic attraction.

BP 61.3 Fri 10:45 ZEU 222

Knotted and unknotted ring polymers under shear — •MAXIMILIAN LIEBETREU and CHRISTOS N. LIKOS — Faculty of Physics, University of Vienna, Austria

The behavior of single 3_1 -knotted (trefoil) rings in a fluid under shear is compared to their unknotted ring polymer counterparts. We simulate flexible polymers of a fixed size in a thermostatted Multi-Particle Collision Dynamics (MPCD) solvent (with fixed control parameters) with Lees-Edwards boundary conditions. We primarily investigate the differences in shape parameters for 3_1 -knotted and 0_1 -unknotted rings in dependency of shear rate, as well as characteristics of average number of beads being part of the knot (knot size), angle between knot center of mass and first principal axis relative to the polymer's center of mass, and correlations between these quantities. We compute the relaxation time of 3_1 -knotted rings and present results on their tumbling- and tank-treading dynamics. We obtain evidence suggesting that on a knotted ring, the 3_1 knot itself develops a tendency to be

located near those beads closest to the orientational axis, aligned with the flow. We also show that the average knot size is decreasing with increasing shear. Preliminary findings indicate the 3_1 -knotted rings responding to lower shear rates than their unknotted counterparts, and suggest a binary-state behavior for the 3_1 -knotted ring under strong shear, with the knot size alternating between rather stable tight and relatively unstable delocalised configurations. Special attention is paid to the correlation between alignment angle and knot size.

Invited Talk

BP 61.4 Fri 11:00 ZEU 222

Protein Folding under Mechanical Load — •MATTHIAS RIEF — Physikdepartment der TU München, James-Frank-Str. 85748 Garching

The development of nano-mechanical tools like AFM and optical traps has made it possible to address individual biomolecules and study their response to mechanical forces. These techniques allow us to study and induce conformational changes of proteins in real time. In my talk, I will show how single molecule mechanical methods can be used to study folding of proteins. Examples will include the folding of the calcium binding protein calmodulin, as well as the folding of a protein with knotted structure.

15 min break

BP 61.5 Fri 11:45 ZEU 222

Entropic vs Energetic stiffness in biopolymers — •TATJANA ŠKRBIČ¹, ACHILLE GIACOMETTI¹, TRINH HOANG², ARTEM BADASYAN³, and RUDOLF PODGORNİK⁴ — ¹University of Venice, Italy — ²Institute of Physics, Hanoi, Vietnam — ³University of Nova Gorica, Slovenia — ⁴University of Ljubljana, Slovenia

Homopolymers form a high temperature swollen (coil) phase and a low temperature phase globular phase. The glassy nature of this ground state stems from the inability of homopolymers to reduce their entropy as temperature is decreased.

Recent attempts to introduce additional ingredients allowing the removal of this glassy ground state and hence the onset of alpha-helical and beta-sheet like structures, characteristic of proteins, will be presented. In particular, it will be shown how the introduction of an entropic stiffness breaks the spherical symmetry of the interactions and leads to the formation of protein secondary structures.

Further, the difference between this entropic stiffness and the conventional energetic stiffness characteristic of semi-flexible polymers will be pointed out, as well as the relevance of the latter for the ground state phase diagram of DNA in a bad solvent.

Finally, the relevance of the presented results for the protein design, as well as for the interpretation of experimental results on the DNA condensation, will be discussed.

References [1] T. Škrbič et al, J. Chem. Phys. (2016) [2] T. Škrbič

et al, Soft Matter (2016) [3] T.X. Hoang et al, Phys. Rev. E (2015)
[4] T.X. Hoang et al, J. Chem. Phys. (2014)

Invited Talk

BP 61.6 Fri 12:00 ZEU 222

All-atom simulations of folding of proteins with topologically complex native structures. — ●PIETRO FACCIOLO and SILVIO A BECCARA — Physics Department , Trento University, Trento, Italy

Investigating protein folding using MD remains a formidable task. Using the Anton supercomputer it is now possible to perform folding simulations of small globular proteins, with folding times in the ms scale. On the other hand, proteins with topologically complex or even knotted native structures can take much longer to fold. Thus investigating these processes by plain MD is well beyond the reach of any present nor foreseen supercomputer.

Our group has developed an enhanced path sampling approach based

on a rigorous variational approximation, which enables to simulate the folding of protein of virtually any size with folding time as long as tens of minutes using all atom force fields. This method has been first validated against the results of Anton and then applied to larger systems with increasingly complex topology. In this talk I will review our recent results concerning the folding of the smallest knotted protein and of a serpin, a large (~400 amino-acid) misfold-prone protein with a very complex native structure architecture.

In both cases we find that, in contrast to what happens to simpler globular proteins, sequence-dependent non-native interactions are playing an important role in guiding the folding process, in particular by ensuring that the native contacts are formed in the right order.

30 min panel discussion