Biological Physics Division
Fachverband Biologische Physik (BP)

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Overview of Invited Talks and Sessions
(Lecture rooms H43, H44, and H45; Poster C)

Plenary Talks with special interest for BP

PV I	Mon	8:30– 9:15	H1	**Merging light with nanoparticles: artificial molecules, photocatalysis, cancer therapy, and solar steam** — •Naomi J. Halas
PV IV	Mon	14:00–14:45	H1	**Recent Advances and Opportunities in Electron Microscopy of Materials** — •Ulrich Dahmen
PV XV	Wed	14:00–14:45	H1	**Taming Molecules in Hybrid Nanosystems** — •Jürgen P. Rabe
PV XXIV	Thu	14:00–14:45	H15	**Single-Molecule Spectroscopy of Biomolecular Dynamics at the Nanoscale** — •Ben Schuler

Invited Talks

BP 2.1	Mon	9:30–10:00	H43	**Multicellular Streaming in Solid Tumours** — •Josef Käs, Franziska Wetzel, Anatol Fritsch, Steve Pawlizak, Linda Oswald, Steffen Grosser, Lisa Manning, Cristina Marchetti, Michael Höckel, John Condeelis
BP 3.1	Mon	9:30–10:00	H44	**Structural Dynamics of Single G-protein Coupled Receptors** — •Emmanuel Margeat
BP 7.1	Mon	11:15–11:45	H45	**Relating biological networks to gene expression patterns** — •Marc-Thorsten Hütt
BP 8.1	Mon	11:30–12:00	H43	**Prospects of super-resolution optical microscopy for studying membrane bioactivity** — •Christian Eggeling, Marco Fritzsche, Erdinc Sezgin
BP 11.4	Mon	16:00–16:30	H43	**Chromophore Photophysics in Fluorescent Proteins of the GFP family** — •Gerd Ulrich Nienhaus
BP 12.1	Mon	15:00–15:30	H45	**Imaging of G-protein coupled receptors while quantifying their ligand-binding free energy landscape to mutiple ligands** — •Daniel J. Müller, David Alsteens, Moritz Pfreundschuh, Patrizia M. Spoerri, Shaun R. Coughlin, Cheng Zhang, Brian K. Kobilka
BP 27.1	Tue	9:30–10:00	H43	**Membrane proteins under voltage: simulations of ion channels and receptors at work** — •Ulrich Zachariae
BP 28.1	Tue	9:30–10:00	H44	**Molecular Bioimaging of Genome Transcription** — •Patrick Cramer
BP 28.5	Tue	11:15–11:45	H44	**The biosynthetic basis of budding yeast cell size control** — •Kurt M. Schmoller, Jonathan J Turner, Mardo Koivomägi, Devon Chandler-Brown, Jan M. Skotheim
BP 29.1	Tue	9:30–10:00	H45	**Cell Migration in Confined Geometries** — •Joachim O. Rädler, Felix J. Segerer, Anna-Kristina Marel, Matthias L. Zorn, Christoph Schreiber, Peter Röttgermann, Alexandra Fink, Florian Thüroff, Erwin Frey
BP 36.1	Wed	9:30–10:00	H43	**Molecular simulation of protein dynamics and function** — •Gerhard Hummer

BP 37.1	Wed	9:30–10:00	H44	**Reconstituting basic mitotic spindles in artificial confinement —** •Marileen Dogterom
BP 38.1	Wed	9:30–10:00	H45	**Optogenetics: Basics, Applications and Chances —** •Ernst Bamberg
BP 38.2	Wed	10:00–10:30	H45	**The mechanical control of CNS development and functioning —** •Kristian Franze
BP 43.1	Wed	15:00–15:30	H43	**Cellular Mechanosensing —** •Rudolf Merkel
BP 44.1	Wed	15:00–15:30	H45	**Physics for the Origins of Life —** •Dieter Braun
BP 57.1	Thu	9:30–10:00	H43	**Monolayer curvature induced nanoscale structures in lipid membranes** — •Friederike Schmid
BP 58.1	Thu	9:30–10:00	H44	**Cytoskeletal coordination —** •Gijsje Koenderink
BP 58.8	Thu	11:45–12:15	H44	**Single molecule studies on myosin motors —** •Claudia Veigel
BP 59.1	Thu	9:30–10:00	H45	**RNA-based gene circuits in vitro and in vivo —** •Friedrich Simmel
BP 65.1	Thu	15:00–15:30	H43	**Design features of a membrane-assisted protein oscillator —** •Petra Schwille

Invited talks of the joint symposium Anomalous Diffusion in Complex Environments (SYAD)
See SYAD for the full program of the symposium.

SYAD 1.1	Thu	15:00–15:30	H15	**Phenomenology of Collective Chemotaxis in Artificial and Living Active Matter —** •Ramin Golestanian
SYAD 1.2	Thu	15:30–16:00	H15	**First-passage times of Markovian and non Markovian random walks in confinement —** •Raphael Voituriez
SYAD 1.3	Thu	16:00–16:30	H15	**Cytoskeleton organization as an optimized, spatially inhomogeneous intermittent search strategy —** •Heiko Rieger, Yannick Schröder, Karsten Schwarz
SYAD 1.4	Thu	16:45–17:15	H15	**Ergodicity violation and ageing in living biological cells —** •Ralf Metzler
SYAD 1.5	Thu	17:15–17:45	H15	**Anomalous diffusion within cells —** Sarah Klein, •Cecile Appert-Rolland, Ludger Santen

Invited talks of the joint symposium Scientometric Maps and Dynamic Models of Science and Scientific Collaboration Networks (SYSM)
See SYSM for the full program of the symposium.

SYSM 1.1	Thu	9:30–10:00	H1	**Science Forecasts: Measuring, Predicting, and Communicating Scientific Developments —** •Katy Börner
SYSM 1.2	Thu	10:00–10:30	H1	**Mapping science with variable-order Markov dynamics reveal overlapping fields and multidisciplinary journals —** •Martin Rosvall
SYSM 1.3	Thu	10:30–11:00	H1	**Network algorithms for reputation and quality in scholarly data —** •Matúš Medo, Manuel Mariani, Yi-Cheng Zhang
SYSM 1.4	Thu	11:15–11:45	H1	**Modeling scientific networks in social media —** •Cassidy Sugimoto
SYSM 1.5	Thu	11:45–12:15	H1	**Modeling scientific collaboration across multiple scales: from individuals to Europe —** •Alexander Petersen

Invited talks of the joint symposium Chimera States: Coherence-Incoherence Patterns in Complex Networks (SYCS)
See SYCS for the full program of the symposium.

SYCS 1.1	Tue	9:30–10:00	H1	**Theory far from infinity: chimera states without the thermodynamic limit —** •Daniel Abrams
SYCS 1.2	Tue	10:00–10:30	H1	**Chimera patterns: Influence of topology, noise, and delay —** •Eckehard Schöll
SYCS 1.3	Tue	10:30–11:00	H1	**Chimera states in quantum mechanics —** •Victor Manuel Bastidas Valencia
SYCS 1.4	Tue	11:15–11:45	H1	**Synchronization in Populations of Chemical Oscillators: Phase Clusters and Chimeras —** •Kenneth Showalter
SYCS 1.5	Tue	11:45–12:15	H1	**Epileptic seizures: chimeras in brain dynamics —** •Klaus Lehnertz

Sessions

BP 1.1–1.3	Sun	16:00–18:30	H16	**Tutorial: Evolutionary Dynamics and Applications to Biology, Social and Economic Systems (SOE/DY/BP/jDPG)**
BP 2.1–2.5	Mon	9:30–11:00	H43	**Physics of Cancer**
BP 3.1–3.8	Mon	9:30–12:15	H44	**Protein Structure and Dynamics**
BP 4.1–4.6	Mon	9:30–11:00	H45	**Colloids and Complex Fluids I (Joint Session BP/CPP/DY)**
BP 5.1–5.11	Mon	9:30–13:00	H51	**Colloids and Complex Fluids II (Joint Session CPP/DY/BP)**
BP 6.1–6.6	Mon	10:00–11:30	H36	**Networks: From Topology to Dynamics I (Joint Session SOE/DY/BP)**
BP 7.1–7.6	Mon	11:15–13:00	H45	**Coupled Problems in Biological Systems (Focus Session)**
BP 8.1–8.4	Mon	11:30–12:45	H43	**Bioimaging and Spectroscopy I**
BP 9.1–9.4	Mon	12:15–13:15	H36	**Evolutionary Game Theory (Joint Session SOE/DY/BP)**
BP 10.1–10.11	Mon	15:00–18:00	H42	**Colloids and Complex Fluids III (Joint Session CPP/DY/BP)**
BP 11.1–11.7	Mon	15:00–17:15	H43	**Bioimaging and Spectroscopy II**
BP 12.1–12.6	Mon	15:00–17:15	H45	**Single Molecule Biophysics**
BP 13.1–13.2	Mon	17:30–19:30	Poster C	**Posters - Anomalous Diffusion in Complex Environments**
BP 14.1–14.3	Mon	17:30–19:30	Poster C	**Posters - Biotechnology and Bioengineering**
BP 15.1–15.4	Mon	17:30–19:30	Poster C	**Posters - Complex Fluids and Soft Matter**
BP 16.1–16.10	Mon	17:30–19:30	Poster C	**Posters - Computational Biophysics**
BP 17.1–17.2	Mon	17:30–19:30	Poster C	**Posters - Coupled Problems in Biological Systems: Model Identification, Analysis and Predictions**
BP 18.1–18.6	Mon	17:30–19:30	Poster C	**Posters - DNA, RNA and Related Enzymes**
BP 19.1–19.11	Mon	17:30–19:30	Poster C	**Posters - Membranes and Vesicles**
BP 20.1–20.4	Mon	17:30–19:30	Poster C	**Posters - Molecular Dynamics**
BP 21.1–21.1	Mon	17:30–19:30	Poster C	**Posters - Nanoparticles, Nanocrystals and Composites**
BP 22.1–22.6	Mon	17:30–19:30	Poster C	**Posters - Neurosciences**
BP 23.1–23.5	Mon	17:30–19:30	Poster C	**Posters - Protein Structure and Dynamics**
BP 24.1–24.6	Mon	17:30–19:30	Poster C	**Posters - Single Molecule Biophysics**
BP 25.1–25.1	Mon	17:30–19:30	Poster C	**Posters - Systems Biology**
BP 26.1–26.5	Tue	9:30–12:15	H1	**Symposium - Chimera States: Coherence-Incoherence Patterns in Complex Networks (SYCS)**
BP 27.1–27.7	Tue	9:30–11:45	H43	**Computational Biophysics**
BP 28.1–28.8	Tue	9:30–12:30	H44	**Systems Biology & Gene Expression and Signalling**
BP 29.1–29.10	Tue	9:30–12:45	H45	**Multicellular Systems**
BP 30.1–30.12	Tue	9:30–13:00	H47	**Microswimmers I (Joint Session with DY)**
BP 31.1–31.4	Tue	12:00–13:00	H43	**Statistical Physics of Biological Systems I (Joint Session with DY)**
BP 32.1–32.4	Tue	14:00–15:00	H36	**Chimera State: Symmetry breaking in dynamical networks (joint session SOE/DY/BP)**
BP 33.1–33.5	Tue	14:00–15:15	H46	**Colloids and Complex Fluids IV (Joint Session DY/BP/CPP)**
BP 34.1–34.6	Tue	14:00–15:30	H47	**Anomalous Diffusion (Joint Session with DY)**
BP 35.1–35.3	Tue	15:00–15:45	H36	**Networks: From Topology to Dynamics II (Joint Session SOE/DY/BP)**
BP 36.1–36.5	Wed	9:30–11:00	H43	**Molecular Dynamics (Focus Session)**
BP 37.1–37.10	Wed	9:30–12:45	H44	**Cell Mechanics and Migration**
BP 38.1–38.5	Wed	9:30–11:15	H45	**Neurosciences**
BP 39.1–39.11	Wed	9:30–12:45	H46	**Active Matter (Joint Session with DY)**
BP 40.1–40.4	Wed	11:30–12:30	H43	**Statistical Physics of Biological Systems II (Joint Session with DY)**
BP 41.1–41.6	Wed	11:30–13:00	H45	**Microswimmers II (Joint Session with DY)**
BP 42.1–42.11	Wed	15:00–18:15	H40	**Biomaterials and Biopolymers I (Joint Session CPP/MM/BP)**
BP 43.1–43.7	Wed	15:00–17:00	H43	**Cell Adhesion**
BP 44.1–44.6	Wed	15:00–16:45	H45	**Biotechnology & Bioengineering**
BP 45.1–45.3	Wed	15:30–16:15	H46	**Statistical Physics in Biological Systems III (Joint Session with DY)**
BP 46.1–46.6	Wed	17:00–19:00	Poster C	**Posters - Biomaterials and Biopolymers**
BP 47.1–47.2	Wed	17:00–19:00	Poster C	**Posters - Active Matter**
BP 48.1–48.20	Wed	17:00–19:00	Poster C	**Posters - Bioimaging and Spectroscopy**
BP 49.1–49.21	Wed	17:00–19:00	Poster C	**Posters - Cell Mechanics and Migration & Physics of Cancer**
BP 50.1–50.7	Wed	17:00–19:00	Poster C	**Posters - Cell Adhesion**
BP 51.1–51.5	Wed	17:00–19:00	Poster C	**Posters - Cytosceletal Filaments**

BP 52.1–52.4	Wed	17:00–19:00	Poster C	**Posters - Multi-Cellular Systems**
BP 53.1–53.11	Wed	17:00–19:00	Poster C	**Posters - Statistical Physics of Biological Systems**
BP 54	Wed	19:00–20:00	H43	**BP Mitgliederversammlung (Annual General Meeting of the Biological Physics Division)**
BP 55.1–55.5	Thu	9:30–12:15	H1	**Symposium - Scientometric Maps and Dynamic Models of Science and Scientific Collaboration Networks (SYSM)**
BP 56.1–56.8	Thu	9:30–12:45	H37	**The Physics of Water Interactions with Biological Matter (Joint Focus Session with CPP)**
BP 57.1–57.10	Thu	9:30–12:45	H43	**Membranes and Vesicles I**
BP 58.1–58.11	Thu	9:30–13:00	H44	**Cytoskeletal Filaments**
BP 59.1–59.5	Thu	9:30–11:00	H45	**DNA, RNA and Related Enzymes**
BP 60.1–60.12	Thu	9:30–13:00	H46	**Pattern Formation (Joint Session with DY)**
BP 61.1–61.6	Thu	11:30–13:00	H45	**Anomalous Diffusion in Complex Environments (Focus Session)**
BP 62.1–62.5	Thu	11:45–13:00	H52	**Biomaterials and Biopolymers II (Joint Session MM/CPP/BP)**
BP 63.1–63.1	Thu	14:00–14:45	H15	**Plenary Talk of Ben Schuler**
BP 64.1–64.5	Thu	15:00–17:45	H15	**Symposium - Anomalous Diffusion in Complex Environments (SYAD)**
BP 65.1–65.4	Thu	15:00–16:15	H43	**Membranes and Vesicles II**
BP 66.1–66.5	Thu	15:00–16:15	H45	**Biomaterials and Biopolymers III (Joint Session BP/CPP/MM)**
BP 67.1–67.6	Thu	15:30–17:00	H47	**Networks: From Topology to Dynamics III (Joint Session DY/SOE/BP)**
BP 68.1–68.4	Thu	16:45–17:45	H43	**Networks - From Topology to Dynamics IV (Joint Session BP/SOE/DY)**

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

Wednesday   19:00–20:00   H43

- Poster Awards
- Report of the current speakers
- Lessons learned and spring meeting Dresden 2017
- Miscellaneous

BP 1: Tutorial: Evolutionary Dynamics and Applications to Biology, Social and Economic Systems (SOE/DY/BP/jDPG)

Current model approaches for collective phenomena in biological, social and economic systems widely employ methods from statistical physics. This sequence of tutorial talks demonstrates how physical concepts allow the formulation of appropriate microscopic models, the numerical and analytical treatment to obtain phase diagrams and macroscopic equations of motion. Host-virus coevolution, social opinion formation and systemic risk of the interbank network are research frontiers illustrating fruitful applications (Session compiled by J.C.Claussen)

Time: Sunday 16:00–18:30   Location: H16

Tutorial   BP 1.1   Sun 16:00   H16
Predicting evolution: statistical mechanics and biophysics far from equilibrium — •Michael Lässig — Institut für theoretische Physik, Zülpicher Strasse 77, D-50937 Köln

The human flu virus undergoes rapid evolution, which is driven by interactions with its host immune system. We describe the evolutionary dynamics by a fitness model based on two biophysical phenotypes of the virus: protein folding stability and susceptibility to human immune response. This model successfully predicts the evolution of influenza one year into the future, which has important consequences for public health: evolutionary predictions can inform the selection of influenza vaccine strains. Based on this example, we discuss the role of statistical mechanics and biophysics in making evolutionary biology a predictive science.

Tutorial   BP 1.2   Sun 16:50   H16
Voter models of social opinion formation. — •Katarzyna Sznajd-Weron — Department of Theoretical Physics, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw

Among many different subjects, opinion dynamics is one of the most studied in the field of sociophysics. In my opinion there are at least two important reasons why physicists study this topic. The first motivation comes from social sciences and can be described as a temptation to build a bridge between the micro and macro levels in describing social systems. Traditionally, there are two main disciplines that study social behavior - sociology and social psychology. Although the subject of the study is the same for both disciplines, the usually taken approach is very different. Sociologists study social systems from the level of the social group, whereas social psychologists concentrate on the level of the individual. From the physicist's point of view this is similar to the relationship between thermodynamics and statistical physics. This analogy raises the challenge to describe and understand the collective behavior of social systems (sociology) from the level of

interpersonal interactions (social psychology). The second motivation to deal with opinion dynamics is related to the development of non-equilibrium statistical physics, because models of opinion dynamics are often very interesting from the theoretical point of view. A good example of such an interesting model is a broad class of voter models, including linear voter model and nonlinear q-voter model introduced in along with its modifications.

Tutorial   BP 1.3   Sun 17:40   H16
Maximum-entropy methods for network reconstruction, systemic risk estimation, and early-warning signals — •Diego Garlaschelli — Lorentz Institute for Theoretical Physics, University of Leiden, The Netherlands

The global financial crisis shifted the interest from traditional measures of "risk" of individual banks to new measures of "systemic risk", defined as the risk of collapse of an entire interbank system. In principle, estimating systemic risk requires the knowledge of the whole network of exposures among banks. However, due to confidentiality issues, banks only disclose their total exposure towards the aggregate of all other banks, rather than their individual exposures towards each bank. Is it possible to statistically reconstruct the hidden structure of a network in such a way that privacy is protected, but at the same time higher-order properties are correctly predicted? In this talk, I will present a general maximum-entropy approach to the problem of network reconstruction and systemic risk estimation. I will illustrate the power of the method when applied to various economic, social, and biological systems. Then, as a counter-example, I will show how the Dutch interbank network started to depart from its reconstructed counterpart in the three years preceding the 2008 crisis. Over this period, many topological properties of the network showed a gradual transition to the crisis, suggesting their usefulness as early-warning signals of the upcoming crisis. By definition, these early warnings are undetectable if the network is reconstructed from partial bank-specific information.

BP 2: Physics of Cancer

Time: Monday 9:30–11:00   Location: H43

Invited Talk   BP 2.1   Mon 9:30   H43
Multicellular Streaming in Solid Tumours — •Josef Käs[1], Franziska Wetzel[1], Anatol Fritsch[1], Steve Pawlizak[1], Linda Oswald[1], Steffen Grosser[1], Lisa Manning[2], Cristina Marchetti[2], Michael Höckel[1], and John Condeelis[3] — [1]Leipzig University — [2]Syracuse University — [3]Albert-Einstein College

As early as 400 BCE, the Roman medical encyclopaedist Celsus recognized that solid tumours are stiffer than surrounding tissue. However, cancer cell lines are softer, and softer cells facilitate invasion. This paradox raises several questions: Does softness emerge from adaptation to mechanical and chemical cues in the external microenvironment, or are soft cells already present inside a primary solid tumour? If the latter, how can a more rigid tissue contain more soft cells? Here we show that in primary tumour samples from patients with mammary and cervix carcinomas, cells do exhibit a broad distribution of rigidities, with a higher fraction of softer and more contractile cells compared to normal tissue. Mechanical modelling based on patient data reveals that, surprisingly, tumours with a significant fraction of very soft cells can still remain rigid. Moreover, in tissues with the observed distributions of cell stiffnesses, softer cells spontaneously self-organize into lines or streams, possibly facilitating cancer metastasis.

BP 2.2   Mon 10:00   H43
Stochastic tunneling and metastable states during the somatic evolution of cancer — Peter Ashcroft[1], Franziska Michor[2], and •Tobias Galla[1] — [1]School of Physics and Astronomy, The University of Manchester, UK — [2]Department of Biostatistics and Computational Biology, Dana-Farber Cancer Institute and Department of Biostatistics, Harvard School of Public Health, Boston, MA, USA

Tumors initiate when a population of cells accumulates a certain number of genetic and/or epigenetic alterations. Sometimes an intermediate mutant in a sequence does not reach fixation before generating a double mutant, this is referred to as 'stochastic tunelling'. Here, we focus on stochastic tunneling in a Moran model. Our analysis reveals fitness landscapes and mutation rates for which finite populations are found in long-lived metastable states. The escape from these states is driven by intrinsic noise, and their location affects the probability of tunneling. In these regimes it is the escape from the metastable states that is the key bottleneck; fixation is no longer limited by the emergence of a successful mutant lineage. We use the Wentzel-Kramers-Brillouin (WKB) method to compute fixation times, successfully validated by stochastic simulations. Our work fills a gap left by previous approaches and provides a more comprehensive description of the ac-

quisition of multiple mutations in populations of somatic cells.

Reference: P. Ashcroft, F. Michor, T. Galla, Genetics 199 (2015) 1213.

BP 2.3   Mon 10:15   H43
Liquid-like and Solid-like Behaviour of Breast Cancer Cell Lines in 3D Aggregates — ●LINDA OSWALD, STEFFEN GROSSER, STEVE PAWLIZAK, ANATOL FRITSCH, and JOSEF KÄS — University of Leipzig, Institute of Experimental Physics I, 04103 Leipzig, Germany

Three-dimensional aggregates of biological cells become increasingly relevant in research as they resemble in vivo situations much closer than two-dimensional assays. These tissue models are usually described by viscous liquid theories on long time scales. Recent experiments on 3D segregation of breast cancer cell lines questioned this approach.

Based on this finding, we create aggregates of MCF-10A, MDA-MB-436, which form compact spheroids, and of MDA-MB-231 cells, forming loose aggregates only. We perform fusion experiments of the spheroids allowing to assess the ratio of tissue surface tension to viscosity. While MDA-MB-436 spheroids fuse mainly as expected from the viscous liquid theory, MCF-10A spheroids show a rich diversity in fusion behaviour, such as changing fusion speeds and complete fusion arrest accompanied by superficial morphological changes.

BP 2.4   Mon 10:30   H43
Comparison of the visco-elastic properties of cancer and normal cells by step-response AFM — ●CARMELA RIANNA, HOLGER DOSCHKE, JENS SCHÄPE, and MANFRED RADMACHER — Institute of Biophysics, University of Bremen, Germany

We have measured the visco-elastic creep response of cancer cells on different stiffness polyacrylamide gels and compared it with normal cells of the same type. In conventional force indentation curves the viscous and elastic properties cannot be measured separately. So, these data are usually only analyzed in terms of elastic response, even though the response of the cell to a moving AFM tip is viscous and elastic at the same time. Applying a force step in contact and recording the creep relaxation of the cell allows separating the viscous and elastic response independently. This can be converted in the storage and loss modulus as is usually done in soft matter rheology. We have cultured cells on three different substrates: polyacrylamide gels of 5 kPa and 50 kPa, respectively, and "infinitely" stiff Petri dishes. Normal cells showed an increase of the storage modulus from 1 kPa, to 1.5 kPa to 2.2 kPa with increasing sample stiffness. Whereas cancer cells showed a storage modulus around 1.2 kPa, more or less independent of sample stiffness. The loss modulus was around 400 Pas for cancer cells, where normal cells showed an increase from 250 Pas, to 600 Pas and to 700 Pas with increasing stiffness. There is a large difference in adaption of cancer and normal cells to the substrate stiffness. Whereas normal cells sense the softness of the substrate and adapt to it, cancer cells do not change their visco-elastic properties according to it.

BP 2.5   Mon 10:45   H43
Cell sorting in breast cancer cell lines: Driven by differential adhesion? — STEVE PAWLIZAK[1], ANATOL FRITSCH[1], ●STEFFEN GROSSER[1], LINDA OSWALD[1], DAVE AHRENS[1], TOBIAS THALHEIM[1], M. LISA MANNING[2], and JOSEF ALFONS KÄS[1] — [1]University of Leipzig, Institute of Experimental Physics I, 04103 Leipzig, Germany — [2]Syracuse University, Department of Physics, Syracuse, NY 13244, USA

Demixing of differentiating cells into different compartments, resulting in tissues with stable boundaries, is a crucial process during embryogenesis, which is usually thought of being driven by differential adhesion of the cells. This stable sorting of cells is disrupted in metastasis, questioning if differential adhesion plays the decisive role here, too.

We use a panel of three different breast cancer cell lines from different sides of the epithelial-mesenchymal transition to test the differential adhesion hypothesis (DAH) in this environment. We employ a variety of measurement techniques to asses mechanical properties of cells on the single-cell level, comprising cell-cell adhesion, cell stiffness, cell shapes, and cadherin densities. We compare these results to multicellular 3D sorting experiments and show that the results are at odds with predictions from the DAH. The behaviour of multi-cellular aggregates even shows deviations from the basic assumption of tissue liquidity on long timescales.

These findings suggest that dynamical effects such as directional motility or jamming might be key players in cancer development.

BP 3: Protein Structure and Dynamics

Time: Monday 9:30–12:15   Location: H44

Invited Talk   BP 3.1   Mon 9:30   H44
Structural Dynamics of Single G-protein Coupled Receptors — ●EMMANUEL MARGEAT — Centre de Biochimie Structurale, UMR 5048 CNRS, INSERM U1054, Université de Montpellier, France

Efficient cell-to-cell communication relies on the accurate signaling of cell surface receptors. Understanding the molecular bases of their activation requires the characterization of the dynamic equilibrium between active and resting states. Here, we monitor, using single molecule Förster resonance energy transfer, the kinetics of the activation of metabotropic glutamate receptor (mGluR), a class C G-protein coupled receptor (GPCR) activated by glutamate, the major excitatory neurotransmitter in the central nervous system. By combining filtered Fluorescence Correlation Spectroscopy (fFCS), excited stated lifetime analysis and Photon Distribution (PDA) analysis on single diffusing receptors, we demonstrate that most receptors oscillate between a resting- and an active- conformation on a sub-millisecond timescale. Interestingly, we demonstrate that differences in agonist efficacies stem from differing abilities to shift the conformational equilibrium toward the fully active state, rather than from the stabilization of alternative static conformations, which further highlights the dynamic nature of mGluRs and revises our understanding of receptor activation and allosteric modulation.

BP 3.2   Mon 10:00   H44
Scaling rules for vibrational energy transport in globular proteins — ●SEBASTIAN BUCHENBERG GEB. WALTZ[1], DAVID M. LEITNER[2], and GERHARD STOCK[1] — [1]Biomolekulare Dynamik Physik Uni-Freiburg — [2]Chemistry University of Nevada/Reno

Computational studies of vibrational energy flow in biomolecules have to date mapped out transport pathways on a case by case basis [1]. To provide a more general approach, we derive scaling rules for vibrational energy transport in a globular protein, which are identified from extensive nonequilibrium molecular dynamics simulations of vibrational energy flow in the villin headpiece subdomain HP36 [2]. We parameterize a master equation based on inter-residue, residue-solvent and heater-residue energy transfer rates which closely reproduces the results of the all-atom simulations. From that fit two scaling rules emerge. The first for the energy transport along the protein backbone which is described by a diffusion model in which the local diffusion strongly depends on the size of the individual amino acid side chain. And the second for the energy transport between tertiary contacts which is based on a harmonic description and depends on the coupling strength of the contact and the charge of the atoms in contact. Requiring only the calculation of mean and variance of relatively few atomic distances, the approach is able to predict the pathways and timescales of vibrational energy flow in proteins.

[1] D. M. Leitner, S. Buchenberg, P. Brettl and G. Stock, J. Chem. Phys. 142, 075101 (2015) [2] S. Buchenberg, D. M. Leitner and G. Stock, submitted (2015)

BP 3.3   Mon 10:15   H44
Peptides in Presence of Aqueous Ionic Liquids: Tunable Co-Solutes as Denaturants or Protectants? — VOLKER LESCH[1], ANDREAS HEUER[1], DIDDO DIDDENS[1], CHRISTIAN HOLM[2], and ●JENS SMIATEK[2] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]Institut für Computerphysik, Universität Stuttgart, D-70569 Stuttgart, Germany

We studied the stability of a small beta-hairpin peptide under the influence of aqueous 1-ethyl-3-methylimidazolium acetate ([EMIM]+ [ACE]-) solution via all-atom molecular dynamics simulations in combination with metadynamics. Our free energy results indicate a denaturation of the peptide structure in presence of the ionic liquid which is

validated by a significant broadening of the end-to-end distance. The radial distribution functions between the ions and the peptide were used for the calculation of the preferential binding coefficients in terms of the Kirkwood-Buff theory. A significant structure dependent binding of acetate to the peptide was found which can be interpreted as the main reason for the denaturation of the native conformation. The outcomes of our simulations allow us to propose a simple mechanism to explain the unfolding of the peptide with regard to the specific properties of ionic liquids. Our results are in good agreement with experimental findings and demonstrate the benefits of ionic liquids as tunable co-solutes with regard to their influence on protein structural properties.

BP 3.4   Mon 10:30   H44

The C-terminus of human copper importer, Ctr1, acts as binding site and transfers copper to Atox1 — ●Michael Kovermann[1,2], Dana Kahra[2], and Pernilla Wittung-Stafshede[2,3] — [1]Fachbereich Chemie, Universität Konstanz, Germany — [2]Department of Chemistry, Umeå University, Sweden — [3]Department of Biology and Bioengineering, Chalmers University of Technology, Sweden

Uptake of copper ions (Cu) into human cells is mediated by the plasma membrane protein Ctr1, followed by Cu transfer to cytoplasmic Cu chaperones for delivery to Cu-dependent enzymes. The C-terminal cytoplasmic tail of Ctr1 is a 13-residue peptide harboring a HCH motif thought to interact with Cu. We here employ biophysical experiments under anaerobic conditions to peptide models of the Ctr1 C-terminus to deduce Cu-binding residues, Cu affinity and ability to release Cu to the cytoplasmic Cu chaperone Atox1. Based on NMR assignments and bicinchoninic acid competition experiments, we demonstrate that Cu interacts in an one-to-one stoichiometry with the HCH motif with an affinity K_D of 10^{-14} M. Removing either the Cys residue or the two His residues lowers the Cu-peptide affinity but site specificity is retained. The C-terminal peptide and Atox1 does not interact in solution in the absence of Cu. However, as directly demonstrated at the residue level via NMR spectroscopy, Atox1 readily acquires Cu from the Cu-loaded peptide. We propose that Cu binding to the Ctr1 C-terminal tail regulates Cu transport into the cytoplasm such that the metal ion is only released to high-affinity Cu chaperones.

30 min break

BP 3.5   Mon 11:15   H44

Dynamics of dissolved BSA studied by QENS: MD simulations compared to experiments — ●Christian Beck[1], Marco Grimaldo[2], Felix Roosen-Runge[2], Tilo Seydel[2], Fajun Zhang[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]Institut Laue - Langevin, Grenoble, France

Recent improvements in the field of quasi-elastic neutron scattering (QENS) offer the possibility to explore simultaneously the global movements and the internal dynamics of proteins in solution [1,2]. While the global diffusion can be described by colloidal models, different non-consistent descriptions exist for the internal dynamics. To address this challenge, scattering functions are calculated from atomically resolved molecular dynamics (MD) simulations of bovine serum albumin in solution for a temperature series crossing the denaturation temperature, analysed with a two-state model of switching diffusing processes and compared with experimental data [1].Furthermore, we implemented the model of fractional Brownian dynamics [3].
For both models, the analysis is expanded onto broader energy windows compared to the experimental one to test the limits of the models and alsoto open the possibility to combine results from different neutron spectrometers such as time-of-flight and backscattering instruments.

[1] M.Grimaldo et al. Phys. Chem. Chem. Phys., **17** (2015) 4645
[2] M.Grimaldo et al. J. Phys. Chem. B **118** (2014) 7203
[3] I.Krasnov et al. Phys. Rev. E **91** (2015) 042716

BP 3.6   Mon 11:30   H44

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 are ubiquitous folding motifs found in proteins. They consist of two alpha-helices wrapped around each other in a super helix configuration. In biological systems, coiled coils 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 find that the pulling force at slow constant pulling speed is independent of either the total length or the contact length of the coiled-coils, and is the same as the force for unfolding a single alpha-helix. The results suggest that short coiled-coils under slow shear strain move via a dislocation mechanism: a defect is created at the pulled end of the helix and travels to the other end of the helix in tens of nanoseconds.

BP 3.7   Mon 11:45   H44

Photo-dynamics of photoactivated adenylyl cyclase LiPAC from the spirochete bacterium *Leptonema illini* strain 3055 — ●Alfons Penzkofer[1], Meenakshi Tanwar[2], Sindu Kandoth Veetil[2], and Suneel Kateriya[2,3] — [1]Fakultät für Physik, Universität Regensburg, Universitätsstraße 31, D-93053 Regensburg, Germany — [2]Department of Biochemistry, University of Delhi South Campus, Benito Juarez Road, New Delhi 110021, India — [3]School of Biotechnology, JNU, New Delhi 110067, India

The photoactivated adenylyl cyclase LiPAC from the spirochete bacterium *Leptonema illini* was synthesized and characterized by absorption and fluorescence spectroscopic methods [1]. LiPAC consists of a BLUF domain and an adenylyl cyclase homology domain. Photo-excitation of fully oxidized flavin in LiPAC resulted in a typical primary BLUF domain photo-cycle dynamics. The quantum efficiency of BLUF domain signaling state formation was determined to be 0.60. Continued blue-light-excitation of LiPAC in the light-adapted state caused irreversible photo-degradation of non-covalently bound flavin to covalently bound fully reduced flavin with a quantum efficiency of 1.1×10^{-5}. At 20 °C the time constant of signaling state recovery to the receptor state after excitation light switch-off was 2.6 s. The protein thermal stability was studied by stepwise sample heating and cooling. A LiPAC melting temperature of 54 °C was determined. Schemes of the primary BLUF domain photo-cycling dynamics and the secondary BLUF domain photo-degradation in the signaling state are presented.

[1] A. Penzkofer et al., Trends in Applied Spectroscopy 11 (2014) 39.

BP 3.8   Mon 12:00   H44

Protein anisotropy modulates the coupling between rotational and translational diffusion under crowding conditions — ●Matthias Roos[1], Maria Ott[1], Marius Hofmann[2], Susanne Link[1], Jochen Balbach[1], Ernst Rössler[2], Alexey Krushelnitsky[1], and Kay Saalwächter[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Germany — [2]Universität Bayreuth, Lehrstuhl Experimentalphysik II, Germany

In vivo molecular motion of biopolymers is known to be strongly influenced by excluded-volume effects caused by the high concentration of organic matter inside cells, usually referred to as crowding conditions. In order to further understand the effects on translational and rotational diffusion, we performed pulsed-field gradient and field-cycling NMR, X-ray scattering and viscosity measurements for three proteins in water solution - αB-crystallin, bovine serum albumin and lysozyme. Our results demonstrate, on the one hand, that long-time translational diffusion quantitatively follows the expected increase of macro-viscosity upon increasing the protein concentration. The behavior of rotational diffusion, on the other hand, turns out to be protein-specific and spans the full range between the limiting cases of full coupling and full decoupling from the macro-viscosity. We show that the anisotropy of inter-protein interactions, in particular of electrostatic nature, is the main factor modulating the (de)coupling between rotational and long-time translational diffusion.

BP 4: Colloids and Complex Fluids I (Joint Session BP/CPP/DY)

Joint session with CPP and DY organized by BP.

Time: Monday 9:30–11:00   Location: H45

BP 4.1 Mon 9:30 H45

Intracellular microfluidics to probe the role of hydrodynamic flows in embryonic cell polarization — Matthäus Mittasch[1], •Peter Gross[2], Stephan Grill[2], and Moritz Kreysing[1] — [1]MPI-CBG, Dresden, Germany — [2]Biotechnolgy Center, TU Dresden, Dresden, Germany

A hallmark of embryogenesis is the development of spatial structure. This process is orchestrated by gene regulatory networks coupled to physical transport mechanisms. Particularly, it was suggested that the polarization of the egg cell of the nematode worm Caenorhabditis elegans, prior to asymmetric cell division, relies on interaction of two protein networks (PAR proteins) coupled to active cortical flows. However, it remains a challenge to perturb intracellular fluid mechanics to demonstrate the causal role of hydrodynamic flows in embryogenesis. Towards this end, we exploited thermo-viscous pumping (Weinert & Braun, J. appl. Phys. 2008) in order to dynamically control hydrodynamic flows inside of living embryos. Specifically, well-defined flow patterns were generated on sub- and cellular length-scales with velocities exceeding wild-type flows significantly, without affecting the biological integrity of the embryo. By application of externally-induced flows we depleted membrane-bound PAR proteins locally, suggesting that hydrodynamic flows are essential to load PAR proteins at the posterior pole. Furthermore, we perform rescue experiments in a non-polarizing embryo, by which the omitted wild-type flow will be applied externally to test if the PAR polarity can be restored artificially.

BP 4.2 Mon 9:45 H45

Phase behavior of dense lysozyme solutions — •Julian Schulze[1], Johannes Möller[2], Michael Paulus[1], Julia Nase[1], Metin Tolan[1], and Roland Winter[3] — [1]Fakultät Physik/Delta, Technische Universität Dortmund,44221 Dortmund ,Germany — [2]ESRF - The European Synchrotron, 38043 Grenoble, France — [3]Fakultät für Chemie und Chemische Biologie, Technische Universität Dortmund, 44221 Dortmund, Germany

In previous studies, small-angle X-ray scattering (SAXS) in combination with liquid-state theoretical approaches and DLVO theory was used to study the intermolecular interaction potential V(r) of lysozyme solutions under the influence of varying environmental conditions such as protein concentration c, temperature T, and pressure p. While the repulsive Coulomb term of the DLVO potential remains almost constant as a function of p, the depth of the attractive part, J(p), exhibits a non-monotonic p-dependence with a minimum at about 2 kbar at constant T. Adding 0.5 M NaCl leads to more prominent short range interactions, especially at high c and low T, and the homogeneous protein solution becomes turbid due to formation of a metastable liquid-liquid phase separation (LLPS) region, where lysozyme forms small droplets of high concentration within the more dilute liquid phase. At elevated pressures, this l-l phase separation is suppressed, but due to the non-monotonic behavior of J(p), a further pressure increase leads to a re-entrant LLPS regime. In this contribution, we will discuss the phase behavior of lysozyme as a function of c, p, and T.

BP 4.3 Mon 10:00 H45

Demixing and Ripening in Gradient Systems — •Christoph Weber[1], Chiu Fan Lee[2] und Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Department of Bioengineering, Imperial College, London

Ostwald ripening in homogeneous mixtures is described by the Lifshitz-Slyozov theory. It captures the phenomenon of smaller droplets that shrink, while larger ones grow. This process is driven by a difference in the Laplace pressures between the drops. Recently, liquid-like drops have been reported in living cells, which ripen in a gradient of a regulating protein component. This protein is known to affect the phase separation properties along the gradient such that drops dissolve at one and grow at the opposite side of the cell. An open question is how an inhomogeneous background affects the ripening law in contrast to the homogeneous Lifshitz-Slyozov theory.

To this end we analytically derived the corresponding growth law using a mean field theory. We find that there is a gradient of supersaturation that leads to a drift and an inhomogeneous growth of drops.

The latter gives rise to a dissolution boundary that moves through the system leaving droplets only at one side of the system.

Using our mean field approach to describe the interactions between multiple drops we discover that a larger gradient of supersaturation not necessarily implies a faster ripening. Instead, droplets can be spatially sorted in size leading an arrest of the ripening dynamics for large times until homogeneous Ostwald-ripening sets in again.

BP 4.4 Mon 10:15 H45

New analysis method for passive microrheology — •Kengo Nishi[1], Maria L. Kilfoil[2], Christoph F. Schmidt[1], and Fred C. MacKintosh[3] — [1]Georg-August-Universität Göttingen, Göttingen, Germany — [2]University of Massachusetts, Amherst, USA — [3]Vrije Universiteit, Amsterdam, Netherland

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. Microrheology is well suited to study rheological properties of materials that are difficult to obtain in larger amounts and also of materials inside of single cells. 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. Here, we discuss how to obtain more accurate values of the real part of the response function by an alternative method using autocorrelation functions.

BP 4.5 Mon 10:30 H45

How to regulate droplet position in a heterogeneous chemical environment? — •Samuel Krüger[1,2], Christoph A. Weber[1], Jens-Uwe Sommer[2,3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Leibniz Institute of Polymer Research Dresden e.V., Dresden — [3]Technische Universität Dresden, Institute of Theoretical Physics, Dresden, Germany

Cells contain chemical components that are not separated from the cytoplasm by a membrane. An example are P-granules in the C. elegans embryo. They are liquid-like structures, that form droplets. They consist of RNA and proteins that are segregated spontanuously from the cytoplasm and are known to play a role in the specification of germ cells. During asymmetric cell division, P granules are segregated to one side of the cell. This segregation is guided by a spatial concentration gradient of the protein Mex-5. We simplify the multicomponent nature of the cytoplasm with a ternary model: The P granule material, the solvent (cytoplasm), and a regulator corresponding to Mex-5. Using this model we aim to understand the physical principles controlling the droplet position in a simplified scenario, where an external potential establishes the regulator gradient. We use the Flory-Huggins mean field theory and calculate the equilibrium solutions by minimizing the free energy functional. There are two equilibrium states. Droplets either localize at high external potential or low external potential. Changing the interaction between the regulator and the solvent we find that the free energy exhibits a kink indicating that the transition between both states being a discontinuous phase transition.

BP 4.6 Mon 10:45 H45

Finding descriptive features for the characterization of the coarsening dynamics of three dimensional foams — •Jonas Dittmann[1], Anja Eggert[2], Martina Lambertus[1], Jannika Dombrowski[3], Alexander Rack[4], and Simon Zabler[1,2] — [1]Lehrstuhl für Röntgenmikroskopie, Fakultät für Physik und Astronomie, Universität Würzburg, Germany — [2]Fraunhofer EZRT, Fürth, Germany — [3]Wissenschaftszentrum Weihenstephan, Technische Universität München, Germany — [4]European Synchrotron Radiation Facility (ESRF), Grenoble, France

Understanding the coarsening behavior of foams is essential for their deliberate design. The coarsening theories by Lifshitz, Slyozov and Wagner (LSW) as well as Glazier provide concise coarsening models with descriptive parameters that may enable systematic studies on the effects of different foam constituents.

Wet polydisperse beta-Lactoglobulin foam was imaged by fast synchrotron micro computed tomography over a period of 15 minutes in intervals of 2 to 5 minutes. The growth behavior of about 2×10^5 pores is individually observed and statistically analyzed as a function of pore radius as well as number of neighboring pores.

The three-dimensional analog of von Neumann's law by Glazier is confirmed as a fitting empirical description of the mean coarsening behavior, whereby the critical number of neighbors discriminating between shrinkage and growth is found to be 13.2 ± 5.5. Qualitative features of LSW theory are observed as well: the pore's growth rate increases with their size and a critical radius can be identified.

BP 5: Colloids and Complex Fluids II (Joint Session CPP/DY/BP)

Time: Monday 9:30–13:00   Location: H51

Invited Talk   BP 5.1   Mon 9:30   H51
Dynamics of thermosensitive core-shell dumbbells as analyzed by rheo-SANS — •Matthias Ballauff — Helmholtz-Zentrum Berlin

We present a study of the dynamics of dumbbell-shaped colloids. The thermosensitive dumbbell-shaped microgels consist of a solid polystyrene core and a thermosensitive shell of cross-linked poly(N-isopropylacrylamide). These colloidal particles are nearly monodisperse as shown by cryogenic transmission electron microscopy. The aspect ratio L* defined by the ratio of the center distance L to the diameter D can be varied between 0.24 and 0.3. The effective volume fraction can be varied by temperature and high volume fractions can be achieved easily because of the thermosensitive shell [1]. We observe the formation of a plastic crystal in these suspensions about of volume fraction of 0.5 as predicted by theory. This is shown from rheological evidence and by the Bragg-reflections of the crystals. For higher volume fraction a glassy state is formed. Moreover, oscillatory experiments in the linear viscoelastic regime and flow curves up to volume fractions of nearly 0.7 have been obtained. Recent studies based on a combination of rheoSANS experiments and BD-simulations revealed the formation of a novel, partially oriented phase formed by dumbbells under shear. All data demonstrate that these particles present a novel model system for the study of the rheology of slightly anisotropic particles.

[1] F. Chu, et al., Macromol. Rapid Comm. 33 (2012) 1042.

BP 5.2   Mon 10:00   H51
Phase diagram of polydisperse colloidal dispersions — •Preecha Kiatkirakajorn[1], Joaquim Li[1], Bernard Cabane[2], Franck Artzner[3], Robert Botet[4], and Lucas Goehring[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Götingen, Germany — [2]LCMD, CNRS UMR 8231, ESPCI, 10 rue Vauquelin, 75231 Paris Cedex 05, France — [3]Institut de Physique, CNRS UMR 6626, Univ Rennes, 35042 Rennes, France — [4]Physique des Solides, CNRS UMR 8502, Univ Paris-Sud, F-91405 Orsay, France

Polydisperse colloidal dispersions have been predicted, for over twenty years, to have a rich and complex phase space of colloidal crystals. However, experiments have consistently suggested that such crystals are kinetically inaccessible, as small amounts of polydispersity poison crystal formation. Here, we show a result of small-angle X-ray scattering experiment of highly polydisperse (yet monomodal) colloidal dispersions in a range of sizes (average size from 8 to 50 nm), with soft, charge-mediated interactions. These dispersions were dialysed and compressed by aqueous solutions of poly(ethylene glycol) to reach 15% to 30% of volume fraction, and crystallize. Their phase diagrams, structure factors and crystal peaks were analysed by the x-ray scattering patterns. We found coexistences of complex crystal structures (two BCC structures and Laves AB2) for the small particle size, and BCC and FCC crystals for the larger particle size. These results show a fractionation among the particles. We further show how this is possible through numerical simulations, which explain how the fractionation occurs and how the particles distribute among the different coexisting phases.

BP 5.3   Mon 10:15   H51
Free energies, liquid and crystal phases of the Asakura–Oosawa model: a density functional theory study — •Mostafa Mortazavifar and Martin Oettel — Institut für Angewandte Physik, Uni Tübingen, Tübingen, Germany

The Asakura–Oosawa(AO) model is a well known model for studying colloid–polymer mixtures in which the depletion interaction between colloidal particles results in a phase diagram similar to molecular liquids. More importantly, it is a generic model system for short range attractive colloidal particles. We have studied the model by means of density functional theory (DFT) by applying a linearization of a two–component fundamental measure hard sphere tensor functional with respect to the second (polymer) component. The linearized functional gives a unified description of gas, liquid, and crystal phases. We have calculated the free energies and phase diagrams for a variety of colloid–polymer size ratios. The results are in good agreement with available simulations. For small size ratios, the model can be mapped exactly to a one–component system with a short–range attractive potential between the colloids. Standard mean field approximations fail in describing the liquid and crystal phases; here our functional offers novel insights how to construct generically density functional descriptions of interparticle attractions.

BP 5.4   Mon 10:30   H51
Crystallization of sheared nearly hard-spheres — •David Richard and Thomas Speck — Staudingerweg 9, 55128 Mainz

Understanding crystallization pathways and kinetics is a long standing challenge in condensed matter science. Additionally, the effect of impurities and external fields is also a matter of debate. In this study, we look at the effect of a simple linear shear flow on the crystallization of nearly hard-spheres [1]. By varying the density from low to high supersaturation, we find a crossover from shear-suppressed crystallization to an enhanced crystallization kinetics. We attribute this crossover under shear to the vanishing nucleation barrier in the quiescent system, at which nucleation is changing from an activated to a diffusive limited process.

[1] Richard, David, and Thomas Speck. 'The Role of Shear in Crystallization Kinetics: From Suppression to Enhancement.' Scientific Reports 5 (2015).

BP 5.5   Mon 10:45   H51
On the influence of the softness of the potential on the phase diagrams of core-shell micelles - a simulation study — •Heiko G. Schoberth, Heike Emmerich, and Thomas Gruhn — Lehrstuhl Material- und Prozesssimulation, Universität Bayreuth, D-95440 Bayreuth

Quasicrystals are of continuous interest due to their fascinating fundamental properties and their promising applications as advanced photonic materials in a range of optical devices. In the last years colloidal quasicrystals have been found in solutions with spherical polymer core-shell micelles. With these colloids and their intriguing possibility to self-assemble in a broad range of nanoscale and microscale quasicrystalline structures, the demand arises of understanding the complex formation mechanism and the thermodynamic stability of these structures. Especially, it is important to find a direct relation between the stability of the structures and the main parameters of the micelle-micelle interaction. We perform coarse-grained molecular dynamics simulation to investigate the dependence of the phase diagram on the softness of the interaction potential. The core-core interaction is modelled by infinite repulsion, whereas the shell-shell interaction is varied from a stiff to a very soft potential. Varying the core to shell radius and packing fraction we study systematically the change in the phase diagram finding domains with 10-,12-,18-,24-fold quasicrystalline symmetries. With increasing smoothness of the potential the phase diagram changes qualitatively and the geometry of the phase boundaries gets more regular.

BP 5.6   Mon 11:00   H51
Estimation of crystal nucleation barriers for colloidal crystals from computer simulations — •Peter Koss[1,2], Antonia Statt[1], Peter Virnau[1], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [2]Graduate School of Excellence Materials Science in

Mainz, Staudinger Weg 9, 55128 Mainz, Germany

A fluid in equilibrium in a finite volume, with a density exceeding the onset of freezing, may exhibit phase coexistence of a crystal nucleus surrounded by liquid. In classical nucleation theory, the barrier of homogeneous nucleation is given by two contributions, the energy gain of creating a droplet and the energy loss due to surface tension of the newly created interface. Using a computational method suitable for the estimation of the chemical potential of dense fluids we obtain the excess free energy due to the surface of the crystalline nucleus. Our novel 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 report that the nucleation barrier for a soft version of the effective Asakura-Oosawa model[1] is compatible with a spherical shape, and consistent with classical nucleation theory [2].

[1] M. Dijkstra, R. van Roij and R. Evans, Phys. Rev. E 59, 5744-5771 (1999).
[2] A. Statt, P. Virnau, and K. Binder, Phys. Rev. Lett. 114, 026101 (2015).

BP 5.7 Mon 11:15 H51

Crystal nucleation in metastable hard sphere fluids by confocal microscopy — Achim Lederer[1] and •Hans Joachim Schöpe[2] — [1]Retsch Technology GmbH, Retsch-Allee 1-5, 42781 Haan, Germany — [2]Eberhards Karls Universität Tübingen, Auf der Morgenstelle 10, 72026 Tübingen, Germany

Crystal nucleation in colloidal hard spheres is a longstanding research topic. Light scattering and confocal microscopy as well as simulations had been carried out to characterize the nucleation process and to get a microscopic picture. In these studies results both differ and agree with each other. It is still unclear whether the large disagreement in the nucleation rate densities between the light scattering experiments and simulations are of physical nature or result from differing data analyses. Furthermore, the temporal evolution of the microscopic structure has not yet been characterized sufficiently. Using laser-scanning confocal microscopy we study crystal nucleation in colloidal hard spheres. The used system has been characterized with extreme care to allow for meaningful comparison with other experiments and simulations. Observing a large sample volume we can analyze the nucleation process with high accuracy. This allows us to obtain meaningful data of the nucleation rate density, critical nucleus size and nucleation barrier. Furthermore, we determine the time-dependent interfacial tension through how the cluster size distribution evolves. Analyzing the nucleation process on a microscopic scale, we confirm the scenario of precursor-mediated crystal nucleation. In addition we show in great detail the structure evolution from precursor to crystal.

15 min. break

Invited Talk   BP 5.8 Mon 11:45 H51

Percolation in colloidal model systems — •Tanja Schilling[1], Hugues Meyer[1], Mohit Dixit[1], Mark Miller[2], and Paul van der Schoot[3] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Department of Chemistry, Durham University, United Kingdom — [3]Theory of Polymers and Soft Matter, Technische Universiteit Eindhoven, 5600 MB Eindhoven, The Netherlands

Connectivity percolation is the transition in which isolated clusters of solid particles in a fluid become connected in some sense to form a system-spanning network. This network has a significant effect on the transport properties of the material on a macroscopic scale. If, for example, an electrically insulating polymer is mixed with conductive fibres such as carbon nanotubes, the conductivity of the composite increases by ten or more orders of magnitude near the percolation transition of the filler material.

We discuss percolation in suspensions of fibres and of platelets. Our study covers the entire range of aspect ratios from spheres to extremely slender rods and infinitely thin disks. The percolation threshold for rod-like particles of aspect ratios below 1000 deviates significantly from the inverse aspect ratio scaling prediction, thought to be valid in the limit of infinitely slender rods and often used as a rule of thumb for fibres in composite materials. We also show the effects of polydispersity on the percolation transition. The main result is that the percolation

threshold shows universal behaviour, i.e. it depends only on certain cumulants of the size distribution.

BP 5.9 Mon 12:15 H51

Towards flexible and dynamic self-assembly from colloids with magnetic anisotropy — •Gabi Steinbach[1,5], Dennis Nissen[2], Manfred Albrecht[2], Ekaterina V. Novak[3], Pedro Sánchez[4], Sofia Kantorovich[3,4], Sibylle Gemming[1,5], and Artur Erbe[5] — [1]Technische Universität Chemnitz, 09107 Chemnitz, Germany. — [2]University of Augsburg, 86159 Augsburg, Germany. — [3]Ural Federal University, 620000, Ekaterinburg, Russia. — [4]University of Vienna, 1090 Vienna, Austria. — [5]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany.

Magnetic colloidal particles are a suitable model system for the study of self-assembly and dynamic processes on the microscale. Here, we illustrate the potential of directed, but flexible bonds for tailored structure formation. As an example, we present a system of colloidal microspheres that have an off-centered net magnetic moment pointing perpendicular to the particle surface. They are an experimental realization of the theoretical model of spheres with radially shifted point dipole (sd-particles). Experimentally we observed the formation of branched structures as result of two coexisting self-assembly patterns, which is untypical for homogeneous systems. We show that the bistability can be explained by an extended model of sd-particles. This framework takes the broad magnetization distribution in the experimental particles into account. We will further show that the interacting particles exhibit interesting non-equilibrium dynamics when exposed to time-dependent fields, leading to reversible structural reconfigurations.

BP 5.10 Mon 12:30 H51

Enhanced magneto-optical response in dispersions of anisometric pigment particles — •Kathrin May, Alexey Eremin, and Ralf Stannarius — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39016 Magdeburg, Germany

Colloidal suspensions of anisometric particles show a variety of unique properties depending on particle concentration and external electric fields, such as the formation of ordered phases, phase separation, electro-optical effects, and non-linear rheology. Electro- and magneto-optical properties of colloids are of particular interest because of the possible applications in electrophoretic ink displays and other technologies. We demonstrate a binary colloidal system with an unusually strong magneto-optical response which is comparable with that of thermotropic liquid crystals. This system is based on a binary mixture of elongated non-magnetic pigment particles and a small volume fraction < 0.1 v/% of spherical magnetic nanoparticles. The birefringence is caused by a partial alignment of the pigment particles, controlled by anisometric agglomerates of the magnetic particles that form in a magnetic field. This effect is discussed in the frame of the Onsager-Lekkerkerker theory of sterical alignment transfer in binary mixtures of colloidal particles.

BP 5.11 Mon 12:45 H51

The initial magnetic susceptibility of cube-like magnetic colloids in dilute suspensions — •Joe Donaldson[1] and Sofia Kantorovich[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Ural Federal University, Lenin av. 51, 620083, Ekaterinburg, Russia

Magnetic nano/micro-particles are currently applied in many diverse research and industrial disciplines. These particles exhibit a number of interesting properties that can be utilised, leading to a number of established and developing applications. Most notably: magnetic drug targeting; magnetic hyperthermia cancer treatment; and ferrofluids. In each of these applications, a crucial piece of information is required; namely, some sort of insight into the magnetic behaviour of these particles. Ideally, one would like some indication of this a priori. As such, we present here theoretical and simulation studies on permanently magnetised particles that are actually cube-like in shape [1]. We have investigated the differences in magnetic behaviour arising from this additional directional interaction, focussing on the initial magnetic susceptibility of low-density suspensions.

[1] J. G. Donaldson and S. S. Kantorovich, Nanoscale, 2015, 7, 3217

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

Time: Monday 10:00–11:30   Location: H36

BP 6.1   Mon 10:00   H36

Revealing physical interaction networks from nonlinear dynamics — Jose Casadiego[1], Dimitra Maoutsa[1], Hauke Hähne[1], Mor Nitzan[2], and ●Marc Timme[1] — [1]Network Dynamics, MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

Structural connectivity of networks reflects the direct physical interactions between pairs of dynamical units, as opposed to effective, functional or other statistical measures of connectivity. How to uncover physical interaction structure from measured time series of networked systems remains an open question. Here we present a dynamical systems' view on collective network dynamics, thereby proposing an approach to reveal physical interaction networks from the nonlinear dynamics they generate. Introducing the notion of *explicit dependency matrices*, we present two examples: one, where the time series consists of the full network states as a function of time, the other, where the time series exhibits only partial information about the full states. We apply the latter to neural circuit dynamics where the observables are spike timing data, i.e. only a discrete, state-dependent output of the neurons. These results may help revealing network structure for systems where direct access to dynamics is simpler than to connectivity.
    For an introductory review of the state of the art, see
J. Phys. A: Math. Theor. 47 343001 (2014)
http://dx.doi.org/10.1088/1751-8113/47/34/343001

BP 6.2   Mon 10:15   H36

Theory and experiments on anomalous critical and supercritical connectivity transitions — ●Jan Nagler — ETH Zurich

The emergence of large-scale connectivity on an underlying network or lattice, the so-called percolation transition, has a profound impact on the system's macroscopic behaviours. There is thus great interest in controlling the location of the percolation transition to either enhance or delay its onset and, more generally, in understanding the consequences of such control interventions. Here we report on the sudden emergence of large-scale connectivity that results from repeated, small interventions designed to delay the percolation transition. These transitions exhibit drastic, unanticipated and sometimes exciting consequences in complex networked systems but also pose experimental challenges. In particular, I will report on both theoretical and experimental progress (D'Souza & Nagler, Nature Physics 11:531, 2015; Nagler et al., unpublished).

BP 6.3   Mon 10:30   H36

What does Big Data tell? Sampling the social network by communication channels — ●János Török[1,2], Yohsuke Murase[3], Hang-Hyun Jo[4,5], János Kertész[2,1,5], and Kimmo Kaski[5] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest H-1111, Hungary — [2]Center for Network Science, Central European University, Budapest H-1051, Hungary — [3]RIKEN Advanced Institute for Computational Science, Kobe, Hyogo 650-0047, Japan — [4]BK21plus Physics Division and Department of Physics, Pohang University of Science and Technology, Pohang 37673, Republic of Korea — [5]Department of Computer Science, Aalto University School of Science, P.O. Box 15500, Espoo, Finland

Big Data has become the primary source of understanding the structure and dynamics of the society at large scale. However, usually one has information only about one of the channels, which should be considered as a sample of the whole. We show by simulations and analytical methods that this sampling may lead to bias. For example, while it is expected that the degree distribution of the whole social network has a maximum at a value larger than one, we get with reasonable assumptions about the sampling process a monotonously decreasing distribution as observed in empirical studies of single channel data. Also we find, that assortativity may occur or get strengthened due to the sampling process. We analyze the far-reaching consequences of our findings.

BP 6.4   Mon 10:45   H36

Effective Distances in Complex Networks — Flavio Iannelli[1], ●Andreas Koher[2], Philipp Hövel[2], and Igor M. Sokolov[1] — [1]Humboldt Universität zu Berlin, Germany — [2]Technische Universität Berlin, Germany

The analysis of global epidemics revealed that physical distances can hardly be used to forecast the outbreak dynamics. Instead, a network-based measure which has been introduced recently [1] allows to predict infection arrival times with a surprisingly high accuracy. The so-called effective distances are solely based on the (weighted) network topology.
    We present an alternative approach, which is motivated by a fundamental property from the theory of random walks: The distribution of first passage times. This random walk based distance allows to forecast disease dynamics on various topologies. For the special case of highly heterogeneous networks it reduces to the previously introduced effective distance.
[1] Brockmann D, Helbing D "The hidden geometry of complex, network-driven contagion phenomena." Science. 2013;342(6164):1337–1342

BP 6.5   Mon 11:00   H36

A Geometrical Approach to Infection Dynamics on Temporal Networks — ●Felix Herrmann[1], Philipp Hövel[1], Vitaly Belik[1], Andreas Koher[1], Hartmut H. K. Lentz[2], and Dirk Brockmann[3,4] — [1]Institut für Theoretische Physik, Technische Universität Berlin — [2]Friedrich-Loeffler-Institut, Greifswald — [3]Institut für Theoretische Biologie, Humboldt-Universität zu Berlin — [4]Robert Koch-Institut, Berlin

We investigate the extension of a recently introduced geometrical approach for the description of spreading processes on static undirected networks [1] to directed temporal networks. Its key quantity is a probabilistically motivated "effective distance" between nodes, which is based on the weights of the links and allows reliable predictions of disease arrival times and the identification of the origin of spreading processes. The approach has already been successfully applied to study infection dynamics on a static undirected air traffic network [1].
    By demonstrating how this approach can be generalized, we contribute to a framework for the investigation of spreading dynamics on temporal networks. Specifically, we consider an empirical livestock trade network in Germany, consisting of 97,980 nodes (agricultural holdings) and 6,359,697 temporal edges (trade events) [2], and use a SIR model to simulate the local dynamics of the nodes. Strong fluctuations in the activity of the nodes render the application of the geometrical approach particularly challenging.
[1] D. Brockmann and D. Helbing, Science 342, 1337 (2013).
[2] H. H. K. Lentz et al., Phys. Rev. Lett. 110, 118701 (2013).

BP 6.6   Mon 11:15   H36

Controlling recurrent epidemics on temporal networks — ●Vitaly Belik[1,2], Florian Fiebig[1], Hartmut H K Lentz[3], and Philipp Hövel[1,4] — [1]Institut für Theoretische Physik, Technische Universität Berlin — [2]Helmholtz Zentrum für Infektionsforschung, Braunschweig — [3]Institute of Epidemiology, Friedrich-Loeffler-Institute, Greifswald — [4]Bernstein Center for Computational Neuroscience Berlin, Humboldt Universität zu Berlin

We consider a rucurrent epidemic on a temporal network. The goal of the control is to reduce the prevalence or make the epidemic extinct, respectively. To this end we propose a protocol based on rewiring the edges away from infected nodes, after they are detected as those: instead of an infected node, we randomly choose a healthy one (or perceived as such). In contrast to coevolutionary adaptive networks, the intrinsic dynamics of the network is taken into account by our approach alongside with the adaptive rewiring. The proposed control scheme significantly expands the range of a disease-free parameter region. For example, on the network of German pig trade, diseases with detection times up to 10 days and infectious periods up to 3 months could be efficiently controlled by our method [1]. Thus changing the behaviour of trading partners could have significant impact on the epidemic outcome.
[1]V Belik, F Fiebig, HHK Lentz, P Hövel arXiv preprint arXiv:1509.04054

BP 7: Coupled Problems in Biological Systems (Focus Session)

Focus session organized by Syn Schmitt and Nicole Radde, University of Stuttgart.

Time: Monday 11:15–13:00   Location: H45

Invited Talk   BP 7.1   Mon 11:15   H45
Relating biological networks to gene expression patterns —
●Marc-Thorsten Hütt — Jacobs University, Bremen, Germany

Understanding, how a gene expression pattern – the simultaneous measurement of gene activity for a large number of genes in a cell – emerges from the dynamics of a gene regulatory network is one of the key challenges at the interface of statistical physics and systems biology.

The last two decades have shown that the statistical physics of complex networks can serve as a powerful toolbox for addressing this challenge. The guiding questions are: (1) How is a gene expression pattern 'generated' by the underlying regulatory network? (2) What functional state (e.g., from the perspective of the cell's metabolic network) does the gene expression pattern define?

At the same time, the conceptual limitations of mapping an intricate biological system onto the formal language of nodes and links have become apparent.

Here I will describe recent developments in this field, starting from investigations of network topology and then moving to dynamics on graphs and, finally, to a network-guided interpretation of gene expression patterns in biology and medicine.

         BP 7.2   Mon 11:45   H45
A basic mechanical model of muscular contraction —
●Michael Günther, Daniel F.B. Haeufle, and Syn Schmitt —
Universität Stuttgart, Institut für Sport- und Bewegungswissenschaft

There is a rich history of quantitative experiments on muscle contraction. Mainly two mathematical approaches are applied to disentangle this hairball. First, A.V. Hill (1938) observed a fibre's steady-state force-velocity relation to be a hyperbola. Later, A.F. Huxley (1957) suggested a mathematical model based on cross-bridges making filaments slide. Using eleven model parameters, Huxley could reproduce in 1973 Hill's relation including its modification from 1964. However, both approaches are not explanatory in a sense that they derive, e.g., the force-velocity relation from basic, physical principles and laws. This led us to ask: what mechanical structure can explain skeletal muscle contractions? As a possible answer, we have worked out a basic mechanical model that can explain, by a force equilibrium between four elements, altogether six characteristic relations of both steady-state and non-steady-state muscular contractions at once. Compared to modern Huxley-type models, the number of parameters is dramatically reduced: we need just six parameters in common plus another two for the steady-state and another three for known microscopic force-length relations specific to non-steady-state responses. We suggest therefore our reduced model to be a promising alternative for advancing causal understanding of the relation between structure and function incorporated into the skeletal muscle machinery.

         BP 7.3   Mon 12:00   H45
Uncertainty analysis for dynamic models in systems biology
— ●Daniel Kaschek — Physikalisches Institut, Universität Freiburg, Deutschland

Dynamic models have gained increasing importance for the way we understand complex behavior in cell biology. Although the structure of such a model may be highly conserved between different cell types, experiments show that the parameter values are not. Therefore, reliable and efficient methods to determine parameter values from cell-type specific, time-resolved data are crucial for precise predictions.

Here, we present a collection of methods to determine parameter values, parameter uncertainty and uncertainty of prediction in non-linear dynamic models. Lie-group theory is employed to detect symmetries in the model and to eliminate structurally non-identifiable parameters. The profile-likelihood is introduced as an indispensable tool to determine parameter confidence bounds and explore the non-linear relationships between parameters. Also model predictions can be associated to special likelihood profiles and their uncertainty can thereby be accurately quantified. Finally, the method of Lagrangian multipliers is presented as a way to exploit the local structure of the likelihood, guide us quickly along the profile paths and make the likelihood-based methods even more efficient.

         BP 7.4   Mon 12:15   H45
Predicted error pushes pointing movements into the goal
— ●Karl Theodor Kalveram[1,2], Tim Lauer[2], Sebastian Babl[2], Christina Binder[2], Anna Klubertanz[2], Kristin Roehr[2], Elena Wicharz[2], Darya Yatsevich[2], and Joachim Vogt[2] — [1]Universitaet Duesseldorf — [2]Technische Universitaet Darmstadt

Movements of a pointer connected to the forearm were perturbed by arbitrary changes of the geometry of the arm-pointer arrangement. Under discontinuous visual feedback (pointer visible only at beginning and ending of the movement), the error at the movement*s first stop was high and varied with the perturbations. Under continuous visual feedback (pointer always visible), the error remained low and was un-correlated with the perturbations. Inspection of the recorded kinematics revealed that neither negative feedback control nor feedforward control through an inverse kinematics model could explain these outcomes. The paper proposes an alternative non-linear mechanism that uses the phase relationship between observed velocity and position to predict the stop position from any interim state of the movement. This provides a prediction of the error, based on which one or several scaled force impulses can be released annihilating the error at movement end.

         BP 7.5   Mon 12:30   H45
Migration patterns of dendritic cells in response to chemokines — ●Veronika Bierbaum, Jan Schwarz, Michael Sixt, and Tobias Bollenbach — IST Austria, am Campus 1, 3400 Klosterneuburg

Dendritic cells are decisive components of the adaptive immune system. When they navigate through tissues, the two chemokines CCL19 and CCL21 guide them directionally. In an experimental-theoretical study, we develop a physical description of dendritic cell migration in response to a given chemokine field. We characterize cell migration as a function of this field through in vitro assays of precisely controlled immobilized chemokine patterns. We monitor cells in varying exponential or linear profiles using time-lapse microscopy. The trajectories of these cells can be characterized in terms of stochastic differential equations, which allow for separation of the stochastic and deterministic contributions to cell directionality and velocity. For CCL21, we find that the cells' directionality is higher in exponential as compared to linear profiles. This observation supports a scenario where the directionality is governed by the signal-to-noise ratio resulting from chemokine binding to the receptor. Cells with a defect in the chemokine signal transduction pathway show reduced ability of CCL21 recognition, consistent with biochemical studies. Our findings indicate that cell directionality, for a range of concentrations, is controlled by the quality of signal transduction.

         BP 7.6   Mon 12:45   H45
The effect of model rescaling and normalization on sensitivity analysis on an example of a MAPK pathway model — Jakob Kirch, Caterina Thomaseth, Antje Jensch, and ●Nicole Radde — Institute for Systems Theory and Automatic Control, University of Stuttgart, Stuttgart, Germany

The description of intracellular processes based on chemical reaction kinetics has become a standard approach, and parameter estimation poses several challenges. Sensitivity analysis can aid model calibration in various ways. Results can for example be used to simplify the model. However, models are usually subject to rescaling and normalization, which changes the variance of the output and hence also influences results of sensitivity analyses.

We investigate the effect of model rescaling and normalization to a reference experiment on the outcome of local and global sensitivity analyses. Results are exemplified on a model for the MAPK pathway. Results for differently scaled and normalized model versions are compared. We show that sensitivity analyses are invariant under simple rescaling of variables and parameters. By contrast, normalization to a reference experiment that also depends on parameters has a large impact on any sensitivity analysis, and in particular makes an interpretation difficult. This dependency should be taken into account when working with normalized model versions.

BP 8: Bioimaging and Spectroscopy I

Time: Monday 11:30–12:45 | Location: H43

Invited Talk | **BP 8.1** | Mon 11:30 | H43
Prospects of super-resolution optical microscopy for studying membrane bioactivity — •Christian Eggeling, Marco Fritzsche, and Erdinc Sezgin — Weatherall Institute of Molecular Medicine, University of Oxford, Oxford, United Kingdom

Molecular interactions in the plasma membrane of living cells are key in cellular signalling. Protein-protein or protein-lipid complexes, the formation of lipid nanodomains (often denoted "rafts"), or diffusional restrictions by the cortical cytoskeleton are considered to play a functional part in a whole range of membrane-associated processes. The direct and non-invasive observation of such interactions in living cells is often impeded by principle limitations of conventional far-field optical microscopes, specifically with respect to limited spatio-temporal resolution. We present how novel details of molecular membrane dynamics can be obtained by using advanced microscopy approaches such as the combination of super-resolution STED microscopy with fluorescence correlation spectroscopy (STED-FCS). We will focus on new insights into the lipid "raft" theory, and on the role of plasma membrane and cytoskeleton organization in the triggering of immune cells, specifically during T-cell activation.

BP 8.2 | Mon 12:00 | H43
Label-free high contrast superresolution microscopy at 100Hz using coherent dark field illumination in TIR mode (TIR-CODAF) — •Dominic Ruh, Felix Jünger, Philipp von Olshausen, and Alexander Rohrbach — University of Freiburg, Department of Microsystems Engineering - IMTEK, Laboratory for Bio- and Nano-Photonics, Germany

Cells are the smallest units of life. A variety of forces constantly act on these complex systems, pushing them out of equilibrium and causing a manifold of signaling events. The investigation of fast dynamic processes in living cells resulting from these forces require fast measurement techniques - faster and more precise than currently available. The technique presented in this work uses a laser beam that illuminates a living, unlabeled cell under an oblique angle. The monochromatic light is multiply scattered at the cellular structures yielding an image of the cell on the camera that is strongly distorted by speckles. However, by sweeping the laser beam along a circular path in the back focal plane of the objective lens during the integration time of the camera (e.g. only some milliseconds), the speckles cancel out and a high contrast image of the cell is obtained. We call this new technique *total internal reflection coherent dark field (TIR-CODAF) microscopy*. In this talk we present a resolution of 150 nm at a frame rate of 100 Hz. Since TIR-CODAF does not rely on fluorescence many thousands of images without visible loss of image quality can be acquired.

BP 8.3 | Mon 12:15 | H43
A novel membrane label for STED nanoscopy of living cardiomyocytes — •Elke Hebisch[1], Stephan E. Lehnart[2], and Stefan W. Hell[1] — [1]Max Planck Institute for Biophysical Chemistry, Department NanoBiophotonics, Am Fassberg 11, 37077 Goettingen, Germany — [2]Research Unit for Cellular Biophysics and Translational Cardiology, Heart Research Center Goettingen, Robert-Koch-Str. 40, 37099 Goettingen, Germany

In heart muscle cells the fast and cell-wide propagation of rhythmic action potentials crucially depends on the architecture and composition of the plasma membrane (sarcolemma) and its extensive invaginations that form a transverse-axial tubular system (TATS). Here we report on the first application of the novel fluorescent membrane label cholesterol-PEG-KK114 (Chol-KK114) for STED nanoscopy of living mouse cardiomyocytes. Chol-KK114 enables fast and nontoxic in vivo labeling of cholesterol-rich cardiac membrane nanodomains. We could observe complex sarcolemmal and intracellular cholesterol signal patterns representing nanodomains sized far below the confocal resolution limit. These signal patterns are rich in detail and highly cell type specific since they could not be observed in HeLa or PtK2 cells. On the sarcolemma, we identified individual cholesterol-rich membrane nanodomains and higher order arrangements into ring structures and patches. Conclusively, we established a novel membrane label for superresolution microscopy of nanodomains in living primary cells.

BP 8.4 | Mon 12:30 | H43
Low-intensity STED microscope with increased image brightness and uncompromised resolution — •Jennifer-Rose Schubert, Claudia Geisler, Britta Vincon, and Alexander Egner — Optical Nanoscopy Dept., Laser-Laboratory, D-37077 Göttingen

Far-field optical microscopy represents a well-established method in the life sciences. Due to diffraction, the resolution is limited to $\sim \frac{\lambda}{2}$ in the focal plane. This constraint can be surpassed by nanoscopic techniques [1]. Amongst others, STED microscopy provides a resolution of up to 20 nm [2]. By definition, resolution enhancement in STED microscopy is achieved by narrowing the effective fluorescent area [3]. This reduction of detection volume depends on the factor of resolution enhancement and is directly linked to a decrease in fluorescence signal which limits the acquisition rate in many cases.
Here, we present a STED technique based on a rotating 1D depletion pattern. This novel STED variant can achieve a higher resolution for a given depletion light intensity as compared to the classical implementation. Furthermore, the overall fluorescence signal detected is higher than for conventional STED microscopy working at the same resolution. Consequently, not only identical super resolution conditions can be realized at lower depletion laser powers but also the acquisition can be sped up. Moreover, both aspects have the potential to drastically reduce photobleaching and sample damage.
[1] Huang, B. et al., Annu. Rev. Biochem., 78, 993-1016 (2009)
[2] Harke, B. et al., Opt. Express, 16, 4154-4162 (2008)
[3] Hell, S. W., Science, 316, 1153-1158 (2007)

BP 9: Evolutionary Game Theory (Joint Session SOE/DY/BP)

Time: Monday 12:15–13:15 | Location: H36

BP 9.1 | Mon 12:15 | H36
Evolutionary ecological-economic modelling: Ecological instability and economic growth — •Sylvie Geisendorf[1], Frank Beckenbach[2], and Christian Klippert[1] — [1]ESCP Europe Campus Berlin, Heubnerweg 8-10, 14059 Berlin, Germany — [2]University of Kassel

The paper proposes an evolutionary ecological-economic model taking into account the complexity of the ecological as well as the economic system. We argue that Economics should consider ecological complexity and the co-dynamics of the economic and ecological system to better understand drivers and restrictions of economic evolution. At the same time, the development of a regenerative resource is affected by the internal growth dynamics of the economy. Given that no economic activity is conceivable without using natural resources and relying on natural systemic services, there is a surprising simplification of the natural system in economic models. The model we propose has three particularities distinguishing it from traditional resource economic models. (1) it implements a multi-dimensional link between the economic and ecological system, considering side effects of the production process like waste or emissions. (2) it uses a difference equation approach for the biological resource instead of the typical differential one, to allow for the whole range of stability regimes and (3) it links this resource system to an evolving, agent-based economy instead of the standard optimization calculus.

BP 9.2 | Mon 12:30 | H36
Changing the rules of the game as an emergent feature of the dynamics — •Darka Labavić and Hildegard Meyer-Ortmanns — Jacobs University Bremen, Bremen, Germany

We consider (N, r) games of competition with N species and $r < N$ prey and predators. Basic reactions include predation, reproduction, decay, and diffusion, without a hard constraint on the occupation num-

ber per site. For special combinations of N and r we observe the option to see games within games for an appropriate choice of parameters. As one of the simplest examples we analyze a $(6, 3)$ game. Once the players segregate from a random initial distribution, domains on a coarse scale emerge, which play a $(2, 1)$-game at their boundaries, while agents inside the domains play rock-paper-scissors (that is, $(3, 1)$), leading to the formation of spirals with species chasing each other. The $(2, 1)$-game has a winner in the end, so that the coexistence of domains is transient, while agents inside the remaining domain coexist, until demographic fluctuations lead to the survival of only a single species. This means that we observe a dynamical generation of multiple scales in space and time with an emerging change of rules on the coarse scale starting from a simple set of rules on the unit scale of the grid. In view of predicting these features, we derive the deterministic limit within a van Kampen expansion. A linear stability analysis reproduces the number of forming domains and their composition in terms of species. A comparison of analytical predictions with Gillespie simulations also reveals the impact that the various sources of stochastic fluctuations have on the dynamics, even on its qualitative features.

BP 9.3   Mon 12:45   H36

A synthetic codon replicator with tRNA — •Simon Alexander Lanzmich and Dieter Braun — Systems Biophysics, Physics Department, Nanosystems Initiative Munich and Center for NanoScience, LMU Munich, Germany

Every evolving system requires the storage and replication of genetic information. Modern biology solves this using an RNA-dominated machinery (ribosome and a pool of tRNAs) to encode proteins. The proteins in turn replicate genetic information. In contrast, early life most probably replicated genes using a pool of short RNA sequences.

To approach above chicken and egg problem, we explore an autonomous, waste-free, and purely thermally driven replication mechanism. Instead of chemical base-by-base replication, it operates on successions of multi-base codons. The molecules used have a hairpin loop at each end and are derived from transfer RNA. They encode and

replicate a binary code at the anticodon sites of tRNA.

Replication of a template succession of tRNAs is facilitated by temperature oscillations and proceeds in three logical steps. (1) Strands with matching anticodons bind to the template. (2) Fluctuations in the bound strands' hairpins allow for the hybridization to neighboring strands. (3) Subsequent heating splits the replicate from the template, freeing both for the next cycle. This physical ligation chain reaction proceeds cross-catalytically. Instead of chemical backbone ligation, matching strands are linked by physical base pairing.

BP 9.4   Mon 13:00   H36

Stepwise cooperation of molecular replicators — •Georg Urtel and Dieter Braun — Systems Biophysics, Ludwig-Maximilians-Universität München, Amalienstr. 54, D- 80799 München, Germany

Life emerged from the ability of informational polymers to pass on sequences to other polymers before they degrade. Before competition between living species, the first selection pressure was to replicate faster than degradation. What were the strategies the molecules could take?

Based on biological evidence, DNA or RNA replicators require a defined binding site to start replication. We study experimentally and theoretically three geometries of the binding site: linear single binding, hairpin binding and two opposing binding locations. The geometries have fundamentally different, increasing replication speeds.

Interestingly, two hairpin replicators cooperate readily and form the fastest replicating geometry. After incomplete replication, they bind by hybridization and cooperate by forming a crossbreed species. This cooperation of two replicators retains most of the sequence information of both hairpins. Under conditions where hairpins are doomed to degrade, their crossbreed is replicating fast enough to survive. As a result, two initially separated hairpins survive by diffusional mixing and the colocalized crossbreeding.

Our experiments show a stepwise evolution of replicator geometries. Already at a molecular level, cooperation was an advantageous strategy under Darwinian evolution.

BP 10: Colloids and Complex Fluids III (Joint Session CPP/DY/BP)

Time: Monday 15:00–18:00   Location: H42

BP 10.1   Mon 15:00   H42

Directed assembly of soft colloids through rapid solvent exchange — •Arash Nikoubashman[1], Victoria E. Lee[2], Chris S. Sosa[2], Robert K. Prud'homme[2], Rodney D. Priestley[2], and Athanassios Z. Panagiotopoulos[2] — [1]Institute of Physics, Johannes Gutenberg University of Mainz, Germany — [2]Department of Chemical and Biological Engineering, Princeton University, USA

We studied the directed assembly of soft nanoparticles through rapid micromixing of polymers in solution with a non-solvent. Both experiments and computer simulations were performed to elucidate the underlying physics and to investigate the role of various process parameters. In particular, we discovered that no external stabilizing agents or charged end-groups are required to keep the colloids separated from each other, when water is used as the non-solvent. The size of the nanoparticles can be reliably tuned through the mixing rate and the ratio between polymer solution and non-solvent. Furthermore, we were able to fabricate a wide variety of patchy colloids, such as Janus particles, when polymer blends were used in the feed stream. Our results demonstrate that this mechanism is highly promising for the mass fabrication of uniformly-sized colloidal particles, using a wide variety of polymeric feed materials.

BP 10.2   Mon 15:15   H42

Directed Assembly of Janus Particles through Flow — •Arash Nikoubashman — Institute of Physics, Johannes Gutenberg University of Mainz, Germany

We investigate the self-assembly of colloidal Janus particles under shear and Poiseuille flow, by employing hybrid molecular dynamics simulations that explicitly take into account hydrodynamic interactions. Under quiescent conditions, the amphiphilic colloids form spherical aggregates with a large size polydispersity. The solvophobic hemispheres are directed towards the core, whereas the solvophilic caps are exposed to the solvent. When sufficiently strong shear is applied, the micelles disaggregate with a consequent decay of the average cluster size. How-

ever, we find an intermediate regime where the balance between rearrangement and dissociation favors the growth of the aggregates, where the majority of clusters consist of 13 particles in an icosahedral arrangement. This bias is due to the high geometric symmetry of the icosahedron, which maximizes the internal bonding energy of the aggregate. Our findings demonstrate how self-assembly can be directed towards specific structures via external fields, and open up new applications for Janus particles, ranging from biotechnology to sensor systems.

BP 10.3   Mon 15:30   H42

Self-organized velocity pulses of dense colloidal suspensions in microchannel flow — •Philipp Kanehl and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Colloids in dense suspension exhibit shear-induced migration and size segregation under pressure driven flow [1]. If the density is increased further, the steady flow becomes unstable and regular oscillations in flow velocity emerge [2]. To develop a theoretical understanding of these oscillations, we simulate colloidal particles with frictional contact under pressure-driven flow in two dimensions using the mesoscale simulation technique of multi-particle collision dynamics.

We present a detailed parameter study on how friction generates transient jamming in the colloidal flow. The jammed regions are unjammed by rarefaction pulses travelling upstream similar to the experimental observations. Moreover, we address the role of fluid permeation and channel confinement.

Finally, a linear stability analysis of a newly developed continuum model predicts scaling laws for stability condition, wavenumber, and pulse speed, which agree well with our numerical data.

[1] P. Kanehl and H. Stark, J. Chem. Phys. 142, 214901 (2015).
[2] L. Isa, R. Besseling, A. N. Morozov, and W. C. Poon, Phys. Rev. Lett. 102, 058302 (2009).

BP 10.4   Mon 15:45   H42

An empirical correction for multiple scattering in integral laser Doppler velocimetry experiments — •Denis Botin[1], Ludmila Marotta Mapa[1,2], Christopher Wittenberg[1], Holger Schweinfurt[1], and Thomas Palberg[1] — [1]Institute of Physics, JGU, D-55099, Mainz, Germany — [2]Federal Univesity of Itajuba, Brazil

Super-heterodyne laser Doppler velocimetry (SHLDV) provides an integral measurement of the velocity distribution in electro-kinetic experiments[1]. This allows simultaneous evaluation of the electro-phoretic and electro-osmotic mobilities of the particles and along the cell wall, respectively [2]. Here, we introduce an extension of the method to the regime of concentrated samples, where multiple scattering affects the signal [3]. Multiple scattering distorts the signal shape, creating an additional hump in the background and prohibiting any meaningful fit. We use an empirical correction scheme for the spectra, in which we fit the multiple scattering contribution and subtract it from the raw data. This leaves the velocity dependent singly scattered contribution unaffected. First applications to measurements of the concentration dependence of the electro-phoretic mobility of charged colloidal spheres are reported.

[1]T. Palberg et al. J. Phys. Chem. 96, 8180 - 8183 (1992)
[2]T. Palberg et al. J. Phys.: Condens. Matter 24, 464109 (2012).
[3]H.C. Van de Hulst., *Multiple Light Scattering: Tables, Formulas, and Applications*, Academic Press, New York., (1980).

BP 10.5   Mon 16:00   H42
Multiscale modelling of complex (macro-)molecular fluid mixtures — •Christoph Junghans[1], Tiago E. de Oliveira[2,3], Paulo A. Netz[2,3], Debashish Mukherji[2], and Kurt Kremer[2] — [1]CCS Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — [2]Max-Planck Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz Germany — [3]Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil

Many biophysical processes in water are determined by the interactions of cosolvents within the hydration shells of dissolved molecules. Computational approaches are mostly limited to the "mid sized" all-atom simulation protocols. While all-atom simulations are suitable in some cases, problems arise when concentration fluctuations are large, thus requiring efficient simulation methods. Therefore, we develop two distinct, yet related, multiscale methods. In one case, we develop a semi-grand canonical MD that heals the particle depletion [1] that uses the AdResS scheme [2], coupled with a metropolis particle exchange criterion. In AdResS, an all-atom region is coupled to a coarse-grained (CG) reservoir, where the particle exchange is performed. In the second protocol, we develop a "parameter free" CG model, which uses cumulative coordination within an iterative procedure [3]. Both methods preserve pair-wise structure of complex fluids and their solvation thermodynamics. We apply these methods to study several cases of (macro)molecular solvation in aqueous mixtures [1,3].

[1] D. Mukherji and K. Kremer, Macromolecules (2013).   [2] S. Fritsch, et al. PRL (2012). [3] T. E. de Oliveira, et al. (2016).

BP 10.6   Mon 16:15   H42
Kinetics of liquid-liquid phase transition in protein solutions exhibiting LCST phase behavior studied by USAXS — •Fajun Zhang[1], Stefano Da Vela[1], Michal Braun[1], Michael Sztucki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

We present the results of the early stage kinetics of liquid-liquid phase separation (LLPS) in protein-salt solutions studied by ultra-small angle x-ray scattering (USAXS). The model system of bovine serum albumin (BSA) with YCl_3 [1,2] shows LLPS and a lower critical solution temperature (LCST) phase behavior and can be rationalized using an ion-activated patchy-colloid model [3]. We focus on the phase transition of the dense liquid phases after a T-jump aiming at the arrested or slowed down kinetics. The USAXS curves of sample solutions after a T-jump exhibit a peak that grows in intensity and shifts to lower q values with time. The characteristic length (ξ) obtained from this scattering peak increases with time approximately as $t^{0.3}$. The interface between the dilute and dense phase is quickly established as a Porod region (q^{-4}) is visible within a few seconds. Thus the kinetics of the intermediate stage of phase transition was followed by USAXS. It is interesting to see that $\xi(t)$ is nearly independent on the jump temperatures (below 40 °C). At a higher temperature jump (45 °C), a slowed down kinetics was observed indicating that the gelation line was approached. [1] F. Zhang, et al. Phys. Rev. Lett. 101, 148101 (2008) Proteins 78, 3450 (2010). [2] F. Zhang, et al. Soft Matter 8,

1313 (2012). [3] F. Roosen-Runge, et al. Sci. Rep. 4, 7016 (2014).

15 min. break

BP 10.7   Mon 16:45   H42
Hydration and hysteresis of triblock copolymers — •Bernhard Schummer, Stefan Gerth, and Randolf Hanke — Universität Würzburg, Lehrstuhl für Röntgenmikroskopie

Ternary polyether are block ABA copolymers consisting of polyethyleneoxide (PEO) (A) and polypropylenoxide (PPO) (B). They change their hydrophilic or hydrophobic balance dramatically with their temperature and their concentration in water. This change causes a micelleisation. In this case P123 will be used as a copolymer and SAXS will be the method of examination. For micelles an appropriate model is the core-shell model where the shell mostly consists of PEO and the core mainly of PPO. In this model the SLD's for core and for shell heavily depend on each other. A new parameter $\kappa = \frac{\rho_c - \rho}{\rho_s - \rho}$ is presented to describe the change of the conformation and hydration of the micelle while including the radii of shell and core. Here ρ_c is the SLD of the core ρ_s the SLD of the shell and ρ the SLD of the solvent. The new parameter indicates that the SLD of the core decreases and thus dehydrates with increasing temperature. For instancethe SLD's of the poloxamer L51 show a similar dependency as P123. The heating and cooling curves of the sample for different small concentrations will be presented and show a hysteresis in the form phase diagram. This can be observed in a diagram where κ is ploted against the temperature. At higher concentrations poloxamers form a liquid crystal. It has already been shown that there is a hysteresis in the cell parameter at high concentrations. This effect can now be attributed to a single component of the system, the form change of the micelle.

BP 10.8   Mon 17:00   H42
Phase behaviour and interactions in a three components γ-globulin based depletion interaction system — •Stefano Da Vela[1], Fajun Zhang[1], Sarah El-Asfar[1], Christian Exner[1], Michael Sztucki[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen — [2]ESRF, Grenoble, France

Aqueous solutions of bovine γ-globulin with polyethylene glycol (PEG) added as non-interacting polymer, provide a tunable protein system for the study of depletion-driven phase behaviour: range and strength of the interaction are adjusted by appropriate choice of PEG molecular weight and concentration. An extensive study of the phase behaviour of the system for different effective attraction strengths reveals a set of conditions for which a Liquid-Liquid Phase Separation (LLPS) phase boundary emerges above the freezing temperature of the solvent. Addition of bovine serum albumin (BSA), results into an effective three components system. BSA, while not inducing depletion interaction on its own, appears to enhance it in presence of PEG, shifting the LLPS boundary to higher temperatures while being preferentially excluded from the resulting protein-dense liquid phase. In order to investigate the effect of BSA on the phase boundaries and on the interaction, phase diagrams as a function of temperature, protein and PEG concentration are presented together with small angle X-ray scattering data. Optical microscopy, turbidimetry and size exclusion chromatography are employed as supplementary techniques. The findings are relevant to the understanding of protein mixtures and their separation.

BP 10.9   Mon 17:15   H42
Clusters of proteins – are they transient or static? — •Michal Braun[1], Marco Grimaldo[1,2], Felix Roosen-Runge[2], Christian Beck[1], Fajun Zhang[1], Frank Schreiber[1], and Tilo Seydel[2] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institut Laue-Langevin, Grenoble, France

Signatures of protein clusters have been observed for globular proteins such as lysozyme [1], crystallins and bovine serum albumin [2,3]. The nature of these clusters, whether static or transient, however, is still a debated question and depends sensitively on environmental conditions. A better understanding would be key to use protein clusters as precursors for protein crystallization or in drug delivery.

We report cluster formation in solutions of β-lactoglobulin (BLG), as systematically investigated using static and dynamic scattering techniques. From small-angle scattering (SAXS/SANS), we obtain a cluster signature from the missing shift of the correlation peak with concentration and related data fitting. Neutron quasi-elastic backscattering (QENS) evidences the formation of oligomers via the short-time

self-diffusion coefficient at nanosecond time scales. Finally, neutron spin-echo spectroscopy (NSE) allows to compare structural information from the structure factor with the dynamical features of collective diffusion on time scales of several tens of nanoseconds, which ultimately allows to determine the nature of the observed protein clusters.

[1] Stradner et al. Nature 432 (2004) 492
[2] Soraruf et al. Soft Matter 10 (2014) 894
[3] Grimaldo et al. J. Phys. Chem. Lett. 6 (2015) 2577

BP 10.10   Mon 17:30   H42

Self-assembled micelles as drug carriers: Influence of molar mass and chain architecture — •Bart-Jan Niebuur[1], Xiaohan Zhang[1], Natalya Vishnevetskaya[1], Petr Chytil[2], Sergey K. Filippov[2], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Garching, Germany — [2]Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic

A promising way to achieve site-specific delivery of anticancer agents is to use the enhanced permeation and retention (EPR) effect of self-assembled polymeric micelles. At this, a low critical micelle concentration (CMC) and particle sizes in the range of 1-100 nm are of importance.

In the present work, we focus on the importance of (i) the overall molar mass and (ii) the chain architecture. We investigate both N-(2-hydroxypropyl) methacrylamide (HPMA) [1] homopolymers with randomly distributed cholesterol side groups and diblock copolymers having a pure HPMA block and an HPMA block with cholesterol. Using fluorescence correlation spectroscopy and small-angle neutron scattering (SANS), the CMC as well as the size and structure of the micelles are determined in phosphate buffer. We find that the CMC decreases with increasing molar mass, but does not depend on chain architecture. The micellar radius is with 4-5 nm in the desired range.

[1] Filippov, S.K. et al., *Biomacromolecules* **13**, 2594 (2012) and **14**, 4061 (2013)

BP 10.11   Mon 17:45   H42

Modeling Viscoelastic Properties of Complex Fluids — •Julius Schulz, Alexander Schlaich, Roland Netz, and Julian Kappler — Fachbereich Physik, Freie Universität Berlin, 14195 Berlin

The viscoelastic response of a complex liquid like water differs significantly from more simple models such as a Lennard-Jones fluid or methane. Using all-atom molecular dynamics simulations, we calculate the frequency-dependent viscosity for two liquids: TIP4P/2005 water and a glycerol/water solution. The corresponding elastic spectrum exhibits two peaks and cannot be described by simple viscoelastic models. We discuss the origins of these features and present a novel extension of the Maxwell model for viscoelastic fluids which is capable of reproducing the relevant features of the frequency-dependent viscosity. Extracted shear relaxation times for the glycerol-water mixtures compare well with experiments.

BP 11: Bioimaging and Spectroscopy II

Time: Monday 15:00–17:15   Location: H43

BP 11.1   Mon 15:00   H43

Cellular Structures Resolved by X-Ray Diffraction with Micro- and Nanometer Beamsize: From Stem Cells to Cardiomyocytes — •Marten Bernhardt[1], Jan-David Nicolas[1], Marius Priebe[1], Markus Osterhoff[1], Carina Wollnik[2], Ana Diaz[3], Marina Eckermann[1], Florian Rehfeldt[2], and Tim Salditt[1] — [1]Institute for x-ray physics, Göttingen — [2]Third Institute of Physics - Biophysics, Göttingen — [3]Paul Scherrer Institut, Villigen

High resolution scanning small angle x-ray scattering (scanning SAXS) enables an access to local cellular structures on a mesoscopic scale. We have performed micro- and nanofocus SAXS recordings on naive human mesenchymal stem cells (hMSCs), neonatal rat cardiomyocytes and other differentiated cell lines and characterized their 2D-diffraction patterns: Results on freeze-dried samples reveal naive hMSCs to be rather weak scatterers with little anisotropic scattering behavior. In contrast, disassembled cells from neonatal rat tissue show a strong anisotropic diffraction signal, that enable us to track down filamentous structures by automated principal component analysis (PCA). These structures can be correlated to the visible light micrograph of fluorescently labeled actin. Successful wet chamber experiments provide a basis for future single cell recordings in chemically fixated and alive states.

BP 11.2   Mon 15:15   H43

Imaging proteins at the truly single molecule level — •Jean-Nicolas Longchamp[1], Stephan Rauschenbach[2], Sabine Abb[2], Conrad Escher[1], Tatiana Latychevskaia[1], Klaus Kern[2,3], and Hans-Werner Fink[1] — [1]Physics Department of the University of Zurich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, DE-70569 Stuttgart, Germany — [3]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Imaging a single protein has been a long-standing dream for advancing structural biology and with this various fields in natural science. Here I will show that, sub-nanometer resolved images of individual folded proteins have been obtained for the first time ever. Electrospray ionization for the specific selection and sound deposition of individual proteins onto ultraclean freestanding graphene in an ultra-high vacuum environment and low-energy electron holography for the non-destructive imaging are combined in a novel experimental workflow.

BP 11.3   Mon 15:30   H43

Developing a modular sensor platform for intracellular environmental sensing — •Torsten Rendler[1], Jitka Slegerova[2], Ondrej Zemek[3], Jan Kotek[3], Andrea Zappe[1], Zhiqin Chu[1], Petr Cigler[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Deutschland — [2]Institute of Organic Chemistry and Biochemistry AS CR, Flemingovo nam. 2, Prague 6, Czech Republic — [3]Department of Inorganic Chemistry, Faculty of Science, Charles University, Hlavova 8, Prague 2, Czech Republic

The development of nano-scaled sensors that can be embedded intracellular without minor modification on the local environments are important for various biological and medical applications. For this purpose we utilize the nitrogen vacancy (NV) center in nanodiamond providing close to single spin sensitivity and nanometer resolution at ambient conditions, providing at the same time long term stability and low cytotoxicity in biological systems. By combining the well-established clinical magnetic resonance imaging (MRI) agent namely Gadolinium with NV spin relaxometry in nanodiamonds, we developed a hybrid sensor that can be adjusted to monitor various physiological quantizes. As an example we demonstrate sensitivity to pH and changes in the redox potential at submicron length scales in a microfluidic channel. Furthermore we introduce our hybrid sensor system into cells and investigate it's response on the local cellular environment. The current work shall open a novel approach for studying subtle changes in physiological conditions, pointing to a new pathway for diagnosis and therapeutics at subcellular level.

15 min break

Invited Talk   BP 11.4   Mon 16:00   H43

Chromophore Photophysics in Fluorescent Proteins of the GFP family — •Gerd Ulrich Nienhaus — Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — Institute of Toxicology and Genetics, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL, USA

Genetically encoded fluorescent proteins (FPs) of the green fluorescent protein (GFP) family have become indispensable as marker tools for imaging live cells, tissues and entire organisms. Great efforts are ongoing in many labs to further optimize their photophysical properties by genetic engineering. The p-HBI chromophore of GFP (or a variant thereof in other FPs), which forms autocatalytically in the interior of the polypeptide chain, is exquisitely sensitive to the protein envi-

ronment. By introducing amino acid modifications, its photophysical properties can be changed, e.g., for the purpose of color tuning. In photoactivatable FPs, chromophore properties can even be controlled by light irradiation, which is of key relevance for super-resolution optical imaging. Photoactivation may occur reversibly, by photoinduced cis-trans isomerization of the chromophore (photoswitching), or by permanent photochemical modifications (photoconversion). Here I shall discuss these photophysical effects in the context of the underlying mechanisms.

BP 11.5   Mon 16:30   H43

Axial super resolved cell dynamics by spectrally coded optical nanosectioning (SpecON) on biocompatible metal-dielectric substrates — Benjamin Schreiber[1], Hannah Heil[1], Martin Kamp[2], Kareem Elsayad[3], and •Katrin G. Heinze[1] — [1]Rudolf Virchow Center, University of Würzburg, Germany — [2]Technische Physik, University of Würzburg, Germany — [3]Advanced Microscopy, Campus Science Support Facilities, Vienna, Austria

Fluorescence microscopy is one major tool to visualize substructures of biological cells down to the single molecule level. While particular powerful in the lateral dimension high-resolution concepts are usually less effective in the axial dimension or compromise temporal resolution.

Here, we show how to overcome this problem by using biocompatible metal-dielectric coated substrates for live cell imaging. As fluorescent emitters can be treated as dipoles they can interact with surface plasmons in metallic interfaces and allows for distance dependent modulation of the emission properties. Thus, it is possible to record the distance-dependent spectral "fingerprint" to determine and visualize fluorophore axial distributions far beyond the Abbe-limit. Compared to respective fluorescence lifetime measurements, spectral changes of the fluorophore emission can be measured with higher temporal resolution. Here we monitor the super-resolved axial movements of living cells particular the dynamics of filopdia in melonama cells, and discuss future perspective for multidimensional imaging.

BP 11.6   Mon 16:45   H43

Non-contact atomic force microscopy of the purple membrane — •Alfred J. Weymouth[1], Katharina Pfeffer[1], Estefania Mulvihill[2], Daniel J. Müller[2], and Franz J. Giessibl[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Biosystems Science and Engineering, ETH Zurich, Basel, Switzerland

Atomic force microscopy is a unique tool for investigating biological samples. Images are normally acquired in tapping mode, in which the tip presses down on the sample with each oscillation. This is relatively non-destructive, requires only a small sample, and can resolve down to the nanometer-scale. (e.g. [1]) However, true non-contact techniques, such as frequency-modulation AFM, have been developed which allow atomic resolution before the tip presses down on the surface. Frequency-modulation AFM has acquired atomic contrast on surfaces in liquid environments. [2] We have started to explore the possibility of using non-contact AFM with a stiff cantilever (a qPlus sensor with k = 3515 N/m) to image biological membranes. As a first sample, we looked at the purple membrane. We present our first results of the membrane islands and atomic resolution of the mica substrate.

[1] M. Pfreundschuh, D. Martinez-Martin, E. Mulvihill, S. Wegmann and D.J. Müller. Nat Protoc, 9, 1113 (2014)

[2] T. Fukuma, K. Kobayashi, K. Matsushige and H. Yamada. Appl Phys Lett, 87, 034101 (2005)

BP 11.7   Mon 17:00   H43

Seeing intermolecular interactions in morphology: AFM-IR of aggregated thin porphyrin films — •Timur Shaykhutdinov, Peter Kate, Simona Pop, Andreas Furchner, and Karsten Hinrichs — Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., ISAS Berlin, Schwarzschildstr. 8, 12489 Berlin, Germany

A comprehensive understanding of hierarchical self-assembly of low-dimensional supramolecular systems is of fundamental importance for applications in the field of nanobiotechnology and bioengineering. Metalloporphyrins are extremely versatile molecular building blocks and serve as active components in a variety of biological systems. Their capability to self-organize over a wide range of length scales spanning from a few nanometers up to hundreds of micrometers is promising for the development of multifunctional biofilms.

Although the morphology of porphyrin aggregates has been studied extensively, their formation mechanisms have remained unclear up till now. In this work we show nanoscale IR spectroscopic evidence of different porphyrin stacking as the underlying cause of morphological patterns of aggregated thin porphyrin films.

Here we apply resonance-enhanced AFM-IR, a high-sensitivity non-destructive nanospectroscopic technique in the fingerprint region, and link intermolecular stacking interactions to nanostructured morphology.

BP 12: Single Molecule Biophysics

Time: Monday 15:00–17:15   Location: H45

Invited Talk   BP 12.1   Mon 15:00   H45

Imaging of G-protein coupled receptors while quantifying their ligand-binding free energy landscape to mutiple ligands — •Daniel J. Müller[1], David Alsteens[1,2], Moritz Pfreundschuh[1], Patrizia M. Spoerri[1], Shaun R. Coughlin[3], Cheng Zhang[4], and Brian K. Kobilka[4] — [1]ETH Zurich, Switzerland — [2]University Leuven, Belgium — [3]University of California San Francisco, USA — [4]Stanford University School of Medicine, USA

Imaging native membrane receptors and testing how they interact with ligands is of fundamental interest in life sciences, but has proven remarkably difficult to accomplish. Here, we introduce experimental and theoretical developments that allow atomic force microscopy (AFM) to simultaneously image native human protease-activated receptors (PAR1) in the functionally important lipid membrane and to quantify their dynamic binding strength to native and synthetic ligands. These binding strengths provide kinetic and thermodynamic parameters of individual ligand-receptor complexes. Recorded in the absence and presence of antagonists, the values describe the ligand-binding free energy landscape of native and synthetic ligands to the G-protein-coupled receptor with remarkable accuracy. We further address the challenge and introduce multifunctional high-resolution AFM to image PAR1 and to simultaneously localize and quantify their binding to two different ligands. Our nanoscopic method opens an exciting avenue to directly image and characterize ligand-binding of native membrane receptors.

BP 12.2   Mon 15:30   H45

How RNA Polymerase II elongates through di-nucleosomal

DNA? — Veronika Fitz[1,2], •Jaeoh Shin[3], Vasily Zaburdaev[3], and Stephan Grill[1,2,3] — [1]Max-Planck-Institute of Molecular Cell Biology and Genetics, D-01307 Dresden — [2]Technical University Dresden, BIOTEC, D-01307 Dresden — [3]Max-Planck-Institute for the Physics of Complex Systems, D-01187 Dresden

RNA polymerase II (Pol II), an enzyme which catalyzes messenger RNA from DNA template, plays a fundamental role in gene regulation. In eukaryotic cells, a large fraction of the DNA molecules are wrapped around nucleosomes, which interfere with the transcription process. Here we study Pol II elongation in di-nucleosomal template by using the optical tweezer setup. Our goal is to understand the role of the neighboring nucleosome on the Pol II elongation, which is relevant in the context of in vivo situation. We found that the Pol II elongation through the first nucleosome depends on the separation between the nucleosomes in a non-monotonous way. We suggest that this effect results from the relative angle between the nucleosomes. To better understand the experimental results, we develop a 2-dimensional random walk model accounting the nucleosomal barrier, backtracking, and the assisting force acting on Pol II. The model reproduces the dynamics of Pol II elongation in agreement with the experimental data without any fitting parameter. Out model shows that the relative strength of the nuclesomal barrier and the assisting force dramatically change the elongation dynamics. We also discuss how the second nucleosome affects the stability of the first nucleosome.

BP 12.3   Mon 15:45   H45

Single-molecule protein nanomechanics of the chaperone DnaK — •Gabriel Zoldak and Matthias Rief — Physik-

Department E22, Technische Universität München James-Franck-Str. 1 85748 Garching Germany

In the last few years, single molecule force spectroscopy has become recognized as an excellent and unique method for probing energy landscapes of large conformational changes in proteins, including protein folding and ligand binding. Conceptually, the force spectroscopy can be applied as a tool for: (1) monitoring single-molecule kinetics with exceptional resolution, and (2) characterizing local mechanics. In the first study, we expand the dynamic range of single-molecule force spectroscopy using optical tweezers by autocorrelation analysis which pushes the time resolution of single-molecule force spectroscopy to ca. 10 microseconds thus approaching the timescales accessible for all-atom molecular dynamics simulations. In the second study, we elucidate the energetic and mechanical changes within the subdomains of the nucleotide binding domain (NBD) of the heat shock protein of 70 kDa (Hsp70) chaperone DnaK upon nucleotide binding. In an integrated approach using single molecule optical tweezer experiments, loop insertions, and steered coarse-grained molecular simulations, we find that the C-terminal helix of the NBD is the major determinant of mechanical stability, acting as glue between the two lobes. After helix unraveling, the relative stability of the two separated lobes is regulated by ATP/ADP binding.

30 min break

BP 12.4   Mon 16:30   H45

Kinesin-1 motors throw each other off the microtubule — •Matthias Rank and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Inside cells, a large number of molecular motors bind to microtubules (MTs) where they perform directed motion. While it is generally accepted that steric hindrance of motors leads to crowding effects, little is known about their specific interactions. We examine a variation of the totally asymmetric simple exclusion process with Langmuir kinetics (TASEP/LK), in which dissociation of molecular motors is enhanced on crowded filaments. We demonstrate that a two-particle "throwing out" interaction can explain recent experimental data for kinesin-1 excellently. Following a theoretical mean-field approach, we derive the phase diagram of the process for important limits. We further extend our results to motors of two different types, and propose an efficient mechanism how they can phase separate on the MT. This can be important for cellular processes requiring ongoing catalytic activity of a specific motor type, and motors which operate cooperatively.

BP 12.5   Mon 16:45   H45

Expanding the Design Space of Synthetic Membrane Pores — •Kerstin Göpfrich[1], Satya Bhamidimarri[2], Alexander Ohmann[1], Iwona Mames[3], Eugen Stulz[3], Mathias Winterhalter[2], and Ulrich Keyser[1] — [1]University of Cambridge, UK — [2]Jacobs University Bremen, Germany — [3]University of Southampton, UK

DNA nanotechnology allows for the creation of membrane-spanning channels with customized functionality. We present three novel designs with channel diameters spanning an order of magnitude from 0.8nm to 8nm. We utilize DNA tile assembly and scaffolded origami with two different scaffold lengths to create channels of variable size and architectural complexity. Bifunctional porphyrin- and cholesterol-tags serve as membrane anchors to facilitate insertion into lipid membranes (J. R. Burns, K. Göpfrich et al., Angew. Chemie, 2013). We compare the conductance of the channels and confirm the correspondence between engineered design and single-channel behaviour. Our channels span three orders of magnitude in conductance, comparable to protein pores encompassing small ion channels as well as large porins. Conductance states are dependent on transmembrane voltage (A. Seifert, K. Göpfrich et al., ACS Nano, 2014). We demonstrate that self-assembly and membrane attachment of simple DNA channels can be achieved within a minute, making their creation scalable for applications in biology (K. Göpfrich et al., Nanoletters, 2015). Our work showcases the versatility of artificial DNA-based pores inspired by the rich structural and functional diversity of natural membrane components.

BP 12.6   Mon 17:00   H45

A coarse grained DNA model for the prediction of current signals in DNA translocation experiments — •Florian Weik — Institut für Computerphysik, Universität Stuttgart, Germany

We present a coarse grained model of DNA in a cylindrical nanopore. It qualitatively reproduces the current modulation in a pore when DNA is present. It extends previous coarse grained and mean field approaches by incorporating a position dependent friction that was shown to be essential to the behavior by Kesselheim et. al. The experimental data of Smeets et. al. as well as the atomistic simulation results by Kesselheim et. al. are reproduced over a wide range of salt concentrations. The model reduces the computational effort by orders of magnitude as compared to all atom simulations and provides a promising starting point into a modeling of the whole translocation process. We combine a representation of the DNA by three beads per base pair with explicit ions, a heuristic friction between the DNA beads and the ions and a continuum approach of the solvent to a correct description of the electrokinetics of the system.

BP 13: Posters - Anomalous Diffusion in Complex Environments

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

BP 13.1   Mon 17:30   Poster C

Spatially Inhomogeneous Search Strategies for Intracellular Transport — •Anne Hafner and Heiko Rieger — Theoretical Physics, Saarland University, Saarbrücken, Germany

Intracellular transport is vital for the proper functioning and survival of a cell. Cargo (proteins, vesicles, organelles, etc.) is transferred from its place of creation to its target locations via molecular motor assisted transport along cytoskeletal filaments. The transport efficiency is strongly affected by the spatial organization of the cytoskeleton, which constitutes an inhomogeneous, complex network. In cells with a centrosome microtubules grow radially from the central microtubule organizing center towards the cell periphery whereas actin filaments form a dense meshwork, the actin cortex, underneath the cell membrane with a broad range of orientations. The emerging ballistic motion along filaments is frequently interrupted due to constricting intersection nodes or cycles of detachment and reattachment processes in the crowded cytoplasm. In oder to investigate the efficiency of search strategies established by the cell's specific spatial organization of the cytoskeleton we formulate a random velocity model with intermittent arrest states. With extensive computer simulations we analyze the dependence of the mean first passage times for different search problems on the structural characteristics of the cytoskeleton, the motor properties and the fraction of time spent in each state.

BP 13.2   Mon 17:30   Poster C

Subcellular Organization of Eukaryotes during Mitosis — Nisha Pawar, •Claudia Donth, and Matthias Weiss — Universität Bayreuth, Experimentalphysik 1

Eukaryotic cells undergo major structural changes at the onset and during mitosis. This includes nuclear envelope breakdown, the formation of a mitotic spindle, disassembly of the Golgi apparatus and a transition of the endoplasmic reticulum from netlike to sheetlike structure.

Using spatially resolved FCS measurements we were able to show that the contiguous fluid of former cytoplasm and nucleoplasm features an anisotropically varying diffusion characteristics in the mitotic spindle area [1]. This affects the preferential direction of long-time diffusion as well as the distribution of nucleocytoplasmic constituents throughout the spindle region.

While being functionally closely related in interphase, ER and Golgi apparatus were found to be inherited separately: After its disassembly, Golgi components are spread throughout the whole cell, while the ER takes on a sheetlike structure that is excluded from the mitotic spindle region. Starting from an unmixed state of ER and Golgi components, Golgi reassembly after cytokinesis appears to be independent of the ER.

[1] N. Pawar, C. Donth and M. Weiss; Curr. Biol. 24, 16, 1905-1908 (2014)

BP 14: Posters - Biotechnology and Bioengineering

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

BP 14.1   Mon 17:30   Poster C

Hydrodynamic Flow Control from Micro- to Picolitres — ●Katja Prasol and Claus Fütterer — Biophysical Tools GmbH/Forschung, 04317 Leipzig, Germany

During the last decade biophysists, biochemists and biologists moved to microfluidics in their applications. Prokaryotic and eukaryotic cells are cultured and investigated in microfluidic chips, they are sorted in microfluidic systems, other molecules, even DNAs, are being observed in micro-droplets.

All of these applications are highly dependent on a precise flow control, which is conventionally done with syringe or peristaltic pumps. However, such approaches have a number of bottlenecks. Smallest irregularities in piston motion of syringe pumps are strongly hydrodynamically amplified in the flow velocity. The peristaltic pump, based on squeezing of tubing, does not allow precise determination of the perfused volume and generates strongly pulsatile flow.

Within our research we focused on the development and testing of novel pressure-driven flow control methods. Recently we developed a new pneumatic flow control principle. Our new system overcomes the bottlenecks of conventional flow control methods including the current state-of-the-art in microfluidic flow control (Fütterer et al., Injection and Flow Control in Microchannels, Lab Chip, 4, 351, 2004). Further, we present data on stability, fast dynamics as well as a number of real and future applications in biology, biophysics and medical research.

BP 14.2   Mon 17:30   Poster C

Exploring the secondary structure of xanthan by atomic force microscopy — ●Julia Teckentrup[1], Orooba Al-Hamood[1], Tim Steffen[2], Hanna Bednarz[2], Volker Walhorn[1], Karsten Niehaus[2], and Dario Anselmetti[1] — [1]Experimental Biophysics, Bielefeld University, Germany — [2]Proteome and Metabolome Research, Bielefeld University, Germany

The polysaccharide xanthan which is secreted by the γ-proteobacterium *Xanthomonas campestris* is an industrial scale used food thickening agent and rheologic modifier. Its great commercial importance calls forth to optimize the xanthan production. By targeted genetic modification the metabolism of *Xanthomonas* can be modified in such a way that the xanthan production efficiency or the shear-thickening potency is optimized.

Using atomic force microscopy (AFM) we analyzed the secondary structure of single xanthan polymers produced by wild-type *Xanthomonas campestris* B100 and several genetically modified variations. We found a wide variation of characteristic differences between xanthan molecules produced by different stems ranging from single linear polymers to branched xanthan double strands. These results can help to get a better understanding of the metabolic pathways that are relevant for xanthan synthesis. Furthermore, variations of the xanthan secondary structure can explain its viscosifying properties.

BP 14.3   Mon 17:30   Poster C

Influence of different hydrophobic tags on structural properties and membrane insertion probability of artificial DNA nanopores — ●Alexander Ohmann, Kerstin Göpfrich, and Ulrich F. Keyser — Cavendish Laboratory, University of Cambridge, CB3 0HE, UK

Biological ion channels are involved in numerous cellular processes and their dysfunction constitutes key events in many pathological processes. It has been shown that the directed folding of DNA allows the fabrication of versatile and programmable synthetic ion channels that can self-insert into the lipid membrane via hydrophobic tags such as cholesterol. However, number and type of hydrophobic tags employed have a significant influence on the structural properties of individual DNA constructs, their behavior at higher concentrations, and their insertion probability into the lipid bilayer. Here, we present initial results on understanding these effects by a thorough analysis of nanoscale DNA constructs assembled entirely from chemically synthetized DNA single strands modified with a variety of hydrophobic tags. The influence on structural properties have been studied on the single molecule level as well as in bulk. Electrophysiological measurements provide insight into their insertion efficiency as well as their characteristics as ion channels. The results of our study greatly enhance our understanding of how to design such artificial ion channels and optimize their insertion efficiency. Making them more adaptable to ambient conditions such as hydrophobicity and salt concentration these synthetic nanopores therefore become increasingly attractive for biomedical applications.

BP 15: Posters - Complex Fluids and Soft Matter

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

BP 15.1   Mon 17:30   Poster C

Margination of rigid spheres in a partially constricted cylinder — ●Christian Bächer and Stephan Gekle — Biofluid Simulation and Modeling, University of Bayreuth, Germany

Previous simulations and experiments have shown the "margination" of rigid spheres suspended in red blood cells flowing through a microchannel: the rigid spheres are pushed towards the wall, whereas the red blood cells concentrate in the inner region of the channel.

To investigate the influence of more complex geometries we simulate margination in a partially constricted cylinder using the Lattice Boltzmann method. This is done using different cylinder lengths and constriction-cylinder ratios. Besides changes in the radial distribution due to the constriction, the density of spheres in flow direction is investigated.

Understanding the influence of a constriction on margination is necessary for efficient drug delivery, especially, in the case of a stenosis.

BP 15.2   Mon 17:30   Poster C

Platelet orientation in laminar flow with no-slip and free-slip boundary conditions — ●Lukas Schrack and Stephan Gekle — Biofluid Simulation and Modeling, University of Bayreuth, Germany

We investigate the orientation of platelet-shaped colloidal particles for a pressure driven laminar flow using Lattice Boltzmann method. The alignment is measured by the Hermans orientation parameter. The radial orientation distribution of platelets within a cylinder and a liquid jet is studied. The liquid jet is simulated by a free moving fluid with variable diameter.

We are interested in the influence of no-slip and free-slip boundary conditions on the orientation parameter especially within the transition zone between a cylinder and a liquid jet.

Our simulation results are compared with experimental data of sodium hectorite measured by small angle X-ray scattering.

BP 15.3   Mon 17:30   Poster C

Finite Element Analysis of the Substrate Effect in Cylindrical Indentation — ●Adrian Fessel and Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen, Deutschland

Indentation tests play an important role in tissue analysis. Various testing scenarios can be simplified to a deformable layer resting on a rigid foundation with an indenter of some shape exerting a normal force on the material surface. Focusing on the case of a flat-ended cylinder as an indenter, we perform a parametric finite element analysis aided by analytical considerations aiming to distinguish non-linear material behavior from thickness effects present in force-indentation measurements at finite indentation depths.

BP 15.4   Mon 17:30   Poster C

Multicomponent nature affects liquid phase-separation as a function of temperature. — ●Omar Adame Arana[1], Christoph A. Weber[1], Andrés F. Diaz Delgadillo[2], Anthony Hyman[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden

Temperature variations affect the fertility of many worm-like species.

Fertility in these organisms has been shown to be correlated with the existence of liquid-like drops which phase separate from the remaining cytoplasm. To understand how temperature affects demixing of these drops, embryos of a certain worm species are experimentally subjected to temperature quenches. In these experiments it is observed that the difference of concentration inside and outside of droplet material shows several plateaus as temperature is increased; a behaviour not possible in binary fluids. An open question is whether the multicomponent nature of the cytoplasm can account for this behavior.

To this end we describe the interior of the cytoplasm as a multicomponent mixture using a Flory Huggins model. In this model interactions between the components are captured by parameters which exhibit a specific dependence on temperature. Exploring several choices of interaction parameters we compute the phase diagrams using a convex hull construction. Then we analyze the behavior of the tie lines and find that the difference between concentrations inside and outside of droplet material can exhibit several plateaus as observed in experiments.

BP 16: Posters - Computational Biophysics

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

BP 16.1   Mon 17:30   Poster C

Contact- and distance-based principal component analysis of protein dynamics — •MATTHIAS ERNST and GERHARD STOCK — University of Freiburg, 79104 Freiburg, Germany

To describe and understand protein dynamics, systematic dimensionality reduction is crucial. This can be accomplished by principal component analysis (PCA), a linear transformation which removes linear correlations of the coordinates by diagonalizing their covariance matrix. Different types of input coordinates can be used, like dihedral angles (dPCA[1]) or various kinds of distances (e.g. conPCA[2]) or cartesian atomic coordinates. Internal coordinates often provides higher resolution, especially for large-amplitude motion as found in folding systems[3]. In contrast to dihedral angles which mainly reflect the behaviour of neighbouring residues in a protein, distances between pairs of atoms also incorporate information about residues further apart in the primary sequence.

We employ PCA and classify the results based on distances between Ca atoms as well as distances between different residues (including side chains) for various types of well-known model problems, like folding of villin headpiece or functional dynamics of BPTI or lysozyme. We show that it can be advantageous to include only a selected set of coordinates for a PCA because the selection of input variables strongly influences the results of a PCA.

[1] Y. Mu, P. H. Nguyen, and G. Stock, Proteins 2005, 58, 45.
[2] M. Ernst, F. Sittel and G. Stock, submitted.
[3] F. Sittel, A. Jain and G. Stock, J. Chem. Phys. 2014, 141, 014111.

BP 16.2   Mon 17:30   Poster C

Structures and Processes in a Quantum Rattle — •AMANDA DIEZ FERNANDEZ, MOLLY STEVENS, and MIKE FINNIS — Imperial College London, United Kingdom

Nanoparticles bring new possibilities to the field of drug delivery engineering. One of the properties nanoparticles for drug delivery must have is a large drug loading capacity and an extended and sustained release. This is necessary to ensure constant drug levels in the target tissue and improve drug efficiency. We recently developed a Quantum rattle based nanoparticle for drug loading and release [1] as well as multimodal imaging capabilities.

In order to understand the key features of the nanoparticle responsible for drug loading and release and to enable further optimisation of these parameters, we have taken a multiscale modelling approach. Firstly, a continuum mathematical model has been developed to describe drug diffusion and sorption in the nanoparticle. In the next phase of the project, Molecular Dynamics simulations are being done to obtain information from lower scales, such as the drug diffusion coefficient inside the pore channels.

REFERENCES:
[1] Gold silica quantum rattles for multimodal imaging and therapy M. Hembury, C. Chiappini, S Bertazzo, T. L. Kalberd, G. L. Driskoe, O. Ogunladed, S. Walker-Samueld, K.S. Krishnai, C. Jumeaux, P. Beard, C.S.S.R.Kumari, A. E. Porter, M.F.Lythgoe, C. Boissièree, C. Sanchez, and M. M. Stevens PNAS, February 17, 2015, vol. 112, no. 7, 1959 1964

BP 16.3   Mon 17:30   Poster C

Modelling and Controlling Electro-Hydrodynamics in Nanopore Translocation Experiments — •ANDREAS J MEYER and PETER REIMANN — Universität Bielefeld

The translocation of biopolymers through nanopores is dominated by several competing effects, namely electrostatic forces resulting from an applied voltage difference, system-intrinsic charges, and the hence induced velocity field of the buffer solution. Since comprehensive molecular-dynamics simulations of translocation processes are practically infeasible, modelling the acting forces demands an effective description of nanoscopic structures and physical parameters. We employ a continuum description via Poisson-Nernst-Planck and Stokes equations for conducting numerical experiments and finding optimized parameter sets or new analysis techniques.

BP 16.4   Mon 17:30   Poster C

Phase Transitions and Defects in a Flocking Model at High Density — •FELIX KEMPF[1], CHRISTOPH A. WEBER[2], and ERWIN FREY[1] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, 80333 Munich, Germany — [2]Department of Biological Physics, Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

To investigate active systems at high densities, we use computer simulations of a flocking model with repulsive interaction. Flocking models implement the core-features of active matter: self-propulsion and mutual alignment. At high densities, our model shows a transition reminiscent of melting in a 2d thermal crystal. Recently, the phase diagram was studied (C. Weber, C. Bock, and E. Frey, Phys. Rev. Lett. 112, 168301 (2014)), an open question was the role of defects in this transition. We now focus on the mutual interaction of dislocations in the crystaline phase. We explore phenomenology and statistics of the mutual interaction of two isolated dislocations in the ordered phase and compare the simulation results to a markovian model. The discrepancy between this simplified model and the statistics of the full simulations reveals that correlations are not negligible for defect interaction. We also observe a faster motion for short dislocation distances, which shows that the mechanisms governing the interactions in the near-range are fundamentally different compared to the far field.

In summary, our work elucidates phenomenology and statistics of the interaction of dislocation pairs in active high-density systems.

BP 16.5   Mon 17:30   Poster C

A mechanism for contraction of cytokinetic actin rings — •FABIAN HUBERTUS KRETEN, CHRISTIAN HOFFMANN, and KARSTEN KRUSE — Universität des Saarlandes, Theoretische Physik, Campus E26, 66123 Saarbrücken

In the late stages of cell division, animal cells are cleaved by contraction of the cytokinetic ring. The ring consists of actin filaments, molecular motors, and other proteins. How this ring generates an average net contractile stress is still poorly understood.

Here, we study a mechanism involving the formation of bipolar filaments by joining polar actin filaments of opposite orientation at their barbed ends. We develop a continuum mean-field model for the dynamics of actin filaments and motors. A linear stability analysis shows that the homogeneous distribution becomes unstable beyond a critical motor strength. Numerical solutions of the full dynamic equations exhibit a backward-bifurcating non-homogenous state with clustered filaments at distinct positions along the ring.

For sufficiently stable bipolar filaments, the distribution is stationary and reminiscent of muscle sarcomeres. In this state, the total stress is higher than in the homogenous state for the same parameters. If the bipolar filaments split fast enough into their polar constituting filaments, oscillatory states can be observed. We discuss these findings in terms of recent experiments.

BP 16.6   Mon 17:30   Poster C
Opposite Translocation of Long and Short Oligomers Through a Nanopore — •Thomas Töws, Sebastian Getfert, and Peter Reimann — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

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

BP 16.7   Mon 17:30   Poster C
New insights to the thermodynamic stability of DNA i-motif: A perspective from advanced computational sampling methods — •Raghvendra Pratap Singh, Vasileios Tatsis, and Andreas Heuer — Corrensstr. 30 , D-48149, Institute of Physical Chemistry, University of Münster

Under high temperature and low pH conditions, cytosine rich stretches of nucleic acids are able to fold in a novel localized tetrameric form via the protonation of N3 nitrogen of Cytosines. The protonation of N3 nitrogen facilitates the nucleic acids to form non Watson-Crick pairing (C+C). Recent studies suggest that this unique fold can be used as a template to create longer quadruplex nanowires for Bionanotechnology applications. The studies suggest that it could be a significant target for certain Cancer treatments. Here we present microsecond long MD simulation using advance-sampling technique of Metadynamics/Bias-exchange Metadynamics for protonated and deprotonated single stranded i-motif at ambient temperature (300K) and in high temperature (500K). Additionally, We studied unfolding simulations of experimentally solved crystal structures along with mutants of the base structure to study the impact of mutations on the thermodynamics of the DNA i-motif. A detailed comparative scenario on the stability and energetics of i-motif and induced mutants will be presented.

References [1] Guéron, M., Leroy, J.L, Current Opinion in Structural Biology 10(3),326-331(2000) [2] Ren, J., Qu, X., Trent, J.O., Chaires, J.B. Nucleic Acids Research 30, 2307*2315 (2002)

BP 16.8   Mon 17:30   Poster C
Interactions between Polyethylene Glycol and Proteins Investigated Using Molecular Dynamics Simulations — Jiajia Zhou[1], Friederike Schmid[1], and •Giovanni Settanni[1,2] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Max-Planck Graduate Center with the University of Mainz

Polyethylene glycol (PEG) is a polymer with a vast range of applications, including medical and biochemical applications. Notwithstanding the widespread use of PEG to improve the therapeuthic efficacy of drugs, proteins, liposomes or nanoparticles through the PEGylation process, the molecular factors at the basis of this behaviour have not been clearly identified, yet. Here we use molecular dynamics simulations to investigate the non-covalent interactions taking place between PEG and several blood proteins. The simulations are used to measure the preferential binding coefficient of PEG for proteins, and reveal recurring patterns of interaction involving specific aminoacids. 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 16.9   Mon 17:30   Poster C
Monte-Carlo-Simulations of Cellular Adhesion — •Filip Savić, Andreas Janshoff, and Burkhard Geil — Georg-August-Universität Göttingen, Institut für Physikalische Chemie, Tammannstraße 6, 37077 Göttingen, Germany

The adhesion of cells to the extracellular matrix is an important process in biology. To understand the physical processes involved in the on state of cellular adhesion, especially the lateral organization of adhesion molecules into clusters, we perform Monte-Carlo-Simulations based on a harmonic multi-spring model involving lipid membranes and their physical properties. Local deformation of the membrane in the vicinity of adhesion clusters facilitates cluster growth while a repulsive interaction between clusters arises due to an interplay of membrane bending rigidity and non-specific repulsion. Balance of this interaction governs cluster size and stability in our simulations.

BP 16.10   Mon 17:30   Poster C
Salting out Constants of Aromatic Compounds - Experiment, Simulation and Kirkwood-Buff Theory — •Jakub Polak, Pavel Vrbka, and Jan Heyda — Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic

Fluctuation theory of solutions, also called Kirkwood-Buff theory (KB), can be used to determine salting out constants of sparingly soluble molecules, from computer simulation data.

In this contribution, we have experimentally determined the limiting activity coefficients for large set of aromatic compounds (benzene, toluene, ethylbenzen and xylenes) in salt solutions (NaCl, Na2SO4, NaSCN). Following a recent simulation study of alkali halides salting-out effect on benzene (dx.doi.org/10.1021/jp5011154), we gained microscopic insight into the role of salts via all-atom molecular dynamics simulations.

The KB analysis of simulation data provide a solid evidence that the preferential binding of salt over water is weakly negative (i.e., salt is weakly depleted) for NaSCN, negative for NaCl, and very negative for Na2SO4, in accord with experimentally determined salting out constants.

The applicability of, in the community frequent, partitioning concepts, as well as the arbitrariness of the selection of 'reference' salt are discussed.

BP 17: Posters - Coupled Problems in Biological Systems: Model Identification, Analysis and Predictions

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

BP 17.1   Mon 17:30   Poster C
Biological cybernetics in human motor control: from single-joint to multi-joint movements — •Alexandra Bayer[1,2], Daniel Häufle[1,2], Michael Günther[1], and Syn Schmitt[1,2] — [1]Institut für Sport- und Bewegungswissenschaft, Universität Stuttgart, Germany — [2]Stuttgart Research Centre for Simulation Technology, Universität Stuttgart, Germany

An open question in motor control is how different and complex movements are planned, controlled and organised in the human body. To investigate this question, biophysical modelling provides a framework to understand human motor control. For this method, physiologically motivated and experimentally validated models are required to predict the dynamic interplay of the neural controller with the musculoskeletal biophysics. Numerous model representations with different levels of detail already exist in literature. Therefore, the main goal of our cybernetic approach was to identify the basic biomechanical and biochemical properties of the neuro-musculoskeletal system for single-joint movements. Using a simple model to perform fast goal-directed arm movements, it was found that in addition to the parameterisation of the force-length curve, the movement velocity strongly depends on the model representing the activation dynamics. Based on these findings, it was possible to construct on overall human model applicable for investigations of complex multi-joint movements. Finally, such a multi-body model was used, for example, to investigate internal loads in human spine during simple movements like sitting down in a seat or during whole-body vibrations.

BP 17.2   Mon 17:30   Poster C
Normalization of Western blot data affects the statistics of estimators — Caterina Thomaseth and •Nicole Radde — Institute

for Systems Theory and Automatic Control, University of Stuttgart, Stuttgart, Germany

Western blotting is a technique for the quantification of proteins, which has made a transition from a purely qualitative to a semi-quantitative method in the last decade. Western blot data are nowadays also frequently used to enrich parameter estimation for models of intracellular processes. This task, however, poses several challenges.

In this work we elaborate on the normalization of data from Western blot experiments and its impact on parameter estimation. Preprocess-ing of Western blot data includes a two step normalization procedure, in which the raw signals are normalized to a loading control and to a reference condition. If the signals themselves are normally distributed, the normalized data are described by ratios of normal distributions, which have some peculiarities that can complicate further analysis. We recapitulate some properties of these ratio distributions and conditions for various approximations that facilitate further analysis. We illustrate results on a case study in which Western blot data are used to infer the fold change in a knockdown experiment.

BP 18: Posters - DNA, RNA and Related Enzymes

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

BP 18.1   Mon 17:30   Poster C
Molecular Dynamics simulations for the detection of unfolding pathways and stable conformations of DNA structures — •Ewa Anna Oprzeska-Zingrebe and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

The formation of specific DNA secondary and tertiary structures has been reported to play a key role in various range of biological processes, such as transcription termination or intermolecular binding. Among them, a pivotal role has been ascribed to DNA i-Motif and G-Quadruplex structures, which due to their biological appearance in telomeric and centromeric DNA are considered as potential targets for various diseases. Recent studies on high-temperature unfolding simulations of the DNA i-Motifs have revealed the existence of stable hairpin configurations as an intermediate step in the unfolding pathway of DNA higher-order structures. In our study, we investigate a simple 7-nucleotide DNA hairpin structure with the sequence d(GCGAAGC) to achieve detailed insight into the stability of DNA hairpin structures and their interaction with the osmolyte urea.

BP 18.2   Mon 17:30   Poster C
Single DNA Molecules and Colloids in a Thermophoretic Trap — •Tobias Thalheim, Marco Braun, Andreas Bregulla, and Frank Cichos — Molecular Nanophotonics Group, Institute of Experimental Physics I, University of Leipzig, Germany

We report on the trapping of single and multiple colloids as well as single DNA molecules in solution. We show, that the actual fuel of Brownian motion - temperature - is also capable of confining Brownian motion. A thermophoretic trap has been developed which employs temperature gradients, which are dynamically generated by the optical heating of a plasmonic structure. An optical feedback mechanism allows to control the number of colloids or molecules in the trap. The study of the motion of two colloids in the trap reveals not only the compression of the mean distance of the two particles in the trap but also a correlation of the spatial distribution of the particles inside the trapping region. The compression of the mean distance of the two colloidal particles suggests that also the macromolecular conformation of a single semiflexible polymer can be compressed by the action of the temperature gradients. First results of experiments on single lambda-DNA molecules provide evidence, that an inhomogeneous temperature profile is able to distort the conformation of the DNA, which paves the way for compression and free expansion experiments of single DNA molecules.

BP 18.3   Mon 17:30   Poster C
The maximum number of independently hybridizing DNA strands — •Mina Mohammadi-Kambs[1], Kathrin Hölz[2], Mark Somoza[2], and Albrecht Ott[1] — [1]Universität des Saarlandes, Department of Experimental Physics — [2]University of Vienna, Institute of Inorganic Chemistry, Faculty of Chemistry

In the cell molecular information processing is based on molecular recognition and binding. Although DNA hybridization is sometimes understood as lock and key interaction, it is not completely clear how the two molecules can identify each other. Even with a few mismatched bases, hybridization still occurs and this makes it difficult to predict hybridization in crowded and competitive environments. Here we study how different strands need to be to avoid competition for the same molecule. In this work we first numerically derive the maximal number of possible sequences, which can coexist without competing to bind to each other's perfect match. Experimentally we determine the appropriate minimum number of mismatched bases and investigate the behavior of DNA in a scenario where many sequences bind to their surface bound complements so that competition is minimized.

BP 18.4   Mon 17:30   Poster C
Subnuclear Microarchitecture is Established when Transcription is Activated in Zebrafish Embryos — •Lennart Hilbert[1,2,3], Yuko Sato[4], Hiroshi Kimura[4], Alf Honigmann[3], Vasily Zaburdaev[2], and Nadine Vastenhouw[3] — [1]Center for Systems Biology Dresden — [2]MPI for Physics of Complex Systems — [3]MPI of Molecular Cell Biology and Genetics — [4]Tokyo Institute of Technology

DNA transcription is a fundamental process of cellular function. Still, the driving forces of spatial organization of the transcription machinery in the nucleus remain poorly understood. Here, we used the onset of transcription in zebrafish embryos as a model system to investigate the contribution of transcription to spatial organization. To enable super-resolution microscopy of subnuclear organization, we dissociated embryos into individual cells. Clones of these cells exhibited transcription onset as seen in embryos. We imaged DNA and active RNA polymerase II (Pol II) in fixed clones by widefield and 3D STED super-resolution microscopy. DNA was first homogeneously distributed but segregated into spatially confined domains after transcription onset. Pol II foci with a granular sub-micron structure were seen. Focus frequency and structural complexity increased with intensifying transcription. After transcription onset, a nucleus-wide, interconnected network of Pol II-compartments formed. Live cell Pol II detection with fluorescence-tagged antibody fragments reproduced the fixed cell results. The techniques enabled by embryo dissociation will support comprehensive assessment of transcription as a driver of subnuclear organization.

BP 18.5   Mon 17:30   Poster C
Measuring DNA translocation forces through MoS2 nanopores — •Dennis Kreft, Sebastian Knust, and Dario Anselmetti — Bielefeld University

We measured the forces acting on a single strand of dsDNA during translocation through nanopores in molybdenum disulfide (MoS2) mono- and bilayer membranes by Optical Tweezers. The system includes a video-based force detection and analysis system allowing for virtually interference-free axial force measurements [1].

Preliminary measurements of the translocation of a λ-DNA dimer through a 40 nm Helium-ion drilled nanopore in a MoS2 bilayer resulted in a force of (4.5 ± 1.5) pN @ 50 mV. We will show further measurements performed with an overall force resolution of 0.5 pN at a sample rate of 2042 Hz.

[1] S. Knust et. al., Rev. Sci. Instrum. **83**, 103704 (2012)

BP 18.6   Mon 17:30   Poster C
Thermally driven length selection increases RNA self-replication rates — •Juan M. Iglesias Artola and Moritz Kreysing — MPI-CBG, Dresden, Germany

It is widely believed that modern life on Earth was preceded by RNA molecules able to store information and to catalyze their own replication. In recent years a vast amount of effort has been dedicated to the understanding of how RNA molecules manage to replicate, and indeed a cross-catalytic replication cycle has been demonstrated experimentally[1]. However, it remains unclear how such multi-component reaction networks[2] could have self-assembled under prebiotic conditions. Particularly problematic seems the strongly non-linear concentration dependence of ligation rates, which necessitates high substrate

concentrations in order to guarantee temporal persistence of the replication cycle. Using the R3C ligase as a model system, we show how a recently described thermally imbalanced micro-environment[3] is suitable to increase ligation rates by orders of magnitude through a) active accumulation of RNA strands in a small compartment, b) selection of successfully ligated products, and c) separation from inhibitory hydrolysis products. For the origin of life, we consider environmentally altered reaction kinetics key to reach reproduction rates in excess of significant decay rates; a pre-requisite not only to sustain reaction of a dilute model replicator, but also a requirement for replication networks to arise spontaneously. Refs.: [1] Lincoln et al. Science 323 (2009), [2] Higgs et al, N. Nat. Rev. Genet. 16 (2015), [3] Kreysing, et al. Nat. Chem. 15 (2015),

BP 19: Posters - Membranes and Vesicles

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

BP 19.1   Mon 17:30   Poster C
Three-dimensional lattice Boltzmann simulations of capsules with viscosity contrast — •Abdallah Daddi-Moussa-Ider[1], Badr Kaoui[2,3,1], and Stephan Gekle[1] — [1]Biofluid Simulation and Modeling, University of Bayreuth, 95440 Bayreuth, Germany — [2]CNRS - University of Technology of Compiègne, UMR 7338 - Biomechanics and Bioengineering, 60200 Compiègne, France — [3]Theoretical Physics I, University of Bayreuth, 95440 Bayreuth, Germany

We study dynamics and deformation of a spherical capsule subjected to shear flow using three-dimensional lattice Boltzmann simulations. The capsule membrane is modeled as a two-dimensional surface exhibiting resistance toward shearing, area dilatation and bending. The two-way coupling, between the fluid and the capsule, is ensured by the immersed boundary method. The viscosity contrast, between the viscosities of the encapsulated and the suspending fluids, is implemented by extending the method proposed in [Kaoui and Harting, Two-dimensional lattice Boltzmann simulations of vesicles with viscosity contrast, Rheologica Acta (2015)] to the three-dimensional case. We benchmarked our method against other previous methods in literature and we got perfect agreement for a wide range of the viscosity contrasts. Afterward we studied shape recovery of a capsule, after cessation of the applied shear flow, and we found that deformation decays exponentially with a characteristic time that depends on the membrane elastic properties and on the viscosity contrast.

BP 19.2   Mon 17:30   Poster C
Neutron Reflectometry Yields Distance-Dependent Structures of Interacting Lipid Membrane Surfaces Decorated with Hydrophilic Polymers — •Ignacio Rodriguez Loureiro[1], Victoria Latza[1], Aurelio Barbetta[1,2], Luca Bertinetti[1], Giovanna Fragneto[3], and Emanuel Schneck[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Institut de Chimie Séparative de Marcoule, France — [3]Institut 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 to determine the distance-dependent structure of interacting lipid membrane surfaces decorated with hydrophilic poly(ethylene glycol) (PEG) brushes. We also have a look at two interacting lipopolysaccharide surfaces.

BP 19.3   Mon 17:30   Poster C
Micropipettes as force sensors in biomechanical studies — •Christian Kreis, Marcin Makowski, Quentin Magdelaine, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

The precise determination of acting forces is fundamentally important for the characterization of mechanical properties of soft matter and biological processes. Optical tweezers and AFM force probes can provide quantitative information on interactions on the micro- and nanoscale. However, these techniques are limited to objects within a certain force and size range. We design micropipette force sensors from glass capillaries and employ these to study the interactions of biological matter with interfaces. The technique enables us to manipulate macroscopic and microscopic objects, with a size range from μm to mm, while measuring forces in the range from pN to mN. Additionally, it allows for quantitative force-shape and force-deformation correlations, as it is purely based on optical high-resolution (and eventually high-speed) imaging involving image cross-correlation analysis. Thus, we can manipulate single cells, multicellular aggregates, cellular tissues and even macroscopic organisms while tracking simultaneously their dynamical response. Here, we present the technique itself, as well as the force calibration of the micropipettes. Finally, we also provide experimental results on the adhesion of eukaryotic flagella to solid surfaces, the propulsion forces of the microalgae *Chlamydomonas* and the elastic properties of multicellular *Volvox* colonies.

BP 19.4   Mon 17:30   Poster C
AFM Study on Cross-linked Nanodisc Systems — •Patrick Paul[1], Dennis Kubiczek[2], Nicholas Bodenberger[2], Frank Rosenau[2], and Kay-E. Gottschalk[1] — [1]Institute of Experimental Physics, Ulm University, Ulm, Germany — [2]Center for Translational Peptide Research, Ulm University, Ulm, Germany

Nanodiscs offer various possibilities in bio nanotechnology [1]. Embedding different proteins in the lipid double layer functionalize them in a designed way [2]. By adding reactive groups to the membrane scaffold proteins (MSP) crosslinking gets possible between the discs.

We present a study of cross-linked nanodiscs to create arrays of functionalized surfaces. With the help of atomic force microscopy we control and monitor sample preparation.

[1] Bayburt et al., J Struct Biol., 1998 Sep;123(1):37-44.
[2] Nath et al., Biochemistry, 2007 Feb 27;46(8):2059-69.

BP 19.5   Mon 17:30   Poster C
Investigating Phagocytic Particle Uptake into Giant Unilamellar Vesicles using Photonic Force Microscopy — •Nicolas Schudell and Alexander Rohrbach — Lab for Bio- and Nanophotonics, University of Freiburg

Particle binding and possible particle uptakes are ubiquitous in cell biology starting and controlling a manyfold of processes. In particular, the immunological process of phagocytosis, the engulfment of a solid particle by a cell, eliminates debris and pathogens by a yet unknown amount of physical and chemical energy. The complex uptake mechanism and the different forces involved in it are only partly understood. In order to unveil the mechanistic principles, GUVs are used as a simplistic biomimetic model of a cell. They allow to investigate the important role of the lipid membrane during particle uptake. Here, we use a Photonic Force Microscope (PFM), based on optical tweezers and ultrafast 3D tracking, to approach an 1 um trapped latex bead to an immobilized GUV, until the uptake occurs. The PFM allows quantifying the position fluctuations of the trapped particle during the uptake process in 3D and with nanometer precision. Thereby, we are able to record force and energy profiles, as well as changes in the viscous drag and stiffness of the membrane. A Helfrich energy model for global and local deformation was developed for the comparison with our experimental data.

BP 19.6   Mon 17:30   Poster C
Hydrogen bond balance and entropy determine the interaction between glycolipid membranes in plant thylakoids — Matej Kanduč[1,2], •Alexander Schlaich[1], Alex de Vries[3], Bruno Demé[4], Roland R. Netz[1], and Emanuel Schneck[5] — [1]Fachbereich Physik, Freie Universiät Berlin, 14195 Berlin, Germany — [2]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [3]Groningen Biomolecular Sciences and Biotechnology (GBB) Institute and Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, The Netherlands — [4]Institut Laue-Langevin, Grenoble, France — [5]Department

of Biomaterials, Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

Naturally stacked biological membranes contain high amounts of glycolipids. Swelling experiments with membranes composed of glycolipids from plant thylakoids revealed that the interaction between these membranes is repulsive only at very low hydration. Even in excess water the membranes stay in close contact, which is in contrast to commonly studied phospholipid membranes.

Using solvent-explicit Molecular Dynamics simulations and taking the chemical potential of water into account, we reproduce the experimentally obtained pressure-distance curves of membranes composed of the plant glycolipid DGDG. Our analysis identifies the hydrogen bond balance and entropic contributions as the key determinants of the interaction. Furthermore, we find that even at the swelling limit the opposing membrane surfaces interact directly via hydrogen bonds.

BP 19.7   Mon 17:30   Poster C

Combination of MD Simulations with Two-State Kinetic Rate Modeling Elucidates the Chain Melting Transition of Phospholipid Bilayers for Different Hydration Levels — ●Bartosz Kowalik[1], Thomas Schubert[2], Hirofumi Wada[3], Motomu Tanaka[2,4], Roland Netz[1], and Emanuel Schneck[5] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institute of Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany — [3]Department of Physics, Ritsumeikan University, Kusatsu, 525-8577 Shiga, Japan — [4]Institute for Intergrated Cell-Material Sciences, Kyoto University, 606-8501 Kyoto, Japan — [5]Biomaterials Department, Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

The phase behavior of membrane lipids plays an important role in the formation of functional domains in biological membranes and crucially affects molecular transport through lipid layers. We investigate the thermotropic chain melting transition from the ordered gel phase to the disordered fluid phase in membranes composed of DPPC by atomistic molecular dynamics simulations in which the membranes are subject to variable heating rates. We find that the transition is initiated by a localized nucleus and followed by the propagation of the phase boundary. A two-state kinetic rate model allows characterizing the transition state in terms of thermodynamic quantities. The extrapolated equilibrium melting temperature increases with reduced membrane hydration and thus in tendency reproduces the experimentally observed dependence on dehydrating osmotic stress.

BP 19.8   Mon 17:30   Poster C

Diffusion of membrane-bound ligand-receptor bonds — ●Henning Stumpf[1], Daniel Schmidt[1,2], and Ana-Sunčana Smith[1,3] — [1]PULS Group, Institut für Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg — [2]II. Institut für Theoretische Physik, Universität Stuttgart — [3]Division of Physical Chemistry, Institute Ruđer Bošković, Zagreb

Protein-mediated membrane adhesion plays a crucial role for many cell functions. In a biomimetic model system, a ligand-decorated membrane adheres to an opposing membrane representing receptors. Prior to formation of a ligand-receptor bond, both individual binders exhibit a protein-specific mobility. However, the mobility of a ligand-receptor bond is significantly decreased compared to the individual binder mobilities. Thus, a bond is often considered as immobile.

In the current work, we address the mobility of a ligand-receptor construct by analytical and numerical means. We calculate the diffusion constant of a single bond as a function of the diffusion constants of the individual binders, the elastic coupling and the affinity. Furthermore, we analyse the thermal induced displacement of the bond and find that it depends sensitively on membrane-mediated correlations between individual bonds. Moreover, entropic contributions of the unbound ligands and receptors in their respective, and possibly

finite, reservoirs allow for a free energy discussion of adhesion domain formation.

BP 19.9   Mon 17:30   Poster C

Hydration Interaction between phospholipid membranes in the presence of co-solutes — ●Anirudh Gupta[1], Alexander Schlaich[1], Dat Pham[2], Matej Kanduč[3], Emanuel Schneck[4], Emma Sparr[2], and Roland R. Netz[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Physical Chemistry, Lund University, 22100 Lund, Sweden — [3]Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [4]Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

We study the interaction between phospholipid bilayers across water in the presence of co-solutes, namely TMAO (Trimethylamine N-oxide) and urea. We investigate the interaction mechanisms and thermodynamics using atomistic simulations at prescribed water chemical potential. Our interaction pressures successfully reproduce experimental data, unveiling that the membranes become more repulsive due to addition of co-solutes, as also indicated by the experiments. TMAO acts as a stabilizer for proteins while urea acts as a denaturant. It is also well known that TMAO is repelled more from proteins than the urea molecules. Our results also indicate that TMAO molecules are repelled further away from the bilayer than urea; however, the effect of both co-solutes on the membrane interaction is similar.

BP 19.10   Mon 17:30   Poster C

Stalk Intermediates on the 'Magic' Lipid Mixture — Yihui Xu and ●Tim Salditt — Institut für Röntgenphysik, Uni Göttingen, Göttingen

Stalk intermediate structures formed by pure lipid mixtures in hydrated air have already been well studied by many groups. Our group has successfully found a few 'magic' lipid mixtures who can form stalk structures at rather high relative humidities. In order to extend this research to a more biologically relevant condition, we are now trying to immerse these 'magic' mixtures into aqueous solution, and promote the stalks structures using detergent/polymers.

BP 19.11   Mon 17:30   Poster C

X-ray reflectivity investgation of structure and kinetics of photoswitchable lipid monolayers — ●Kuntal Chatterjee[1], Björn Haushahn[1], Chen Shen[1,3], Sven Festersen[1], Jonas Warias[1], Benjamin Runge[1], Franziska Reise[4], Thisbe Lindhorst[4], Beate Klösgen[3], Olaf Magnussen[1,2], and Bridget Murphy[1,2] — [1]Institute for Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — [2]Ruprecht Heansel Laboratory, University of Kiel, 24098 Kiel, Germany — [3]University of Southern Denmark, 5230 Odense M, Denmark — [4]Otto Diels Institute of Organic Chemistry, University of Kiel, 24118 Kiel, Germany

The mechanical and dynamic properties of phospholipid membranes are of importance for important biological functions, such as switching of embedded proteins. In order to investigate these properties we study model systems in which amphiphilic photoswitchable molecules are integrated into Langmuir films of phospholipids. we have modified glycolipids to contain an azobenzene photoswitch between the chain and the head group and successfully embedded those in a monolayer of dipalmitoylphosphatidylcholine (DPPC). This allows us to reversibly change the azobenzene-glycolipid orientation between trans- and cis-conformation by illumination with UV and blue light. We have followed the structural changes in this model membrane and the switching kinetics of the system with Langmuir isotherms and in situ X-ray reflectivity at the LISA diffractometer P08, PETRA III. This work is funded by SFB 677. The LISA instrument at PETRA III is funded by BMBF 05K13FK2.

BP 20: Posters - Molecular Dynamics

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

BP 20.1   Mon 17:30   Poster C

Competition of Electrostatic vs. Hydrophobic Forces in the Central Core Region of Amyloid beta Fibrils — ●Felix Hoffmann, Gül Bekcioglu-Neff, and Daniel Sebastiani — Mar-

tin Luther Universität Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle

Amyloidogenic peptides aggregated to large molecular assemblies are a hallmark of several diseases including Parkinson's, Huntington's, and

Alzheimer's disease as well as type II diabetes. Despite that each of these diseases gives rise to a very distinctive clinical picture, amyloid fibrils share the cross-beta structure as a common structural feature. Within this structure, peptide strands are linked via lateral beta-sheet-turn-beta-sheet motifs resulting in fibre-like aggregates with diameters of a few nanometers and lengths up to several micrometers.

The central question addressed is how electrostatic and hydrophobic interactions compete within the central core region of Abeta(1-40) fibrils. By means of extensive molecular dynamics simulations we investigated a series of rationally mutated Abeta(1-40) variants which introduce electrostatic forces in the central core region of the fibril. Our study shows considerable structural differences compared to existing models of wild type Abeta(1-40) fibrils. [1] Further, we computed NMR chemical shifts and NMR order parameters which are in good agreement with experimental findings and thus validate our computational approach. [1]

[1] F. Hoffmann, G. Bekcioglu, J. Adler, D. Huster, and D. Sebastiani, in preparation.

BP 20.2   Mon 17:30   Poster C

Molecular Evolution — ●Emanuel Gregor Worst[1], Philipp Zimmer[2], Eva Wollrab[1], Karsten Kruse[2], and Albrecht Ott[1] — [1]Saarland University, Biological Experimental Physics, Postfach 151150, 66041 Saarbrücken — [2]Saarland University, Theoretical Biological Physics, Postfach 151150, 66041 Saarbrücken

From the origin of life Darwinian evolution has continuously led to new and different species that make up a highly complex biosphere. Reproduction in conjunction with variation leads to the permanent selection and emergence of new species. How Nature avoids an evolutionary stall and keeps on innovating remains poorly understood. Many aspects of Darwinian evolution have been described by experimental as well as theoretical approaches. However, a realization of Darwinian evolution on long time scales that does not end up in the selection of a single fittest evolutionary winner is still lacking. We introduce an experimental system that consists of linear DNA molecules of a given length that are able to reproduce in a template-directed way. Longer molecules emerge by spontaneous ligation. A DNA species is formed by DNA strands that feed on shorter strands and that eventually outcompete other existing DNA molecules. An evolutionary stall is avoided if these new species serve as a niche that future mutants feed upon. Our molecular evolutionary system is principally able to progress indefinitely.

BP 20.3   Mon 17:30   Poster C

Quantitative assessment of sampling quality of molecular dynamics simulations of biomolecular systems — ●Mike Nemec and Daniel Hoffmann — Bioinformatics - Center for Medical Biotechnology, University of Essen, Germany

Typical biomolecular systems have huge, rugged energy landscapes. Although Molecular Dynamics (MD) simulations only sample tiny fractions of these landscapes, these samples are often used for inferring properties of the biomolecular systems, such as thermodynamic averages or conformational states. It is therefore a critical question, how well MD simulations actually sample these systems. Here we show how the quality of the sampling can be assessed by a combination of two measures, the mixture of configurations between MD trajectories and the effective sample size. We report numerical results from extensive MD simulations of two polypeptides in aqueous solution, Met-Enkephalin (5 residues) and HIV-1 gp120 V3 (35 residues), with various sampling protocols, namely conventional MD and two enhanced sampling algorithms aMD and scaledMD.

BP 20.4   Mon 17:30   Poster C

Electrophoretic Mobilization of Neutral Solutes in Salty Solutions — Tomas Krizek[1], Anna Kubickova[1], Pavel Coufal[1], Pavel Jungwirth[2], ●Jan Heyda[3], and Vladimir Vladimir[2,3] — [1]Department of Analytical Chemistry, Faculty of Science, Charles University in Prague, Prague, Czech Republic — [2]Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Center for Biomolecules and Complex Molecular Systems, Prague, Czech Republic — [3]Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic

UV-absorbing neutral substances are commonly used as markers of mean electroosmotic flow in capillary electrophoresis. However, it was recently found both experimentally and computationally (dx.doi.org/10.1002/elps.201300544) that some of the markers have dispositions to be mobilized with respect to the electroosmotic flow. The mobilization is caused by interactions of the marker molecule with components of background electrolyte.

In this work, 'amide' markers in combination with selected background electrolyte cations were studied. On the basis of this set of experiments, some general trends in the mobilization of markers were discussed and some favorable and unfavorable marker-cation combinations were pointed out.

BP 21: Posters - Nanoparticles, Nanocrystals and Composites

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

BP 21.1   Mon 17:30   Poster C

Binding of plasma proteins to nanoagents studied by fluorescence correlation spectroscopy — Judith J. Mittag and ●Joachim O. Rädler — LMU Munich, Faculty of Physics

Nano drug carriers for medical applications are a topic of growing interest in interdisciplinary life sciences. In this context, functionalizing of the nanoparticle surface is generally desired to achieve engineered interactions with cells. Recent studies have emphasized the fascinating role of blood plasma proteins that obscure or enhance specific surface recognition, thereby affecting the mechanism of action and fate of nanoparticles within living systems. Hence, a detailed understanding of the protein corona composition and exchange kinetics in biological

environments is required. Fluorescence correlation spectroscopy (FCS) is a highly sensitive technique that offers the possibility of studying the binding of fluorescently labeled proteins like albumin, fibrinogen or transferrin to nanocarriers. We measure the kinetics of protein corona formation on silica nanoparticles in a model plasma and show that coarse-grained modeling based on non-Langmuir differential rate equations reproduces the data. In addition, we determined the binding affinities, encapsulation efficiency and the temperature-dependent release of thermosensitive liposomes in buffer and in blood plasma. Current work includes the interaction of nanoagents with special proteins like von Willebrand factor. Apart from being the largest protein in blood, it is shear sensitive and therefore might give access to new effects that are not considered or understood yet.

BP 22: Posters - Neurosciences

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

BP 22.1   Mon 17:30   Poster C

Putative role of stochastic resonance in tinnitus — ●Christian Schuetz[1,2], Patrick Krauss[1,2], Claus Metzner[2], and Holger Schulze[1] — [1]Experimental Otolaryngology, ENT-Hospital, University of Erlangen, Germany — [2]Department of Physics, Biophysics Group, University of Erlangen, Germany

Maladaptive processes within the auditory system following damages

of the inner ear are discussed as the origin of the phantom perception of tinnitus. Models of tinnitus development postulate that acoustic trauma initially leads to reduced input into auditory nerve fibers. Remarkably, the neural activity within the central auditory pathway increases. This finding led to models of increased neuronal gain underlying the perception of tinnitus, but the source and control of this gain still remains elusive. We here investigate the role of stochastic resonance in neural sensory systems and its putative influence on the

development of tinnitus. We construct a biologically plausible neural network of leaky integrate-and-fire neurons that models the auditory system and adjusts the appropriate level of noise via a feedback loop to maintain maximum information transmission in terms of mutual information. So far, we were able to show in our model that reduced input leads to increased network activity, which is perfectly consistent with experimental data. Furthermore, by adding plasticity to our model we demonstrate how long-term auditory phantom percepts, namely tinnitus, may emerge from short-term changes of processing dynamics.

BP 22.2   Mon 17:30   Poster C

How to estimate a threshold: theoretical limitations and practical implications — ●Achim Schilling, Patrick Krauss, Konstantin Tziridis, and Holger Schulze — Experimental Otolaryngology, ENT-Hospital, University of Erlangen

We present a novel and robust method to universally estimate physiological and behavioral thresholds using the example of measurements of auditory brainstem responses (ABR) and pre-pulse inhibition (PPI) of acoustic startle responses (ASR). By definition the threshold defines the weakest stimulus strength that evokes a response significantly different from the non-stimulus condition. It is common practice that for threshold estimation measurements of physiological or behavioral responses to stimulus intensities that are close to the putative threshold are carried out. Unfortunately, the signal-to-noise ratio (S/N) naturally is worst near the threshold, since the intensities of evoked responses are positively correlated with stimulus strength. Here we demonstrate that thresholds may be estimated without any near threshold measurements if data are fitted to a generalized logistic function and an additive term representing the measured signal amplitude to the non-stimulus condition is added. We demonstrate that the goodness of fit becomes best if the supporting points are located within the area of the logistic function with the highest gradients, also referred to as its dynamic range, i.e. in a range with good S/N. To become independent from the number of measurement repetitions and the absolute noise level we perform stepwise subsampling with increasing sample-size followed by extrapolation and estimation of the asymptote.

BP 22.3   Mon 17:30   Poster C

Analyzing and modeling dynamics of cortical steady state responses to long lasting stimuli — ●Patrick Krauss[1,2], Achim Schilling[1], Konstantin Tziridis[1], Claus Metzner[2], and Holger Schulze[1] — [1]Experimental Otolaryngology, ENT-Hospital, University of Erlangen — [2]Department of Physics, Biophysics Group, University of Erlangen

We present a novel method for analyzing and modeling high-dimensional data such as multichannel cortical recordings, which is derived from multidimensional scaling (MDS). A fundamental shortcoming of classical MDS is the impossibility of assigning coordinates in target space to new points without re-running the entire scaling procedure. To overcome this problem we construct a mapping matrix M from high-dimensional state space to target space while preserving all mutual Euclidean distances. We use our method to reveal the relation between auditory perception and neuronal activity. The temporal development of the spatial activity pattern across the recording channels corresponds to a trajectory in a high-dimensional state space. Projecting trajectories with the matrix M reveals attractor-like dynamics. Remarkably, this finding remains undiscovered when performing other dimensionality reduction methods such as PCA or ICA. In addition, we use an animal model to induce tinnitus. Our method enables inferring the pitch of the tinnitus precept from recorded neuronal data, which we validate using a behavioral tinnitus assessment paradigm. Finally, inverting the matrix M results in a simple generator model of stimulus specific attractor dynamics.

BP 22.4   Mon 17:30   Poster C

Tailored Multielectrode Array as an Interface for Neuronal Networks — ●Norman Shepheard[1,2], Matthias Schürmann[3], Ulrich Rückert[2], Barabara Kaltschmidt[3,4], Christian Kaltschmidt[3], and Andy Thomas[1,5] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Ger-

many — [2]Cognitronics and Sensor Systems, Bielefeld University, Germany — [3]Cell Biology, Bielefeld University, Germany — [4]Molecular Neurobiology, Bielefeld University, Germany — [5]Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Institute for Metallic Materials, Dresden, Germany

To study neuronal network functions one need the appropriate interface to read out the action potential and to stimulate the neurons. We demonstrate a process to grow guided neuron networks in vitro, as well as to build multielectrode arrays (MEAs), which provides an electrode arrangement fitting to the desired network layout. Soma localization to one electrode is a key point for measurements in networks.

The fabrication of MEAs was done with UV-laser lithography and sputtered thin layers of titanium, titanium nitride for electrodes and silicon nitride as an insulator. The long time stable adhesion layer system is made of (3-aminopropyl)triethoxysilane, glutaraldehyde and poly lysine on top. The patterning of the adhesion layer system for guided neuronal networks is made via UV-laser lithography as well.

This flexible approach allows cell body localization of the neurons and neurite guidance as shown in the results. The network designs fits to the self-built MEAs.

BP 22.5   Mon 17:30   Poster C

Mechanotransduction in the pentamere organ of the Drosophila larva — ●Achintya Prahlad[1], Martin Göpfert[2], and Christoph Schmidt[1] — [1]DPI Göttingen — [2]Schwann-Schleiden Research Centre, Göttingen

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

Several molecular and anatomical aspects of these organs have been studied. However, an understanding of the internal transduction mechanics is still elusive. The cilia are not directly accessible, so a first step is to study the mechanics of the entire organ. Our specific question is how it deforms in response to muscle contractions - which is important since the basis of locomotion of the Drosophila larva is a complex peristaltic wave of muscle contractions.

We are using a preparation of the larva under buffer solution that allows us to directly contact the lch5. Our approach is to provide controlled push/pull stimuli to the organ using a tungsten needle, and to measure the mechanical relaxation. We are also using laser ablation to cut the tense ligament that the organ is attached to and observe the ensuing deformation of the sensory dendrites.

BP 22.6   Mon 17:30   Poster C

The effect of noise on the transition to chaos in random neural networks — ●Sven Goedeke[1,4], Jannis Schuecker[1,4], Markus Diesmann[1,2,3], and Moritz Helias[1,3] — [1]Inst of Neurosci and Medicine (INM-6) and Inst for Advanced Simulation (IAS-6) and JARA BRAIN Institute I, Jülich Research Centre — [2]Department of Psychiatry, Psychotherapy and Psychosomatics, Medical Faculty, RWTH Aachen University — [3]Department of Physics, Faculty 1, RWTH Aachen University — [4]These authors contributed equally

Networks of randomly coupled rate neurons display a transition to chaos at a critical coupling strength (Sompolinsky et al. 1988, PRL). The dynamics close to the transition – at the edge of chaos – provides a powerful substrate for computations. Here, we investigate the effect of additive white noise, representing intrinsic stochasticity or external inputs, on the transition. We develop the dynamical mean-field theory yielding the autocorrelation function. Solving the eigenvalue problem for the maximum Lyapunov exponent allows us to analytically determine the transition from non-chaotic to chaotic activity. Increasing the noise amplitude shifts the transition to larger coupling strengths, i.e., chaos is suppressed. The decay time of the autocorrelation function does not diverge at the transition, but peaks slightly above the critical coupling strength.

BP 23: Posters - Protein Structure and Dynamics

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

BP 23.1   Mon 17:30   Poster C
Structural Changes of Human IgG Antibody under High Hydrostatic Pressure — •Nico König[1,2], Julian Schulze[1], Karin Julius[1], Michael Paulus[1], Clara Grüning[2], Philipp Ellinger[2], Matthias Voetz[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund — [2]Bayer Technology Services GmbH, Leverkusen

A new trend in food industry is to pasteurize foodstuff via high pressure. It is therefore of interest if proteins withstand a high hydrostatic pressure treatment conserving their native structure. In the future this question might also be of relevance in the life science industry.

We report on the investigation of the human antibody Immunoglobulin G (IgG) under high hydrostatic pressure. IgG antibodies play a crucial role in the adaptive immune system of vertebrates. The tips of the Y-shaped IgG antibody represent the paratopes which bind their respective epitopes on the antigen (e.g. other proteins or small molecules). The high binding affinity and engineering of antibodies opens a wide range of applications within the life science industry.

Thus, for future applications of high-pressure treatment in the life science industry it is interesting to investigate the behaviour of IgG antibodies under high hydrostatic pressure. We conducted high-pressure small-angle X-ray scattering (SAXS) experiments on IgG to check for structural changes. Additional experiments were performed using circular dichroism spectroscopy (CD) and dynamic light scattering (DLS).

BP 23.2   Mon 17:30   Poster C
Protein folding investigated by SANS/SAXS small angle scattering and neutron spin-echo — •Felix Ameseder[1], Aurel Radulescu[2], Olaf Holderer[2], Andreas Stadler[1], and Dieter Richter[1] — [1]Forschungszentrum Jülich GmbH, Neutron Scattering, JCNS/ICS-1 — [2]Forschungszentrum Jülich GmbH, Neutron Scattering, JCNS-FRMII

The process of protein folding is highly dependent on the amino acid composition as well as on the solution condition, especially on the presence of denaturant. Our approach is to describe the folding by coefficient dimension of polymer scaling laws, and measure the folding as a function of denaturant type and denaturant concentration which has proved to be promising in singlemolecule FRET experiments. Here, we use SANS/SAXS to determine the structure of bovine serum albumin m=66kD in H20/D2O buffer solution and at various concentrations of guanidine hydrochloride and β-mercaptoethanol as additional solvent. The global dynamics of native and unfolded BSA is investigated with dynamic light scattering spectroscopy. The advantage of neutron spin-echo spectroscopy is used to cover a time range up to 140ns with spacial resolution from $q = 0.05 A^{-1}$ to $q = 0.17 A^{-1}$. SANS and SAXS results of native BSA show agreement with coherent scattering intensities calculated from crystal structure model of a respective monomer. All scattering data of unfolded structures reveal distinct evidence of the lost of internal order. NSE measurements of disordered structures reveal a contribution of internal dynamics to global diffusion.

BP 23.3   Mon 17:30   Poster C
On the α-Helical Coiled Coil to β-Sheet Conversion in Regenerated Hornet Silk — •Andreas Schaper[1], Taiyo Yoshioka[2], Tsunenori Kameda[2], Kohji Tashiro[3], Takashi Nemoto[4], and Tetsuya Ogawa[4] — [1]Philipps University, Marburg, Germany — [2]National Institute of Agrobiological Sciences, Tsukuba, Japan — [3]Toyota Technological Institute, Nagoya, Japan — [4]Kyoto University, Uji, Japan

Alpha-helices, alpha-helical coiled coils and β-sheets are fundamental principles of chain folding in fiber-forming proteins. Evolution has been creating numbers of different structures by varying the intrinsic properties of the amino acid sequences as well as the pathway the fibrillar structures are produced. Studies of protein denaturation as it is initiated by solvents, inappropriate pH level, elevated temperature or other forms of stress, including mechanical deformation and distortion, are key for solving fundamental questions regarding the stability of native α-helix structures and their tendency to undergo amyloid or amyloid-like structure formations under non-physiological conditions.

Resuming our recent studies of the structural details of native silk from the hornet Vespa mandarinia [1], here we report X-ray and electron diffraction observations of regenerated silk under different drawing regimes. We succeeded in evaluating the transformation from a dominant four-strand alpha-helical coiled coil [1,2] to an advanced twisted cross-beta state.

[1] T. Kameda et al., J. Struct. Biol. 185, 303 (2014); [2] R.D.B. Fraser and D.A.D. Parry, J. Struct. Biol. 192, 528 (2015)

BP 23.4   Mon 17:30   Poster C
Dissociation dynamics of the viral protein hemagglutinin and the cellular receptor sialic acid analyzed by single-molecule force spectroscopy — •Valentin Reiter[1], Sumati Bhatia[2], Daniel Lauster[3], Manuel Gensler[1], Luis Cuellar[2], Rainer Haag[2], Andreas Herrmann[3], and Jürgen P. Rabe[1] — [1]Department of Physics + IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Department of Chemistry, Freie Universität Berlin — [3]Department of Biology, Humboldt-Universität zu Berlin

The trimeric transmembrane protein hemagglutinin (HA) comprises over 80% of the envelope proteins present in the influenza virus and it has an essential role in the reproduction of the virus in epithelial cells by binding to sialic acid (SA) containing glycoproteins [1]. Binding of nanoparticles to the HA can hinder cell attachment and inhibit viral infection [2]. For the development of more potent inhibitors, the binding should be understood on the single-molecule level. Scanning force microscope (SFM) based single-virion force spectroscopy has proven to be a valuable tool to directly probe molecular interactions of virion-cell binding and precisely determine pN-ranged forces that govern the receptor ligand dissociation [3]. Using immobilized single proteins and SFM cantilevers functionalized with SA we measured the rupture forces of single HA-SA bonds under dynamic loads and derive a significantly larger dissociation rate and rupture length compared to single virion experiments [3] which will be discussed. [1] G. M. Whitesides et al., Angew. Chem. Int. Ed. 1998, 37, 2754; [2] I. Papp et al., ChemBioChem 2011, 12, 887; [3] C. Sieben et al., PNAS, 2012, 109, 13626.

BP 23.5   Mon 17:30   Poster C
Particle-based computer simulations of protein self-assembly in shear flow — •Fabian B. Fuchs, Nikolas Schnellbächer, and Ulrich S. Schwarz — University of Heidelberg, BioQuant, ITP

Many proteins self-assemble into supramolecular complexes, with examples ranging from small signaling complexes through clathrin coats or viral capsids to large scale cytoskeletal structures like actin networks or the mitotic spindle. Many of them, most prominently the viral capsids, can also be studied outside the cellular context. As an important step towards more complex environments, here we study protein self-assembly in hydrodynamic flow. To include hydrodynamic interactions, we have developed a novel hybrid algorithm embedding proteins in an explicit solvent. The proteins are propagated using molecular dynamics with protein reactions being implemented through reactive patches on their surface. The solvent is realized using Multi Particle Collision Dynamics (MPCD). As paradigmatic examples with anisotropic intermediates, we examine the assembly of rods and rings as a function of concentration, shear flow and binding rate constants.

BP 24: Posters - Single Molecule Biophysics

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

BP 24.1   Mon 17:30   Poster C
Knotting and Unknotting of a single protein with optical tweezers — •Fabian Ziegler[1], Nicole Lim[1], Soumit Mandal[2], Benjamin Pelz[1], Wei-Ping Ng[2], Sophie Jackson[2], and Matthias Rief[1] — [1]Physik-Department E22, TU München (Germany) — [2]University of Cambridge (UK)

Spontaneous folding of a polypeptide chain into a knotted structure remains one of the most puzzling and fascinating features of protein folding. However the observed kinetics are on the timescale of minutes and thus hard to reproduce with atomistic simulations yet.

Former studies could not distinguish between folding and knotting steps in the formation of the knotted native structure, as it has generally not been possible to control the topology of the unfolded state. We have overcome this problem with Single-molecule Force Spectroscopy by variation of pulling directions and can provide direct evidence that a threading event associated with knot formation significantly slows down folding of native UCH-L1, an important enzyme in the proteosomal degradation that has mutations linked to Parkinson's disease and has been identified as a target for treatment of Alzheimer's disease.

Our results highlight the complex nature of the folding of a knotted protein, and detect many additional intermediate structures. Mechanical stretching of knotted proteins is also important for understanding the possible implications of knots in proteins for cellular degradation. Our results might therefore indicate one possible answer to the often raised question about functions and reasons for knotted structures in proteins.

BP 24.2   Mon 17:30   Poster C
Direct observation of the intermolecular association of PGL-3, a liquid protein droplet component. — •Jose A. Morin[1,2], Shambaditya Saha[3], Anthony Hyman[3], and Stephan Grill[2,3] — [1]Max Plank Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Biotechnology Center, Technical University, Tatzberg 47, 01307 Dresden, Germany — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany

P granules, the germ line determinants in C. elegans, are an excellent example of spatiotemporal cytoplasmatic organization. During the first cell division these non-membranous organelles undergo a liquid-liquid phase separation and become localized to the posterior half of the cell. It have been shown that PGL-3, a key component of P granules, is capable of phase separation by it self into a liquid phase in the test tube. In this work we address the molecular causes for liquid formation in protein systems. We have stablished a single molecule experimental assay to measure the interaction energy between individual PGL-3 proteins. Using the manipulation capabilities of our dual trap optical tweezers, a single molecule force spectroscopy technique, we place two PGL-3 coated beads into close proximity to accurately measure the interaction kinetics between a small number of PGL-3 proteins. Our data exhibit a rich kinetic behavior, where transient interactions can be clearly distinguished from the background and therefore the frequency and time duration of this interactions accessed. Moreover, a cooperative association between these proteins can be hinted.

BP 24.3   Mon 17:30   Poster C
Complex Folding Kinetics of the SAM-I Riboswitch Expression Platform Revealed by Single-molecule FRET and HMM Analysis — •Christoph Manz[1], Andrei Yu Kobitski[1], Bettina Keller[2], Ayan Samanta[3], Andres Jäschke[3], and Gerd Ulrich Nienhaus[1,4] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany — [2]Institute of Chemistry, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [3]Institute of Pharmacy and Molecular Biotechnology, University of Heidelberg, Im Neuenheimer Feld 364, 69120 Heidelberg, Germany and Molecular Biotechnology, Im Neuenheimer Feld 364, 69120 Heidelberg, Germany — [4]Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801, USA

Isolated aptameric domains of riboswitches have been studied intensively, whereas detailed knowledge on interactions between the aptamer and the expression platform of entire riboswitches is still lacking. We have studied the structure and dynamics of a complete S-adenosylmethionine-I riboswitch (SAM-I RS) at different Mg^{2+} and ligand concentrations by using single-molecule Förster resonance energy transfer (smFRET). To observe conformational changes in real time, we performed Mg^{2+} and SAM titration experiments on freely diffusing and on surface-immobilized SAM-I RS, using various FRET-labeled constructs. Data were analyzed with a newly developed hidden Markov model and an optimization procedure for photon-based smFRET data, yielding a detailed folding pathway for the SAM-I RS.

BP 24.4   Mon 17:30   Poster C
Nanomechanics of Fluorescent DNA-Dyes on DNA investigated by Magnetic Tweezers — •Ying Wang, Andy Sischka, Volker Walhorn, Katja Tönsing, and Dario Anselmetti — Experimental Biophysics and Applied Nanoscience, Physics Department, Bielefeld University, Universitätsstrasse 25, 33615 Bielefeld, Germany

Fluorescent DNA-dyes are broadly used in many biotechnological applications for detecting and imaging DNA in cells and gels. Their specific and selective interaction alters the structural and nanomechanical properties of DNA and affects biological processes that are associated with it. Although interaction modes like intercalation and minor grove binding already have been identified, associated mechanic effects like local elongation, unwinding, and softening of the DNA often remain poorly understood. We used magnetic tweezers in order to quantitatively investigate the impact of three DNA-binding dyes (YOYO-1, DAPI and DRAQ5) in a concentration dependent manner. By extending and overwinding individual, torsionally constrained, nick-free dsDNA molecules, we measured the contour lengths and molecular forces which allow estimation of several thermodynamic and nanomechanical binding parameters. Whereas for YOYO-1 and DAPI the binding mechanisms could be allocated to bis-intercalation and minor groove binding, respectively, DRAQ5 exhibited both binding modes in a concentration dependent manner.

BP 24.5   Mon 17:30   Poster C
Construction of an Optical Trap for Single Molecule Measurements on Nucleosomes — •Andreas Weissl[1], Pascal Hauenstein[1], Philip Ketterer[1], Corinna Lieleg[2], Fabian Kilchherr[1], Jonas Funke[1], Philipp Korber[2], Henrik Dietz[1], and Matthias Rief[1] — [1]Physik Department, Technische Universität München, Am Coulombwall 4a, Garching bei München, Germany — [2]Adolf-Butenandt-Institute, University of Munich, Munich, Germany

The folding of nucleosome arrays to chromatin fibres and higher order structures plays a major regulatory role in processes related to DNA transcription and replication in eukaryotic cells. A fundamental understanding of this mechanism requires insight in the formation of chromatin fibres on the molecular level.

We report on the construction of an optical trap suitable to perform single molecule measurements on nucleosomes. To push force resolution to its limits we realised a intensity feedback control that stabilised the laser intensity 0.05%. To be able to measure the same molecule in different buffer conditions we built a multi channel microfluidic setup, where we are to quickly move to various channels with different buffers.

We use this setup in a Dumbbell assay to measure the stacking force of two single nucleosomes. To conjugate the beads with the nucleosomes DNA nanostructured handles are employed. Mainly for two reasons: First, the increased stiffness compared to dsDNA handles reduces the noise, especially at low forces. Second, due to the high control over DNA nanostructures, we are able to control the orientation of the nucleosome interaction with respect to the direction of the force applied.

BP 24.6   Mon 17:30   Poster C
Splitting of plasmid ds-DNA on ultrathin films of alkylamines on graphite — •Caroline Falk[1], Nikolai Severin[1], Lei Tang[2], Stefan Zauscher[2], and Jürgen P. Rabe[1] — [1]Department of Physics & IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Mechanical Engineering and Materials Science, Duke University

DNA replication is an important process in the human body. Replication of double-stranded (ds)-DNA requires unwinding of the helical structure and local melting of ds-DNA into two single strands [1]. The exact mechanism of the initial melting is still unknown. DNA, when stretched in solution, overwinds and melts [2]. This was argued to

give insight onto the replication mechanism. It is difficult, however, to access the direct conformational changes during stretching in solution. Recent work demonstrated that this transition can be imaged with scanning force microscopy on a graphite surface coated with an alkylamine layer [3]. ds-DNA can be controlled by an amphiphilic layer, since the DNA conformation depends on the amphiphile concentration. In particular we analyzed different DNA lengths on the same surface, and we found that at a specific concentration of octadecylamine the

ds-DNA plasmid ring splits into two single strands at one position. The splitting can be analyzed as a function of total plasmid length, ultrathin amphiphilic film and base pairs.

1. D.Coman, I.M.Russu, Journal of Biological Chemistry 280, 20216 (2005). 2. J.Adamcik, S.Tobenas, G.Di Santo, D.Klinov, G.Dietler, Langmuir, 25, 3159 (2009). 3. H.Liang, N. Severin, W.Zhuang, J.P.Rabe, submitted.

BP 25: Posters - Systems Biology

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

BP 25.1   Mon 17:30   Poster C
Evolutionary accessibility of fitness landscapes with multiple alleles — •Marcin Zagórski[1,2], Zdzisław Burda[3], and Bartek Wacław[4] — [1]IST Austria, Klosterneuburg, Austria — [2]Institute of Physics UJ, Kraków, Poland — [3]AGH, Kraków, Poland — [4]University of Edinburgh, Scotland

The question of accessibility of global fitness maximum has a long history. On the one hand, increasing size of fitness landscape results in higher number of local fitness peaks that act as evolutionary dead-ends making global peak inaccessible. On the other hand, with increasing dimensionality of fitness landscape local peaks become saddle points

keeping the global peak accessible. For the fitness landscape with two alleles (genes being ON or OFF) the former picture dominates. However, it is unclear how considering multiple alleles will affect the accessibility. To address this issue, we performed exhaustive enumeration of all accessible pathways for fitness landscapes with up to 16 alleles and 2^{28} genotypes. We also run Moran type simulation of population evolution to independently verify our conclusions. The resulting estimates of asymptotic accessibility give 12%, 50%, 69%, 81% for fitness landscapes with 2, 4, 8 and 16 alleles respectively. Interestingly, this increase in accessibility is connected with higher evolutionary access time, causing evolutionary adaptation to take longer on fitness landscapes with multiple alleles.

BP 26: Symposium - Chimera States: Coherence-Incoherence Patterns in Complex Networks (SYCS)

Time: Tuesday 9:30–12:15   Location: H1

Invited Talk   BP 26.1   Tue 9:30   H1
Theory far from infinity: chimera states without the thermodynamic limit — •Daniel Abrams — Northwestern University, Evanston, IL, USA

Chimera states are surprising symmetry-broken patterns in networks of coupled oscillators which often coexist with fully symmetric states. Much of the theory for chimera states focuses on networks with an infinite number of oscillators. In this talk, I will discuss some new results for the finite-N case, showing that stable chimera states are possible with as few as 4 oscillators. This suggests that they may be easily constructed in experimental or engineered systems, and may even occur naturally.

Invited Talk   BP 26.2   Tue 10:00   H1
Chimera patterns: Influence of topology, noise, and delay — •Eckehard Schöll — Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Chimera patterns, which consist of coexisting spatial domains of coherent and incoherent dynamics, are studied in networks of oscillators involving amplitude as well as phase dynamics, complex hierarchical (fractal) topologies, noise, and delay. We show that a plethora of novel chimera patterns arise if one goes beyond the Kuramoto phase oscillator model. For the FitzHugh-Nagumo system, the Van der Pol oscillator, and the Stuart-Landau oscillator with symmetry-breaking coupling we find various multi-chimera patterns [1], including amplitude chimeras and chimera death [2]. To test the robustness of chimera patterns, we study small-world and hierarchical topologies. We also address the robustness of amplitude chimera states in the presence of noise [3], and the emergence of coherence-resonance chimeras [4]. If delay is added, the lifetime of transient chimeras can be drastically increased, and novel phenomena like stochastic resonance of delayed-feedback chimeras can arise.

[1] I. Omelchenko et al., Phys. Rev. Lett. 110, 224101 (2013). I. Omelchenko et al., Phys. Rev. E 91, 022917 (2015). I. Omelchenko et al., Chaos 25, 083104 (2015). [2] A. Zakharova, M. Kapeller, and E. Schöll, Phys. Rev. Lett. 112, 154101 (2014). [3] S. Loos, J. C. Claussen, E. Schöll, and A. Zakharova, Phys. Rev. E (2016), arXiv:1508.04010v2. [4] N. Semenova, A. Zakharova, V. Anishchenko, and E. Schöll (2016), arXiv:1512.07036.

Invited Talk   BP 26.3   Tue 10:30   H1

Chimera states in quantum mechanics — •Victor Manuel Bastidas Valencia — Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, 117543 Singapore, Singapore

Chimera states are a hallmark of self-organization in non-linear dynamical systems [1]. These intriguing states are characterized by the spatial coexistence of synchronized and desynchronized motion in a complex network [2,3]. In this talk, I will discuss the emergence of Chimera states in a network of N coupled quantum van der Pol oscillators with a ring topology. Among the diverse quantum signatures of Chimera states, I will describe the formation of Chimera-like quantum correlations in the network. In addition, I will show how Chimera states can be characterized by using concepts of quantum information theory such as the quantum mutual information. By using this approach, one can show that Chimera states exhibit lower mutual information than a synchronized state, but higher mutual information than a desynchronized one, which extends in a natural way the definition of chimera states to quantum mechanics [4].

[1] M. J. Panaggio and D. M. Abrams, Nonlinearity **28**, R67 (2015).
[2] Y. Kuramoto and D. Battogtokh, Nonlin. Phenom. in Complex Syst. **5**, 380 (2002)
[3] D. M. Abrams and S. H. Strogatz, Phys. Rev. Lett. **93**, 174102 (2004).
[4] V. M. Bastidas, I. Omelchenko, A. Zakharova, E. Schöll, and T. Brandes, Phys. Rev. E **92**, 062924 (2015).

15 min. break

Invited Talk   BP 26.4   Tue 11:15   H1
Synchronization in Populations of Chemical Oscillators: Phase Clusters and Chimeras — •Kenneth Showalter — West Virginia University, Morgantown, USA

We have studied heterogeneous populations of chemical oscillators to characterize different types of synchronization behavior. The formation of phase clusters in stirred suspensions of Belousov-Zhabotinsky oscillators is described, where the (global) coupling occurs through the medium. We then describe the formation of phase clusters and chimera states in populations of photosensitive oscillators. The nonlocal coupling occurs via illumination intensity that is dependent on the state of each oscillator. The behavior of oscillators in ring configurations as a function of the number of oscillators is described, including traveling

cluster states.

References: A. F. Taylor et al., Angewandte Chemie Int. Ed. 50, 10161 (2011); M. R. Tinsley et al., Nature Physics 8, 662 (2012); S. Nkomo et al., Phys. Rev. Lett. 110, 244102 (2013); J. F. Totz et al., Phys. Rev. E 92, 022819 (2015).

Invited Talk   BP 26.5   Tue 11:45   H1
Epileptic seizures: chimeras in brain dynamics — •Klaus Lehnertz — Universität Bonn

Epilepsy is a complex malfunction of the brain that affects approximately 50 million people worldwide. Epileptic seizures are the cardinal symptom of this multi-facetted disease and are usually characterized by an overly synchronized firing of neurons. Seizures can not be controlled by any available therapy in about 25% of individuals, and knowledge

about mechanisms underlying generation, spread, and termination of the extreme event seizure in humans is still fragmentary.

There is now increasing evidence for the existence of large-scale epileptic networks in which all constituents can contribute to the generation, maintenance, spread, and termination of even focal seizures as well as to the many pathophysiologic phenomena seen during the seizure-free interval. Using concepts and analysis tools from nonlinear dynamics, statistical physics, synchronization and network theory, significant progress has been made over the last decade in characterizing the connection structure of large-scale epileptic networks and in understanding their long-term dynamics. Model simulations of complex oscillator networks with connection structures seen in human epilepsies indicate that seizure-like activities can be regarded as self-initiated and self-terminated chimera states. Altogether, findings open promising directions for the development of new therapeutic possibilities.

BP 27: Computational Biophysics

Time: Tuesday 9:30–11:45   Location: H43

Invited Talk   BP 27.1   Tue 9:30   H43
Membrane proteins under voltage: simulations of ion channels and receptors at work — •Ulrich Zachariae — University of Dundee, Dundee, United Kingdom

Electrochemical ion gradients across biological membranes generate membrane voltage and drive the function of essential membrane proteins. We use sustained transmembrane electrochemical gradients in molecular dynamics simulations to investigate the function of ion channels and receptors under voltage. In our work on potassium channels, we find that a mechanism involving electrostatic interaction between close ion pairs in the ion selectivity filter underlies high-efficiency conduction near the diffusion limit. Evidence for the existence of close ion contacts additionally comes from crystallography. We show that this mechanism is also exquisitely selective for the conduction of potassium vs. sodium ions. Our simulations reveal the determinants of ion discrimination in the channels under actual permeation conditions.

While voltage sensing in ion channels is a widely studied phenomenon, the effects of membrane voltage on other membrane proteins are not as well understood. G-protein coupled receptors (GPCRs), which transduce signals across the membrane and form most human drug targets, have been shown to be regulated by voltage as well. However, the nature of the voltage sensor has remained elusive. Our simulations reveal the motion of a conserved voltage-sensor in class A GPCRs, whose functional implications will be discussed.

**   BP 27.2   Tue 10:00   H43
Electrochromic shift calculations reveal spectral tuning in animal rhodopsins** — •Florimond Collette, Marcel Schmidt am Busch, and Thomas Renger — Institut für Theoretische Physik, Johannes Kepler Universität Linz, Altenberger Strasse 69, 4040 Linz, Austria

Rhodopsins are biological pigment-protein complexes found in photoreceptor cells of the retina. Within the framework of a two-step quantum chemical/electrostatic calculation scheme [1] that has recently been successfully applied to reveal the functional states of BLUF photoreceptors [2], we estimated absorption shifts of the retinal chromophore for a series of site-directed mutants. We eventually explain the variations of the maximal absorbance in the red- and green-sensitive visual pigments. Our results are in excellent agreement with recent experimental studies [3] and suggest that the maximum spectral sensitivity in animal rhodopsins is dominated by electrostatic tuning.

[1] T. Renger et al., *Photosynth. Res.* **116**, 367 (2013).
[2] F. Collette et al., *J. Phys. Chem. B* **118**, 11109 (2014).
[3] W. Wang et al., *Science* **338**, 1340 (2012).

**   BP 27.3   Tue 10:15   H43
The internal dynamics and early adsorption stages of fibrinogen investigated by molecular dynamics simulations** — Stephan Köhler[1], Friederike Schmid[1], and •Giovanni Settanni[1,2] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Max-Planck Graduate Center with the University of Mainz

Fibrinogen, a plasma glycoprotein of vertebrates, plays an essential role in blood clotting by polymerizing into fibrin upon activation. It also contributes, upon adsorption on material surfaces, to determine

their biocompatibility and has been implicated as a cause of thrombosis and inflammation at medical implants. Here we present the first fully atomistic simulations of the initial stages of the adsorption process of fibrinogen on mica and graphite surfaces. The simulations reveal a weak adsorption on mica that allows frequent desorption and reorientation events. This adsorption is driven by electrostatic interactions between the protein and the silicate surface as well as the counter ion layer. Preferred adsorption orientations for the globular regions of the protein are identified. The adsorption on graphite is found to be stronger with fewer reorientation and desorption events, and showing the onset of denaturation of the protein.

**   BP 27.4   Tue 10:30   H43
Folding of small knotted proteins: Insights from a mean field coarse-grained model** — Saeed Najafi and •Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz, Germany

A small but relevant number of known protein structures features a knot. Understanding the process of folding from a swollen unknotted state to the biologically relevant native conformation is, for these proteins, particularly difficult, due to their rate-limiting topological entanglement. In this talk I will present and discuss a novel coarse-grained model, dubbed Elastic Folder Model (EFM), developed to contribute shedding some light on the problem of knotted protein folding. The EFM is a minimalistic, structure-based model where the information about the knotted conformation is encoded in bonded angular interactions only; this potential, which does not favor the formation of native contacts, is parametrized through a stochastic search scheme in parameter space. The optimal knotting pathways of the two smallest known proteins, obtained through this approach, are consistent with the results derived by means of coarse-grained as well as full atomistic simulations.

15 min break

**   BP 27.5   Tue 11:00   H43
Inferring Co-evolution in proteins and RNA by Maximum Entropy Based Approaches** — •Alexander Schug — Karlsruher Institut für Technologie, Steinbuch Centre for Computing

Protein function often requires a protein to form a complex or adopt multiple conformations during its functional cycle. The increasingly ubiquitous availability of sequential information for many protein families has given rise to a Maximum Entropy based approach called Direct Coupling analysis [1], which traces amino acid co-evolution to extract contact maps out of only sequence information. This is sufficient information for the blind prediction of quaternary and tertiary protein [2,3] or RNA structures [4]. Residue co-evolution therefore guarantees the structural stability of a protein including its functional conformations. Similarly, we can infer mutational landscapes and capture epistatic couplings between residues, and assess the dependence of mutational effects on their sequence context [5]. We find an about 40% in explicative power as compared to approaches neglecting epistasis.

References
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[4] De Leonardis E et al., NAR (2015), doi: 10.1093/nar/gkv932
[5] Figliuzzi M et al., Mol Biol Evol (2015), doi: 10.1093/mol-bev/msv211

BP 27.6   Tue 11:15   H43

Bending algorithms for soft objects: Challenge and bane — •Achim Guckenberger, Marcel Schraml, and Stephan Gekle — Biofluid Simulation and Modeling, Universität Bayreuth, Germany

Vesicles, capsules and red blood cells all share a common property, namely the resistance towards bending of their surface, an important ingredient for quantitative simulations. Unfortunately, accurate computation of these bending forces on typical surface discretizations such as flat triangles is far from being trivial.

Starting from the famous Helfrich model, we present and analyze five substantially different algorithms for the computation of the force density on triangulated meshes. Their quality is evaluated quantitatively by comparing with the analytically obtained values for the typical red blood cell shape. Furthermore, we consider the behavior of an elastic capsule in a linear shear flow using the boundary integral and the Lattice Boltzmann method. Comparisons with the existing literature are provided. We finally make a suggestion for the choice of the appropriate bending algorithm based on the presented results.

BP 27.7   Tue 11:30   H43

Exploring Gliding Motility: Model of Helical Transport of Cell Surface Proteins in Flavobacterium johnsoniae — •Mei-Hsien Tu[1], Hirofumi Wada[2], and Hsuan-Yi Chen[1] — [1]Department of Physics, National Central University, Jung-Li 32001 Taiwan — [2]Department of Physics, Ritsumeikan University, Kusatsu, 525-8577 Shiga, Japan

Cells of Flavobacterium johnsoniae exhibit rapid gliding on a solid surface powered by the migration of surface adhesive proteins SprB along a left-handed helical loop on cell surfaces. We develop a model of rigidly coupled adhesins on a helical loop to study the mechanism of this gliding motility. The model takes into account the helical geometry of the loop and the stochastic binding/unbinding dynamics of SprB. The numerical calculations reproduce the main features for the movement of Flavobacterium johnsoniae observed in the experiments. Cell body translation along its long axis displays a bidirectional motion via spontaneous symmetry breaking as predicted in a previous simple one-dimensional model. However, this linear movement has a characteristic switching length comparable to cell length due to end effect. As a cell undergoes translation, the cell body rotates counterclockwise about its principle axis when viewed from its rear. Cells with helical loop that makes one full turn from one pole of the cell to the other pole show left-turn trajectories. Furthermore, SprBs with strong binding at a cell pole naturally introduce an asymmetric distribution of the force generation to uplift the cell body and achieve the end-over-end flipping.

BP 28: Systems Biology & Gene Expression and Signalling

Time: Tuesday 9:30–12:30   Location: H44

Invited Talk   BP 28.1   Tue 9:30   H44

Molecular Bioimaging of Genome Transcription — •Patrick Cramer — Max Planck Institute for Biophysical Chemistry, Göttingen

Our laboratory studies the molecular mechanisms of eukaryotic gene transcription by integrated structural biology and elucidates the systemic principles of genome regulation with the use of funcitonal genomics and computational biology. Based on crystal structures of RNA polymerase II in different functional states we obtained a molecular movie of transcription (Cheung and Cramer, Cell 2012). With the use of functional genomics we elucidated how the transcription cycle is coordinated with co-transcriptional events (Mayer et al., Science 2012), and how a mechanism of transcriptome surveillance removes aberrant non-coding RNAs (Schulz, Schwalb et al., Cell 2013). Unexpected insights into transcription regulation came from the crystal structure of RNA polymerase I (Engel et al., Nature 2013). We have also used cryo-electron microscopy (cryo-EM) to resolve the architecture of an early Pol II elongation complex bound by the capping enzyme, which explains how capping occurs when the RNA first emerges from the Pol II surface (Martinez-Rucobo, Mol. Cell 2015). In my talk I will concentrate on our latest work where we combined different structural biology techniques to provide insights into the mechanism of gene regulation during transcription initiation, which requires the coactivator complex Mediator (Plaschka et al., Nature 2015). We reconstituted a recombinant, functional 15-subunit core of the Mediator complex and used cryo-EM and crosslinking to determine the architecture of the RNA polymerase II-Mediator core initiation complex. This work indicates how Mediator controls transcription and opens the way to the assembly and structural analysis of larger initiation complexes containing additional factors. I will present the latest unpublished work and demonstrate that cryo-EM enables us to obtain near-atomic resolution for large macromolecular assemblies, including mammalian RNA polymerase II.

BP 28.2   Tue 10:00   H44

Modeling of Colicin E2 Expression — •Matthias Lechner[1], Mathias Schwarz[2], Madeleine Opitz[1], and Erwin Frey[1] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München — [2]Institute for Biological and Medical Imaging, Technische Universität München and Helmholtz Zentrum München, Neuherberg, Germany

Regulation of mRNA translation plays a crucial role in many bacterial pathways. For this purpose, possible regulatory components are small, non-coding RNAs (sRNAs) or mRNA-binding proteins. An important system that includes a combination of these modes is the Colicin E2 system, in which SOS responses trigger the expression of the toxin colicin and its release protein. We present a simple, yet comprehensive, model of the colicin E2 regulatory network, and study both its deterministic and stochastic dynamics in detail. Its regulation can be reduced to three components: free mRNA, the mRNA-binding protein CsrA, and an effective sRNA that regulates CsrA. For the stationary state, we show that the production rate of sRNA tunes the magnitude of intrinsic fluctuations and the sharpness of mRNA thresholds. To study the dynamics, we incorporate a stochastic SOS response system into our model. The CsrA regulation filters out short-lived activation peaks, and delays the release of toxin after prolonged SOS signals. Our model thus describes Colicin E2 expression dynamics in detail and reveals the importance of the specific components for toxin release. Moreover, we give an outlook on the role of further components.

BP 28.3   Tue 10:15   H44

Control of single cell somitogenesis — •Jose Negrete JR[1], Laurel Rohde[2,3], Ravi Desai[2,3], Andrew C. Oates[2,3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Francis Crick Institute, London, United Kingdom — [3]University College London, United Kingdom

Embryo somitogenesis is preceded by the spatiotemporal evolution of a kinematic wave of cyclic genes such as her1. It is conjectured that this wave is at the same time modulated by the presence signaling gradients. In this work we have developed a theoretical formalism for analyzing the dynamics of her1 at the single cell level. Remarkably these cells show an oscillatory transient when they are disassociated from the embryo and positioned far from each other, suggesting that autonomous dynamics play an important role in somitogenesis. We have been able to identify the key parameters that are modulated during the evolution of her1 and from these we developed predictions that can be tested in experiment. In particular the parameters of the reaction rates of her1 are non-stationary suggesting that these are controlled by the signaling system.

BP 28.4   Tue 10:30   H44

Physical limits to spatiotemporal cellular signaling — •Vaibhav Wasnik[1] and Karsten Kruse[2] — [1]Saarland University, Saarbrucken, Germany — [2]Saarland University, Saarbrucken, Germany

Cells need to respond to spatiotemporal signals. Physical limits on the detection of such signals are poorly understood. Here we study the de-

tection of spatiotemporal Ca^{2+}-signals by the conventional Protein Kinase C-α (PKC$-\alpha$). Protein kinases C are ubiquitously expressed and, together with Calmodulin, form the basic read-out module for Ca^{2+}-signals. In order to activate PKC-α, it needs to simultaneously bind to Ca^{2+} and to Diacylglycerol (DAG) on the plasma membrane. On the membrane, PKC-α forms clusters. We explore the consequences of cluster formation for signal transduction. In particular we show that PKC-α acts as a low pass filter and determines the accuracy of the readout. Our study highlights the possible role of collective effects for cellular signal transduction.

30 min break

Invited Talk   BP 28.5   Tue 11:15   H44
The biosynthetic basis of budding yeast cell size control —
•Kurt M. Schmoller, Jonathan J Turner, Mardo Koivomägi, Devon Chandler-Brown, and Jan M. Skotheim — Stanford University, Stanford, US

Cell size is an important physiological trait that sets the scale of all biosynthetic processes. Although physiological studies have revealed that cells actively regulate their size, the molecular mechanisms underlying this regulation have remained unclear. Using quantitative single cell microscopy, we identified the molecular mechanism coupling growth and division in budding yeast. As cells grow, they dilute a cell cycle inhibitor while keeping the upstream activator at a constant concentration, which results in a continuously increasing probability for cell cycle entry. Size control itself is ensured by a differential dependence of activator and inhibitor synthesis rates on cell size. We anticipate that such differential size dependence of protein synthesis may be a universal mechanism for cells to coordinate their proteome with cell size.

BP 28.6   Tue 11:45   H44
Integration of morphogen signals in neural tube patterning — •Marcin Zagórski[1], Anna Kicheva[1,2], Gašper Tkačik[1], James Briscoe[2], and Tobias Bollenbach[1] — [1]IST Austria, Klosterneuburg, Austria — [2]The Francis Crick Institute, London, UK

Early in vertebrate development, different neuronal subtypes are generated from neural progenitor cells arrayed along the dorsal-ventral axis of the neural tube. This pattern of neural progenitors is established by the morphogens Shh and BMP which form opposing concentration profiles and control the expression of target genes at defined positions. How the two morphogen signals are integrated to control target gene expression is poorly understood. To address this, we exposed naïve chick neural plate explants to a broad range of defined concentrations of the two morphogens. This allowed the construction of a decoding map that describes the dependence of the target gene expression pattern on the two morphogen concentrations. Strikingly, we obtained a similar map by using a maximum likelihood estimation method to extrapolate neural tube pattern from in vivo measurements of morphogen signaling profiles and gene expression. Both decoding maps correctly predicted target gene boundary shifts in embryos with altered Shh signaling. Moreover, a simple model of a gene regulatory network that integrates the morphogen signals was sufficient to recapitulate this behaviour, providing mechanistic insight into the observed shifts in target gene domains.

BP 28.7   Tue 12:00   H44
Stochasticity in DNA Replication of Archaea — •Jens Karschau[1], Ulrik Günther[2,3], and Alessandro de Moura[4] — [1]MPI PKS, Dresden, Germany — [2]MPI CBG, Dresden, Germany — [3]TU Dresden, Dresden, Germany — [4]University of Aberdeen, Aberdeen, UK

DNA is the building plan of every living organism, which is contained in either a linear or circular chromosome. Replicating this chromosome begins from origins—the starting points from which DNA–copying forks emerge. We previously showed for the linear case that finite ends set optimal configurations for origins to give fast overall replication time. This depends on their probability to activate as well as their relative distance to another [1].

Here, we discuss replication on a circular chromosome: where forks never stop at any ends, walk around the circle, and finally coalesce with another. The process bears similarity to a nucleation and growth process on a ring—as is in bacteria and archaea, with the latter carrying multiple origins. On the one hand, we again show that the optimal location of origins strongly depends on origin distance as well as their activation probability in conditions allowing for the chromosome to be copied only once. On the other hand, under favourable conditions, simultaneous re–replication with clustered origins in nearby groups actually minimises chromosomal duplication times. We relate our findings to published experimental data to distinguish between settings for optimal growth of an archaeal species.

[1] J Karschau, JJ Blow, APS de Moura, PRL, 2012.

BP 28.8   Tue 12:15   H44
A coarse-grained growth control theory for growth transitions — •Severin Schink[1], David Erickson[2], Ulrich Gerland[1], and Terence Hwa[2,3] — [1]Physics of Complex Biosystems, Physics Department, Technical University of Munich, Germany — [2]Department of Physics, University of California at San Diego, La Jolla, CA, USA — [3]Section of Molecular Biology, Division of Biological Sciences, University of California at San Diego, La Jolla, CA, USA

A grand challenge of systems biology is to predict the kinetic response of living systems following environmental perturbations. This task is typically approached in a bottom-up manner, by characterizing the temporal changes in gene expression patterns resulting from the applied perturbation, and deducing the underlying regulatory network. Progress towards quantitative predictive models has been limited however. A fundamental obstacle has to do with the large number of unknown interactions and parameters which vastly outnumber accessible data collected even by high-throughput methodology. In this study, we choose a top-down approach, based on phenomenological growth laws, previously developed for steady state growth. We extend these to the kinetic regime, and develop a coarse-grained flux-driven regulation theory to describe bacterial growth transitions and gene expression in response to transient nutrient changes. The theory is conceptually simple, analytically solvable, and captures the kinetics of bacterial growth transitions that occurs in response to nutrient up-shifts and down-shifts (also called diauxic shifts) quantitatively without free parameters.

BP 29: Multicellular Systems

Time: Tuesday 9:30–12:45   Location: H45

Invited Talk   BP 29.1   Tue 9:30   H45
Cell Migration in Confined Geometries — •Joachim O. Rädler[1], Felix J. Segerer[1], Anna-Kristina Marel[1], Matthias L. Zorn[1], Christoph Schreiber[1], Peter Röttgermann[1], Alexandra Fink[1], Florian Thüroff[2], and Erwin Frey[2] — [1]Faculty of Physics and Center for NanoScience Ludwig-Maximilians-Universität München — [2]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München

Epithelial cell migration is of prominent importance in wound healing, embryonic development, and cancer progression. Attempts to capture cellular hydrodynamics are currently progressing, yet it remains challenging to bridge multicellular motility to single cell migration. The talk intends to provide a perspective on how the study of cell migration in confining geometries facilitates and enhances the analysis of collective motility. Using time-lapse microscopy we study the directed flow of Madin Darby canine kidney (MDCK) cells in micro-channels. We also examine one of the hallmarks of active matter, the spontaneous emergence of vortices, in defined circular micropatterns with a fixed number of cells. The emergence of vortex states is reproduced by computer simulations based on a generalized Potts model. In agreement with experiment the model shows that vortex stability depends on the interplay of the spatial arrangement and internal polarization of neighboring cells. We will furthermore demonstrate that micropatterned surfaces allow the guidance of single cells and hence open up novel approaches to probe single-cell migration.

BP 29.2   Tue 10:00   H45
Dynamics of model cell monolayers — •Damir Vurnek[1],

Sara Kaliman[1], Carina Wollnik[2], Florian Rehfeldt[2], Diana Dudziak[3], and Ana-Sunčana Smith[1,4] — [1]PULS group, Institute for Theoretical Physics I, FAU, Erlangen — [2]3rd institute of Physics - Biophysics, GAU, Göttingen — [3]University Hospital, Erlangen — [4]Division of Physical Chemistry, IRB, Zagreb

Morphogenesis and wound healing both require migration of a large number of constituent cells. This still unresolved problem of collective cell migration is addressed by using MDCK II model epithelium grown on collagen I coated glass substrates. We look at the global development of an initially droplet seeded system of cells which is allowed to expand freely over time. Large scale experiments spanning days and multiple connected fields of view are analyzed with particle image velocimetry of live fluorescent samples. This approach allows for both microscopic and macroscopic (millimeter) scales. As the whole edge, from the colony border up to the contact inhibited centre, is examined continuously new correlation length scales are uncovered. We analyze the connections between these scales and the perpetually increasing velocity of the colony border. Our recent findings push the limits of cooperative cell motion numbers into a previously unreported regime where thousands of cells act at the same time in a coordinated fashion.

BP 29.3   Tue 10:15   H45

Differential motility of *Neisseria gonorrhoeae* within bacterial micro-colonies determines the dynamics of colony merging — •Wolfram Pönisch[1], Christoph Weber[1], Khaled Alzurqa[2], Hadi Nasrollahi[2], Nicolas Biais[2], and Vasily Zaburdaev[1] — [1]Max Planck Institut für Physik Komplexer Systeme, Dresden, Germany — [2]Brooklyn College, New York, USA

Many bacteria possess type IV pili, several microns long filaments that protrude out of the cell membrane. Retraction of pili can generate pulling forces of up to 180 pN. These forces allow cells to attach and move over surfaces. Pili also mediate attractive cell-to-cell interactions that lead to the formation of microcolonies. In this project we examine microcolonies of *Neisseria gonorrhoeae*, the causative agent of the second most common sexually transmitted disease, gonorrhea. By tracking single cells inside of a microcolony, we were able to measure the mean square displacement of cells as a function of their position in a colony and to characterize their motility. We observe that cells close to the surface of the colony are considerably more motile than cells in the inner bulk. A simulation model of individual cells interacting via pili is used to unravel the mechanisms that cause this observation, for example by identifying differences in the number of interacting pili. We suggest that the position-dependent motility of cells in a colony determines the peculiar dynamics of merging microcolonies. The coalescence process is characterized by a fast approach of the colonies that is followed by a slow relaxation to the spherical shape.

BP 29.4   Tue 10:30   H45

Effect of flow and peristaltic mixing on bacterial growth in a colon-like geometry — •Jonas Cremer, Igor Segota, Markus Arnoldini, Alex Groisman, and Terence Hwa — University of California San Diego, 9500 Gilman Dr, La Jolla, CA 92093, USA

The large intestine harbors bacteria from hundreds of species with bacterial densities reaching up to 10^{12} cells per gram. Many different factors influence bacterial growth dynamics and thus bacterial density and microbiota composition. One dominant force is flow which can in principle lead to a washout of bacteria from the proximal colon. Active mixing by contractions of the colonic wall together with bacterial growth might counteract such flow-forces and allow high bacterial densities to occur. As a step towards understanding bacterial growth in the presence of mixing and flow, we constructed an in-vitro setup where controlled wall-deformations of a channel emulate contractions. We investigate growth along the channel under a steady nutrient inflow. In the limits of no or very frequent contractions, the device behaves like a plug-flow reactor and a chemostat respectively. Depending on mixing and flow, we observe varying spatial gradients in bacterial density along the channel. Active mixing by deformations of the channel wall is shown to be crucial in maintaining a steady-state bacterial population in the presence of flow. The growth-dynamics is quantitatively captured by a simple mathematical model, with the effect of mixing described by an effective diffusion term.

BP 29.5   Tue 10:45   H45

Predicting leaf growth by conformal map — •Karen Alim[1], Shahaf Armon[2], Eran Sharon[2], Boris I. Shraiman[3], and Arezki Boudaoud[4] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Racah Institute for Physics,

Hebrew University, Jerusalem, Israel — [3]KITP, University of California, Santa Barbara, U.S.A. — [4]Laboratoire Reproduction et Développement des Plantes & Laboratoire Joliot-Curie, INRA, CNRS, ENS, Université de Lyon, Lyon, France

The dynamics and patterns of growth lie at the heart of morphogenesis, the shaping of an organ or organism. Here, we investigate the local growth throughout plant leaves. We perform a conformal map between the contours at successive stages during the growth of a leaf. Based on the mapping we predict the local displacement field in the leaf blade. The predicted displacement field agrees with the experimentally measured displacement field to 92%. The observed growth is not a mere dilation but dominated by a combination of dilation, rotation and reflection. Yet, we find that the complex growth characteristics are captured by a conformal map. The constraints implied by a conformal map on local growth dynamics suggest local regulation of growth at play.

30 min break

BP 29.6   Tue 11:30   H45

Biaxial nematic order in liver tissue — •Andre Scholich[1], Hidenori Nonaka[2], Hernán Morales-Navarrete[2], Fabián Segovia Miranda[2], Kirstin Meyer[2], Yannis Kalaidzidis[2], Marino Zerial[2], Benjamin Friedrich[1], and Frank Jülicher[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Max-Planck-Institut für Zellbiologie und Genetik, Dresden

Tissue cells typically exhibit an anisotropic distribution of membrane proteins that characterizes a structural polarity of the cell. This 'cell polarity' is linked to function, such as directed transport. In cellular monolayers and various epithelial tissues, cells are known to exhibit a vectorial cell polarity with distinct domains of apical and basal membrane proteins at opposite sides of the cell that face the two boundary surfaces of the flat tissue. Here, we analyze cells of a bulk tissue, the liver. We propose a concept of biaxial cell nematic to describe the distinct anisotropy of membrane proteins in hepatocyte liver cells. Analyzing high-resolution two-photon microscopy images of mouse liver, we find spatial patterns of aligned cell axes at the tissue scale. These spatial patterns characterize liver tissue as a biaxial nematic. Spatial patterns are well-accounted for by a curvilinear reference system set by structural landmarks of large veins within the liver tissue. We discuss minimal mechanisms of cell-scale interactions that can account for the emergence of these tissue-scale patterns.

BP 29.7   Tue 11:45   H45

Driving forces of cellular arrangement during early embryogenesis of *Caenorhabditis elegans* — •Rolf Fickentscher, Philipp Struntz, and Matthias Weiss — University of Bayreuth, Bayreuth, Germany

We have studied mechanical cues in the early embryogenesis of the model organism *Caenorhabditis elegans* by means of a custom-made lightsheet microscope. This approach enabled us to acquire the trajectories and division axes/times of cells in embryos with fluorescently labeled nuclei over several hours. Furthermore, imaging membrane labeled embryos revealed cellular volumes and shapes as a function of time. In order to alter time and length scales during embryogenesis, we have used RNAi methods and different temperatures.

We had shown earlier that cellular trajectories can be modeled accurately in a purely mechanical framework during early embryogenesis [1], i.e. early cell organization is determined by the cells' quest for a position with least repulsive interactions among themselves and the eggshell. By altering the temperature, we show now that cellular velocities in the embryo exhibit an Arrhenius-scaling. Hence biochemical processes like adhesion and remodeling of the cytoskeleton determine the forces which then drive cellular motion. Furthermore, our data highlights a correlation between cell volumes and the respective cell-cycle durations. Based on our experimental data, we propose a minimal model for this phenomenon and relate it to observations in RNAi-treated animals.

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

BP 29.8   Tue 12:00   H45

Tissue level optical benefits of photoreceptor nuclei inversion — •Kaushikaram Subramanian[1], Zuzanna Blaszczak[2], Alfonso Garcia Ulloa[1], Martin Weigert[1], Irina Solovei[4], Jochen Guck[3], and Moritz Kreysing[1] — [1]MPI-CBG, Dresden, Germany — [2]Cavendish Lab, Cambridge Univ, UK — [3]BIOTEC, TU Dresden,

Germany — [4]Dept of Biology, LMU Munich, Germany

With the photoreceptor cells lying at the back, the retina has a counter intuitive optical design that necessitates propagation of light through hundreds of microns of neural tissue prior to detection. Retina has a high cell density (3-5 times higher than brain) and a large volume-fraction of nuclei that can potentially scatter light. During postnatal retinal development the photoreceptor nuclei in nocturnal mammals invert their chromatin architecture [1]. Based on interferometric measurements and simulations, it was suggested that scattering in the retina is reduced by this chromatin re-arrangement and that the individual nuclei possess the optical quality of lenses [2]. Subsequently, predictions about light transmission at tissue level were made. Using the concept of modulation transfer we aim to experimentally verify the simulation based predictions on tissue level optical benefit stemming from this nuclear inversion. Specifically we will present a comparative optical characterisation of wild type and a transgenic mice retina lacking inverted nuclei. Further results indicate optical quality of the retina improve during terminal retinal development, the period in which the unique inversion of nuclei takes place. References: [1] Solovei et al, Cell, 137(2) (2009) [2] Błaszczak et al, Opt Express, 22(9) (2014)

BP 29.9   Tue 12:15   H45
Mechanosensitive regulation of cell extrusions during pupal morphogenesis of the fly wing — •Marko Popovic[1], Raphael Etournay[2], Franz Gruber[2], Matthias Merkel[1], Amitabha Nandi[1], Corinna Blasse[2], Gene Myers[2], Guillaume Salbreux[1], Suzanne Eaton[2], and Frank Julicher[1] — [1]Max Planck Institute for Physics of Complex Systems, Dresden — [2]Max Planck Institute of Molecular Biology and Genetics, Dresden

The fly wing is a double layered epithelium which significantly reshapes during pupal stages of development. Cell extrusion is a process by which cells are expelled from the epithelium. It allows the tissue to re-duce the number of cells during pupal development and thus to adjust the stress in the tissue. Although extrusion rates are reproducible in wild type experiments they exhibit quantitatively different behavior in genetically and mechanically perturbed wings. How the extrusions are controlled is yet unknown. Motivated by the experimentally obsevred extrusion patters we construct a model of mechanosensitive regulation of cell extrusions. In combination with a simple continuum model, previously used to describe the fly wing development [Etournay et. al. eLife 2015], it yields a dynamical equation for extrusion rates with a single relaxation time-scale.

BP 29.10   Tue 12:30   H45
Accumulation of mutations for tumour initiation: extreme value statistics in a neutral Moran process — •Philip Greulich[1,2] and Benjamin D. Simons[1,2] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, UK — [2]Gurdon Institute, University of Cambridge, Cambridge, UK

To initiate tumour growth, usually several mutations need to accumulate in at least one tissue cell. Some mutations may be (quasi-) neutral alone, but the epistatic interplay of a critical number of neutral mutations may lead to a selective advantage over normal cells, which can trigger tumour growth. Here I study a model for neutral competition of renewing tissue (stem) cells which accumulate random neutral mutations over time (Moran process). The quantity of interest is the "tumour-initation risk", the probability that at least one cell acquires a threshold number of mutations, which is supposed to trigger further events towards tumour progression. By studying the extreme value statistics of mutation numbers, which are correlated between related cells, I show how this risk scales with the tissue size and with time. Thereby, I will reason how neutral competition of stem cells can reduce the risk of tumour initiation compared to non-competitive stem cells that divide only through asymmetric divisions.

BP 30: Microswimmers I (Joint Session with DY)

Time: Tuesday 9:30–13:00   Location: H47

Invited Talk   BP 30.1   Tue 9:30   H47
Amoeboid swimming — •Chaouqi Misbah — CNRS and Univ. Grenoble, France

Microorganisms, such as bacteria, algae, or spermatozoa, are able to propel themselves forward thanks to flagella or cilia activity. By contrast, other organisms employ pronounced changes of the membrane shape to achieve propulsion, a prototypical example being the Eutreptiella gymnastica. Cells of the immune system as well as dictyostelium amoebas, traditionally believed to crawl on a substratum, can also swim in a similar way. We develop a model for these organisms. It is shown that fast propulsion can be achieved with adequate shape adaptations. We investigate the effect of confinement. A complex picture emerges. In particular it is found that optimal swimming can be obtaiend for a special confinement, and that the nature (pusher or puller) of the swimmer depends on confinement. The swimmer is often found to excecute ample excursion (navigation) in the channel.

BP 30.2   Tue 10:00   H47
Meandering liquid crystal droplet swimmers — •Carsten Krüger, Corinna Maass, Christian Bahr, and Stephan Herminghaus — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Liquid crystal microswimmers immersed in an aqueous surfactant solution at concentrations above the critical micelle concentration show self-propelled motion. The droplets dissolve into surfactant micelles [1], producing an inhomogeneous surfactant distribution in the continuum, propelling the droplets via Marangoni flows at the interface [2,3].

Below the nematic-isotropic transition we observe regular meandering trajectories, which change to a persistent random walk when the droplets are made isotropic by heating. This offers a unique possibility to tune the swimming behavior. We observe a distortion of the nematic director field, with the central defect pulled towards the droplet apex, but angled away from the direction of motion. This is consistent with a constant torque caused by a distortion of the defect pattern by the external and internal flow fields, acting against the elastic field associated with the nematic order. It also gives rise to the twofold symmetry break required for helical motion, as proposed by theory, e.g. in [4].

We use polarized microscopy to observe defect structures, PIV to image flow fields and are able to track freely moving droplets in 3D with a light sheet setup. [1] K. Peddireddy et al., Langmuir 28, 12426 (2012). [2] S. Herminghaus et al., Soft Matter 10, 7008 (2014). [3] C. C. Maass et al., Annu. Rev. Cond. Mat. 7, in press (2016). [4] H. Crenshaw, Amer. Zool. 36, 608 (1996).

BP 30.3   Tue 10:15   H47
Dynamical density functional theory of microswimmers — •Andreas M. Menzel, Arnab Saha, Christian Hoell, and Hartmut Löwen — Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany

Microswimmers are found in nature in the form of self-propelling microorganisms, or they can be realized artificially, e.g. as Janus particles propelling due to self-induced phoretic effects. To describe and predict the collective behavior of many such interacting microswimmers on the mesoscopic level, statistical approaches are necessary.

Along these lines, we here report on a newly established dynamical density functional theory (DDFT). This theory includes steric as well as hydrodynamic interactions between individual swimmers within dilute and moderately concentrated suspensions of microswimmers. Minimal model microswimmers are considered. They self-propel by setting the surrounding fluid into motion, which leads to additional hydrodynamic interactions. Both pusher and puller swimming mechanisms are taken into account.

Via numerical simulations, our DDFT is demonstrated to reproduce effects recently observed in agent-based simulations. In a spherical trapping potential, this includes the formation of density rings and the self-organization in a symmetry-breaking state that resembles a hydrodynamic fluid pump. An additional instability is predicted that destabilizes the pumping state.

BP 30.4   Tue 10:30   H47
Dynamics of a single self-propelled particle — •Christina Kurzthaler, Sebastian Leitmann, and Thomas Franosch — Department for Theoretical Physics, University of Innsbruck, Innsbruck, Austria

The dynamics of a single self-propelled particle in two dimensions is analyzed in terms of the intermediate scattering function, i.e. the characteristic function of the random displacements. Its analytical solution is derived by solving the Fourier transform of the Fokker-Planck equation which has the form of a complex Mathieu equation. Exact expressions for the mean-square displacement and non-Gaussian parameter are obtained as derivatives of the intermediate scattering function. For large wave numbers, oscillations in the intermediate scattering function reflect the persistent swimming motion, whereas at small wave numbers diffusive behavior emerges with an effective diffusion coefficient depending on the velocity and rotational diffusion of the swimmer.

BP 30.5 Tue 10:45 H47
Droplet swimmers in complex geometries: Autochemotaxis and trapping at pillars. — •Chenyu Jin, Corinna Maass, Carsten Krüger, and Stephan Herminghaus — MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany

Many organisms communicate by trail mediated signalling or autochemotaxis: their motion is influenced by their own emission of a chemical attractant or repellent, diffusing slowly compared to typical agent velocities. This causes gradient forces acting both on themselves as well as on other individuals. Meanwhile, geometrical confinement also influences the behaviour of microswimmers, e.g., pusher-type swimmers attach to curved interfaces depending on the interplay of hydrodynamic interaction and trajectorial persistence. It is of high biological relevance to have a well-controlled, tunable artificial model system exhibiting these traits.

A promising candidate are self-propelling liquid crystal droplets in an aqueous surfactant solution. They gain propulsion energy by micellar solubilisation, with filled micelles acting as a chemical repellent. We can tune the key parameters swimmer size, velocity and persistence length. We use microfluidic pillar arrays of variable radii to provide a convex wall to attract the swimmer, bend its trajectory and to force it to revert to its own trail. Hence, we investigate the interplay of wall attraction, persistence of motion, and negative auto-chemotaxis. We observe repulsion for highly curved surfaces, stable trapping at large pillars, and a narrow transition region, where negative autochemotaxis makes the swimmers detach after a single orbit.

15 min break

BP 30.6 Tue 11:15 H47
Dimensionality matters in the collective behaviour of active emulsions — •Corinna Maass, Carsten Krüger, and Stephan Herminghaus — MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany

Microswimmer systems like plankton constitute an important part of our ecosystem. The description of such systems is complex, as it involves large numbers of agents, long range hydrodynamic interactions and nontrivial boundary conditions like turbulent flows and complex interfaces. They exhibit rich and sometimes puzzling behaviour like the high species diversity referred to in the Plankton Paradox, or self organised bioconvection of gravitactic bacteria. This complexity makes them hard to treat analytically and numerically. Large scale simulations usually have dimensional restrictions or exclude hydrodynamic interactions, which has to be considered in comparisons with natural systems. Simple, tunable artificial swimmer systems can help bridging this gap.

Our experimental system consists of an active emulsion of self propelling liquid crystal droplets under variable microfluidic confinement and with tunable buoyancy. While changing the system's geometry from a quasi 2D confinement to a full 3D bulk reservoir, we observe a pronounced transition from only transient local aggregation over line formation to a large scale clustering phase stabilised by self-generated convection patterns. We studied this clustering behaviour in more detail with respect to reservoir height and buoyancy.

BP 30.7 Tue 11:30 H47
Quantification of modular phoretic micro-swimmers — •Ran Niu, Christopher Wittenberg, Julian Weber, Denis Botin, and Thomas Palberg — Institut f. Physik, JGU Mainz, Staudingerweg 7, D-55128 Mainz, Germany

We have studied the swimming behavior of modular phoretic 2D micro-swimmers with particular focus on collective and cooperative effects[1,2]. These were exploited to proceed from isolated electrolyte releasing particles, driven by electro-osmotic flow field across a charged

substrate, to multi-component complex, capable of self-generated, self-directed motion, transport and release of cargo and mutual long ranged interactions. Using optical techniques, such as microscopy and super-heterodyne laser doppler velocimetry, we accurately measured and characterized the swimmer properties and dynamics. From PH gradient measurements and particle tracking, we quantified the electric field and flow field around electrolyte releasing particle. The dependence of field strength on time and the size of electrolyte releasing particle were also determined. This provides the base for the quantitative understanding and establishing of a reliable model.
[1] T. Palberg, H. Schweinfurth,T. Koller,H. Muller,H.J. Schope, and A Reinmuller, European Physics Journal Special Topics 2013, 222:2835-2853. [2] A. Reinmuller, H.J. Schope, and T. Palberg, Langmuir 2013, 29:1738*1742.

BP 30.8 Tue 11:45 H47
Confinement of Single Microswimmers in Circular Microfluidic Chambers — •Tanya Ostapenko, Thomas Böddeker, Christian Kreis, Fabian Schwarzendahl, Marco G. Mazza, and Oliver Bäumchen — Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

The characteristics of active fluids, such as suspensions of biological microswimmers, may not only originate from the mutual interactions between the constituents, but also from interactions with interfaces and confining walls. In fact, the natural habitats of many living organisms are complex geometric environments, rather than bulk situations. The influence of interfaces on the dynamics was recognized as an important factor, and there are differences in the way that pusher-type swimmers (e.g. *E. coli*) and puller-type swimmers (e.g. *C. reinhardtii*) behave close to flat interfaces. Using experiments and simulations, we report on the dynamics of single puller-type swimmers in 2D circular microfluidic chambers. We find that the radial probability distribution of trajectories displays a characteristic wall hugging effect, where swimmers remain trapped at a concave interface for decreasing chamber size. For trajectories in the vicinity of the concave wall, an alignment of the local swimming direction with the local wall tangent is observed. In contrast, the swimmers tend to scatter off convex interfaces with short interaction times. Based on geometric arguments involving the swimmer's persistence length, we explain this entrapment effect at concave interfaces.

BP 30.9 Tue 12:00 H47
Tumbling of an E. coli: role of rotation-induced polymorphism and external shear — •Tapan Chandra Adhyapak and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D - 10623 Berlin, Germany

Many multiflagellated bacteria such as E. coli adopt a run-and-tumble strategy to detect and direct themselves in chemical gradients in their surroundings. Tumbles are events which mark nearly abrupt changes in the direction of straight runs of the bacterium. Reversal of rotation of one or more of the flagella, which under normal rotation act as the propelling part of the bacterium, initiates these tumbles. Simultaneously, flagella that are reverse rotated are observed to undergo a series of polymorphic transitions between different flagellar states [1].

To understand the need, if there is any, of these transitions for an effective tumbling event has remained a long-standing problem. We present here a detailed numerical investigation unraveling the correlation between flagellar conformational changes and an efficient tumbling strategy for E. coli. Importance of these transitions in comparison to the contribution from hydrodynamic and steric interactions [2] will be addressed. At the end the nature of a tumbling event in sheared environment will also be discussed.
[1] R. Vogel and H. Stark, Phys. Rev. Lett. **110**, 158104 (2013).
[2] T.C. Adhyapak and H. Stark, Phys. Rev. E **92**, 052701 (2015).

BP 30.10 Tue 12:15 H47
Sperm Cells in Structured Microchannels — •Sebastian Rode, Jens Elgeti, and Gerhard Gompper — Theoretical Soft Matter and Biophysics, Institute of Complex Systems (ICS-2) , Forschungszentrum Jülich, 52425 Jülich, Germany

At low Reynolds numbers and in confinement, the directed motion of a self-propelled microswimmer is strongly influenced by steric and hydrodynamic surface interactions [1-2]. Our mesoscale hydrodynamics simulation allow the study of various flagellated and ciliated microorganisms in this environment, ranging from a single flagellated sperm cell to multiciliated microswimmers. In particular, we have studied the motion of sperm in geometrically structured (zig-zag) microchannels.

This is an interesting geometry for the manipulation and sorting of sperm cells. In general, sperm swim along the channel walls, but can be deflected from the wall at sharp bends. We found that the effective adhesion of a sperm cell to a curved surface depends both on the envelope of its sinusoidal beating shape and on the orientation of its beating plane. We present a heuristic argument explaining this dependence by an interplay of steric and hydrodynamic surface interactions. Our results are in qualitative agreement with recent microfluidic experiments and might provide a better insight in the mechanisms of sperm navigation under strong confinement.

[1] J. Elgeti et al., Rep. Prog. Phys. 78, 056601 (2015)
[2] J. Elgeti et al., Biophys. J. 99, 1018 (2010)

BP 30.11   Tue 12:30   H47
Cross-stream transport of asymmetric particles driven by oscillating shear — •Matthias Laumann[1], Paul Bauknecht[2], Stephan Gekle[2], Diego Kienle[1], and Walter Zimmerman[1] — [1]Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Biofluid Simulation and Modeling, Universität Bayreuth, 95440 Bayreuth, Germany

We study the dynamics of asymmetric, deformable particles in oscillatory, linear shear flow. By simulating the motion of a dumbbell, a ring polymer, and a capsule we show that cross-stream migration occurs for asymmetric elastic particles even in linear shear flow if the shear rate varies in time. The migration is generic as it does not depend on the particle dimension. Importantly, the migration velocity and migration direction are robust to variations of the initial particle orientation, making our proposed scheme suitable for sorting applications of various elastic Janus-like particles.

BP 30.12   Tue 12:45   H47
Calibration method for pH measurements with spatial and temporal resolution — •Julian Weber — Staudingerweg 7, 55128 Mainz

According to the framework of modular microswimmers, the field flow around involved particles is of great interest and can be measured by Doppler velocimetry. Here I present a special method for measuring the pH gradient around a cationic exchange resin. First gradient measurements are demonstrated.

BP 31: Statistical Physics of Biological Systems I (Joint Session with DY)

Joint session with DY organized by BP.

Time: Tuesday 12:00–13:00   Location: H43

BP 31.1   Tue 12:00   H43
Interplay of directed transport and diffusive motion inside cellular protrusions — •Isabella Krämer and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität, München, Deutschland

Linear cellular protrusions are characterized by their finger-like structure that is connected to the cell body at one end, the base, and extends into the surroundings at the other end, the tip. A membrane enclosing the protrusion separates the inside from the extracellular and prevents in- and outflux other than at the base. Inside the protrusion bundles of parallel actin filaments are embedded into cytoplasm so that different types of motion interact: directed transport of cargo towards the tip on the actin filaments and diffusive motion inside the cytoplasm.

Motivated by this biological process we study the steady-state behaviour of a totally asymmetric simple exclusion process (TASEP) that is weakly coupled to different diffusive environments and focus on systems that are closed at the tip of the TASEP. We derive an exact equation that relates the average total occupation on the TASEP to the average total occupation on the diffusive lattice coupled to it. This mass balance equation represents a global detailed balance for the exchange between the two lattices, where detailed balance does not hold locally for any pair of sites but for the two lattices in total. We show that the steady-state profile on the TASEP is given by a localized domain wall whose position can be determined using the mass balance equation. By further exploiting this equation we find an analytic expression for the nearest-neighbour correlations on the TASEP.

BP 31.2   Tue 12:15   H43
Physical driving of chemical reactions — •Vladimir Palyulin and Ulrich Gerland — Theory of Complex Biosystems, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Out-of-equilibrium physical processes can generate a chemical disequilibrium, if a suitable coupling mechanism exists. Such a physical driving of chemical reactions is relevant in contexts ranging from prebiotic evolution to atmospheric chemistry. Inspired by recent microfluidic experiments, we introduce a minimal model that couples biased diffusion as a generic form of physical non-equilibrium to reversible dimerization as the simplest nonlinear reaction. The model demonstrates explicitly that the effective coupling strength, i.e. the amplitude of the chemical response to a given amount of physical driving, depends on the boundary conditions as well as the relative speeds of the physical and chemical kinetics.

BP 31.3   Tue 12:30   H43
Growth and Division of Active Droplets: A Model for Protocells — David Zwicker[1,2], •Rabea Seyboldt[1], Christoph A. Weber[1], Anthony A. Hyman[3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA — [3]Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany

It has been proposed that during the early steps in the origin of life, small droplets could have formed by phase separation from a surrounding complex mixture. These droplets could have provided chemical reaction centers to generate and evolve organic molecules. However, whether these droplets could divide and propagate is unclear. Here we study the dynamics of such droplets by combining the physics of phase separation with chemical reactions that are maintained away from thermodynamic equilibrium by an external supply of energy. Outside the droplets, these reactions turn precursors into droplet material, which then gets incorporated into droplets, where it is eventually converted into a waste product that leaves the droplet. Surprisingly, our theoretical study shows that the resulting chemically driven fluxes can lead to shape instabilities that trigger division of droplets into two smaller daughters, which can then grow again. Therefore, chemically active droplets can exhibit cycles of growth and division that resemble the proliferation of living cells. Dividing active droplets could serve as a model for prebiotic protocells, where chemical reactions in the droplet play the role of a prebiotic metabolism.

BP 31.4   Tue 12:45   H43
Robustness of nucleosome patterns in the presence of DNA sequence-specific free energy landscapes and active remodeling — •Johannes Nuebler[1], Benedikt Obermayer[2], Wolfram Moebius[3], Michael Wolff[1], and Ulrich Gerland[1] — [1]Physik-Department, TU München, James-Franck-Str. 1, 85748 Garching — [2]Max-Delbrück-Center for Molecular Medicine, Robert-Rössle-Str. 10, 13125 Berlin — [3]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Proper positioning of nucleosomes in eukaryotic cells is important for transcription regulation. When averaged over many genes, nucleosome positions in coding regions follow a simple oscillatory pattern, which is described to a surprising degree of accuracy by a simple one-dimensional gas model for particles interacting via a soft-core repulsion. The quantitative agreement is surprising given that nucleosome positions are known to be determined by a complex interplay of mechanisms including DNA sequence-specific nucleosome affinity and active repositioning by remodeling enzymes. We rationalize the observed robustness of the simple oscillatory pattern by showing that the main effect of several known nucleosome positioning mechanisms is a renormalization of the particle interaction. For example, "disorder" from sequence-specific affinities leads to an apparent softening, while active remodeling can result in apparent softening for directional sliding or

apparent stiffening for clamping mechanisms. We suggest that such parameter renormalization can explain the apparent difference of nu-

cleosome properties in two yeast species, S. cerevisiae and S. pombe.

BP 32: Chimera State: Symmetry breaking in dynamical networks (joint session SOE/DY/BP)

Time: Tuesday 14:00–15:00   Location: H36

BP 32.1   Tue 14:00   H36

Controlling Chimera States - The influence of excitable units
— •Philipp Hövel[1,2], Thomas Isele[1], Johanne Hizanidis[3,4], and Astero Provata[3] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Humboldt Universität zu Berlin, Germany — [3]National Center for Scientific Research "Demokritos", Athen, Greece — [4]Crete Center for Quantum Complexity and Nanotechnology, University of Crete, Heraklion, Greece

We explore the influence of a block of excitable units on the existence and behavior of chimera states in a nonlocally coupled ring-network of FitzHugh-Nagumo elements. The FitzHugh-Nagumo system, a paradigmatic model in many fields from neuroscience to chemical pattern formation and nonlinear electronics, exhibits oscillatory or excitable behavior depending on the values of its parameters. Until now, chimera states have been studied in networks of coupled oscillatory FitzHugh-Nagumo elements. In the present work, we find that introducing a block of excitable units into the network may lead to several interesting effects. It allows for controlling the position of a chimera state as well as for generating a chimera state directly from the synchronous state.

BP 32.2   Tue 14:15   H36

Stability analysis of long-living transient amplitude chimeras — •Liudmila Tumash, Anna Zakharova, Judith Lehnert, and Eckehard Schöll — Institut für Theoretische Physik,TU-Berlin, Hardenbergstr 36, 10623 Berlin, Germany,

Chimera states are characterized by a spontaneous break-up of a network of identical elements into coexisting domains of coherent (synchronized) and incoherent (desynchronized) dynamics. We study networks with coupled phase and amplitude dynamics. In contrast to classical phase chimeras, pure amplitude chimeras exhibit domains of coherent and incoherent dynamics with respect to the amplitude, but the phases are always regular and correlated. These states are long-living transients. In this work we investigate networks of Stuart-Landau oscillators with symmetry-breaking non-local coupling, in which amplitude chimeras can occur [1]. We verify the hypothesis that amplitude chimeras represent saddle-states in a high-dimensional phase space by calculating the Floquet exponents and the corresponding Floquet eigenvectors. In this way we can explain the dependence of the transient times upon coupling strength, coupling range and network size.

[1] A. Zakharova, M. Kapeller, E. Schöll, Phys. Rev. Lett. **112**, 154101 (2014).

BP 32.3   Tue 14:30   H36

Chimera patterns under the impact of noise — •Sarah A. M. Loos[1], Jens Christian Claussen[2], Eckehard Schöll[1], and Anna Zakharova[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany — [2]Computational Systems Biology Lab, Campus Ring 1, Jacobs University Bremen, D- 28759 Bremen, Germany

We investigate two types of chimera states, i.e., patterns consisting of coexisting spatially separated domains with coherent and incoherent dynamics, under the influence of noise [1]. Both chimera states arise in ring networks of Stuart-Landau oscillators with symmetry-breaking coupling [2]. Amplitude chimeras are characterized by temporally periodic dynamics throughout the whole network, but spatially incoherent behavior with respect to the amplitudes in a part of the system. They are long-living transients. Chimera death states generalize chimeras to stationary inhomogeneous patterns (oscillation death), which combine spatially coherent and incoherent domains. We analyze the impact of random perturbations on their occurrence and on their lifetimes, addressing the question of robustness of chimera states in the presence of additive white noise.
[1] S. A. M. Loos et al., arXiv:1508.04010v2, (2015).
[2] A. Zakharova et al., Phys. Rev. Lett. 112, 154101 (2014).

BP 32.4   Tue 14:45   H36

A classification scheme of chimera states — •Felix P. Kemeth[1,2], Sindre W. Haugland[1,2], Lennart Schmidt[1], Ioannis G. Kevrekidis[2,3], and Katharina Krischer[1] — [1]Physik-Department, Nonequilibrium Chemical Physics, Technische Universität München, James-Franck-Str. 1, D-85748 Garching, Germany — [2]TUM Institute for Advanced Study, Lichtenbergstraße 2a, D-85748 Garching, Germany — [3]The Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544, USA

The vast and continuously growing number of chimera or chimera-like states discovered in recent years demands a classification of the various manifestations of these dynamical hybrid states. We propose systematic and reductive approaches to characterize chimera states in systems with and without spatial extent, respectively. For locally and non-locally coupled systems, that is for systems involving a spatial extension, we apply a discrete version of the Laplace operator on spatio-temporal data sets exhibiting coexistence of coherent and incoherent regions. Regarding its statistical properties we introduce a detailed classification of chimera states into groups sharing the same qualitative behavior. For globally coupled systems without a spatial dimension, the statistics of pairwise Euclidean distances between all oscillators allow a similar analysis. This classification helps clarify the different facets of chimera states and broadens our understanding of this peculiar phenomenon.

BP 33: Colloids and Complex Fluids IV (Joint Session DY/BP/CPP)

Time: Tuesday 14:00–15:15   Location: H46

BP 33.1   Tue 14:00   H46

Rheo-Chaos of Frictional Grains — •Matthias Grob, Annette Zippelius, and Claus Heussinger — Institut für Theoretische Physik, Georg-August Universität, Göttingen, Deutschland

A two-dimensional dense fluid of frictional grains is shown to exhibit time-chaotic, spatially heterogeneous flow in a range of stress values, σ, chosen in the unstable region of s-shaped flow curves. Stress controlled simulations reveal a phase diagram with reentrant stationary flow for small and large stress σ. In between no steady flow state can be reached, instead the system either jams or displays time dependent heterogeneous strain rates $\dot{\gamma}(\mathbf{r}, t)$. The results of simulations are in agreement with the stability analysis of a simple hydrodynamic model, coupling stress and microstructure which we tentatively associate with

the frictional contact network.

BP 33.2   Tue 14:15   H46

From classical to quantum and back: A Hamiltonian scheme for adaptive multi-resolution classical/path integral simulations — •Karsten Kreis[1,2], Mark E. Tuckerman[3,4,5], Davide Donadio[1,6], Kurt Kremer[1], and Raffaello Potestio[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Department of Chemistry, New York University (NYU), New York, NY 10003, USA — [4]Courant Institute of Mathematical Sciences, NYU, New York, NY 10012, USA — [5]NYU-East China Normal University Center for Computational Chemistry at NYU Shanghai, Shanghai 200062, China —

[6]Department of Chemistry, University of California Davis, One Shields Ave., Davis, CA 95616, USA

Quantum delocalization of atomic nuclei affects the physical properties of many hydrogen-rich liquids and biological systems. To accurately model these effects, Feynman's path integral formulation of quantum statistical mechanics is typically employed, which implies a substantial increase in computational overhead. By restricting the quantum description to a small spatial region, this cost can be significantly reduced. Herein, we derive and validate a rigorous, Hamiltonian-based scheme that allows molecules to change from quantum to classical and vice versa on the fly as they diffuse through the system, both reducing overhead and making quantum grand-canonical simulations possible. Our adaptive resolution approach paves the way to efficient quantum simulations of biomolecules, membranes, and interfaces.

BP 33.3   Tue 14:30   H46
All-Atom and Coarse-Grained Molecular Dynamics Simulation of Ionic Liquids — •Tamisra Pal and Michael Vogel — Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstrasse 6, 64289 Darmstadt

Room temperature Ionic Liquids (RTILs) have garnered much interest in the last few years as they possess tremendous potential for application in industry as reaction media. The high complexity of these liquids originating from their self-assembly or nano-scale aggregate formation motivates us to understand more on their dynamics. We have employed molecular dynamics simulation for RTILs to connect the length and time scales of simulation models with different levels of molecular resolution provided by the mapping scheme. Specifically, we have investigated a coarse grained (CG) model of 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF_6]) and its all-atom (AA) description, at various temperatures. In this way, we unravel the different dynamical modes associated with dynamic heterogeneity and structural relaxation and we quantitatively compare the characteristic time scales from the two model systems to ascertain the effects of coarse graining on the dynamical behavior. The spatial and temporal aspects of molecular dynamics have been studied via calculating non-Gaussian parameters, particle displacement distributions, overlap functions and dynamic susceptibilities. Our simulation results provide a microscopic understanding to the presence of "fast" and "slow" moving particles contributing to dynamic heterogeneity and their relevance for the structural relaxation of ionic liquids.

BP 33.4   Tue 14:45   H46
Equilibrium interfacial free energies and Turnbull coefficient for bcc crystallizing colloidal charged sphere suspensions — •Thomas Palberg[1], Patrick Wette[2,3], and Dieter M. Herlach[2] — [1]Institut f. Physik, Johannes Gutenberg Universität, 55099 Mainz, Germany — [2]Institut f. Materialphysik im Weltraum, DLR, 51147 Köln, Germany — [3]Space Administration, DLR, 53227 Bonn, Germany

The interfacial free energy (IFE) is a central quantity in crystallization from the meta-stable melt. In suspensions of charged colloidal spheres, nucleation and growth kinetics can be accurately measured from optical experiments. We here re-analyze the strictly linear increase of previously reported CNT-effective non-equilibrium IFEs estimated from such experimentsutilizing classical nucleation theory (CNT). For five aqueous suspensions of charged spheres and one binary mixture, we utilize a simple extrapolation scheme and interpret our findings in view of Turnbull's empirical rule. Our first estimates for the reduced equilibrium IFE, $\sigma_{0,bcc}$, between coexisting fluid and bcc-crystal phases are on the order of a few $k_B T$. Their values are not correlated to any of the electrostatic interaction parameters but rather show a systematic decrease with increasing size polydispersity and a lower value for the mixture as compared to the pure components. At the same time, σ_0 shows an approximately linear correlation to the entropy of freezing. The equilibrium interfacial free energy of strictly monodisperse charged spheres may therefore be still greater.

BP 33.5   Tue 15:00   H46
Size matters: can we use a Hamiltonian adaptive resolution scheme to simulate an open system? — •Robinson Cortes-Huerto, Maziar Heidari, and Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz, Germany

Finite size effects are ubiquitous in molecular dynamics simulations. Apart from the obvious implicit size effects due to periodic boundary conditions, explicit size effects are consequence of simulating a fixed and relatively small number of particles. In particular, measurements of density fluctuations within a sub-domain of a periodic simulation box are strongly dependent on the sub-domain size. These effects can be neglected by carrying out computer simulations for extremely large systems. An alternative solution is to use the Hamiltonian adaptive resolution scheme (H-AdResS), where the computational cost reduces substantially by embedding a relatively small high resolution portion of the system in a larger region at low resolution. Our main goal is to explore the viability to perform grand canonical simulations using this dual-resolution approach. In particular, we propose to use H-AdResS to calculate thermodynamic properties of prototypical molecular liquids in an effective open boundary simulation framework. To this end, we calculate Kirkwood-Buff integrals that connect radial distribution functions, available from molecular dynamics simulations, to thermodynamic properties such as the isothermal compressibility. We compare these results with measurements performed in the fully atomistic case and assess whether an adaptive resolution simulation reproduces the behaviour expected from an open simulation setup.

BP 34: Anomalous Diffusion (Joint Session with DY)

Time: Tuesday 14:00–15:30   Location: H47

BP 34.1   Tue 14:00   H47
Diffusion and subdiffusion of interacting particles on comblike structures — •Pierre Illien[1], Olivier Bénichou[2], Gleb Oshanin[2], Alessandro Sarracino[2], and Raphaël Voituriez[2] — [1]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, UK — [2]Laboratoire de Physique Théorique de la Matière Condensée, Université Pierre-et-Marie-Curie, Paris, France

The subdiffusive motion of tracers in crowded media, e.g., biological cells, is widespread, and has motivated a large amount of theoretical work related to diffusion in complex media. Comblike structures have received a particular interest as they constitute minimal models of systems with geometrical constraints. Here, we investigate the effect of excluded-volume interactions on tracer diffusion on such lattices.

We study the dynamics of a tracer particle (TP) on a comb lattice populated by randomly moving hardcore particles. When the TP is constrained to move on the backbone of the comb and in the limit of high density of the particles, we present exact analytical results for the cumulants of the TP position, showing a subdiffusive behavior $t^{3/4}$. At longer times, a second regime is observed where standard diffusion is recovered, with a surprising nonanalytical dependence of the diffusion coefficient on the particle density. When the TP is allowed to visit the teeth of the comb, we unveil a rich and complex scenario with several successive subdiffusive regimes, resulting from the coupling between the geometrical constraints of the lattice and particle interactions. In this case, remarkably, the presence of hard-core interactions asymptotically speeds up the TP motion along the backbone of the structure.

BP 34.2   Tue 14:15   H47
Anomalous transport of circular swimmers in disordered structures: classical edge-state percolation — •Thomas Franosch[1], Walter Schirmacher[2], Benedikt Fuchs[3], and Felix Höfling[4] — [1]UIBK Innsbruck — [2]Universität Mainz — [3]Med.-Uni Wien — [4]FU Berlin

Recently micron-sized self-propelled particles have been realized as model systems [1] for complex living organisms such as bacteria. If the agent is asymmetric a natural circular motion [2] emerges which yields characteristic skipping orbits when interacting with boundaries.

Here, we investigate by molecular dynamics simulations the dynamics of circular swimmers in a two-dimensional model with randomly distributed scatterers. For small radii of the swimming motion the agents orbit only around isolated clusters of scatterers, while at large radii diffusive behavior emerges. A de-localization transition occurs which is generated by percolating skipping orbits along the edges of obstacle clusters. Directly at the transition the mean-square displace-

ments displays subdiffusive transport. The dynamic exponents differ from those of the conventional transport problem on percolating systems, thus establishing a new dynamic universality class [3]. Last, we draw an analogy to the field-induced localization transition in magnetotransport in 2D electron gases in a disordered array of antidots.

[1] F. Kümmel, et al., Phys. Rev. Lett. **110**, 198302 (2013).
[2] S. van Teeffelen and H. Löwen, Phys. Rev. E **78**, 020101(R) (2008).
[3] W. Schirmacher, B. Fuchs, F. Höfling, and T. Franosch, Phys. Rev. Lett. (2015, in print).

BP 34.3　Tue 14:30　H47
Scales of Function Spaces for Weyl Fractional Calculus — •Tillmann Kleiner and Rudolf Hilfer — Institute for Computational Physics, University of Stuttgart, Germany

Anomalous diffusion models are frequently based on fractional differential equations [1]. Analytical investigations of these mathematical models require suitable function spaces on which the fractional derivatives operate as continuous operators. This contribution introduces function spaces suitable for Weyl fractional calculus. Scales of locally convex spaces with topology generating seminorms are constructed using weighted maximal functions. These scales are sets of spaces partially ordered by inclusion. Minimal and maximal spaces with respect to this ordering are determined such that Weyl fractional derivatives operate on them continuously or isomorphically. Such spaces can also be determined for sets of linear combinations of these operators with orders restricted to some fixed subset of $\mathbb{C}$. Inclusions of spaces within the scale correspond to continuous injections with dense range. As a result the investigated operators and their inverses are continuous extensions from the subspace of test functions for all suitable spaces.
[1] *Applications of Fractional Calculus in Physics*, edited by R. Hilfer (World Scientific, Singapore, 2000).

BP 34.4　Tue 14:45　H47
A simple non-chaotic map generating subdiffusive, diffusive, and superdiffusive dynamics — Lucia Salari[1], Lamberto Rondoni[1,2], Claudio Giberti[3], and •Rainer Klages[4,5] — [1]Dipartimento di Scienze Matematiche, Politecnico di Torino — [2]GraphenePoliTO Lab, Politecnico di Torino and INFN Sezione di Torino — [3]Dipartimento di Scienze e Metodi dell' Ingegneria, Universita di Modena e Reggio E. — [4]Max Planck Institute for the Physics of Complex Systems, Dresden — [5]School of Mathematical Sciences, Queen Mary University of London

Consider equations of motion that generate dispersion of an ensemble of particles in the long time limit. An interesting problem is to predict the diffusive properties of such a dynamical system starting from first principles. Motivated by numerical results on diffusion in polygonal billiards, we introduce an interval exchange transformation lifted onto the whole real line that mimicks deterministic diffusion in these billiards. By definition our simple map model is not chaotic, in the sense of exhibiting a vanishing Lyapunov exponent. We show analytically that it nevertheless displays a whole range of normal and anomalous diffusion under variation of a single control parameter [1].
[1] L. Salari et al., Chaos **25**, 073113 (2015)

BP 34.5　Tue 15:00　H47
Localisation of ballistic tracers in the two-dimensional Lorentz model interpreted as a renormalisation group flow — •Felix Höfling — Fachbereich Mathematik und Informatik, Freie Universität Berlin — Max-Planck-Institut für Intelligente Systeme, Stuttgart, und IV. Institut für Theoretische Physik, Universität Stuttgart

The Lorentz model serves as a minimal model to explain many facets of the rich phenomenology of anomalous transport, as frequently observed in porous materials and cellular transport [1]. Here, I will discuss the localisation transition of "ballistic" tracers (subject to Newton's equations of motion) in the two-dimensional, overlapping Lorentz model. Extensive simulations provide evidence for the universality of the dynamic critical exponent, which has been crucial in the interpretation of recent studies [2,3]. The long-time asymptotes, however, are obscured by non-universal corrections to scaling, explaining the contradicting values for the diffusivity exponent in the literature. A spectral analysis of the obtained correlation functions allows for an interpretation of the dynamics as an renormalisation flow of the transport at long times and gives insight into the fixed point structure of the RG flow.
[1] F. Höfling and T. Franosch, Rep. Prog. Phys. **76**, 046602 (2013).
[2] S. K. Schnyder, M. Spanner, F. Höfling, T. Franosch, and J. Horbach, Soft Matter **11**, 701 (2015).
[3] W. Schirmacher, B. Fuchs, F. Höfling, and T. Franosch, arXiv:1511.05218, Phys. Rev. Lett. in print (2015).

BP 34.6　Tue 15:15　H47
Non-adiabatic quantum pumping by a randomly moving quantum dot [1] — •Daniel Waltner[1] and Stanislav Derevyanko[2] — [1]Faculty of Physics, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel

We look at time dependent fluctuations of the electrical charge in an open 1D quantum system represented by a quantum dot experiencing random lateral motion. In essentially non-adiabatic settings we study both diffusive and ballistic (Levy) regimes of the barrier motion where the electric current as well as the net pumped electric charge experience random fluctuations over the static background. We show that in the large-time limit, the wavefunction is naturally separated into the Berry-phase (BP) component (resulting from the singular part of the wave amplitude in the co-moving frame) and the non-adiabatic correction (arising from fast oscillating, slow decaying tails of the same amplitude). Based on this separation we report two key results: firstly, the disorder averaged wave function and current are asymptotically mainly determined by the same BP contribution that applies in the case of adiabatic motion. Secondly, after a short transition period the pumped electric charge exhibits fluctuations that grow much faster than predicted by the adiabatic theory. We also derive the exact expressions for the average propagator (in the co-moving basis representation) for the diffusive and ballistic types of motion considered.

[1] S. Derevyanko, D. Waltner, J. Phys. A **48** (2015) 305302

BP 35: Networks: From Topology to Dynamics II (Joint Session SOE/DY/BP)

Time: Tuesday 15:00–15:45　　　　　　　　　　　　　　　　　　　　　　　Location: H36

BP 35.1　Tue 15:00　H36
Collective Failure due to Multistability in Oscillator Networks and Power Grid — •Debsankha Manik[1], Dirk Witthaut[2], and Marc Timme[1] — [1]Network Dynamics Group, Max Planck Institute for Dynamics anf self-Organization, 37077 Göttingen — [2]Forschungszentrum Jülich, Institute of Energy and Climate Research Systems Analysis and Technology Evaluation (IEK-STE), 52425 Jülich

Networks of phase oscillators model the collective dynamics of various interacting physical and biological systems, ranging from electric power grid operation to neuronal rhythms. Here we show that the number of stable steady states in phase oscillator systems scales with the length of the topological cycles in the network such that for non-global coupling, multistable steady states may emerge. The clustering of similar natural frequencies favour fewer stable states, whereas homogeneous

frequency distributions favour more. Intriguingly, multistability prevails even under conditions for which stable states have been claimed to be unique. This multistability may have significant impact on the collective dynamics of such networks: for example, in power grids where the transmission lines have structural limitations on the maximum load they can safely carry, perturbations may induce switching to different steady states, strongly alter the flow patterns, and in turn yield a collective failure of the grid.

BP 35.2　Tue 15:15　H36
Geometric organization of real multiplex networks — •Kaj Kolja Kleineberg[1], Marian Boguna[1], M. Angeles Serrano[1], and Fragkiskos Papadopoulos[2] — [1]Departament de Fisica Fonamental, Universitat de Barcelona, Marti i Franques 1, 08028 Barcelona, Spain — [2]Department of Electrical Engineering, Computer Engineer-

ing and Informatics, Cyprus University of Technology

Real complex networks are organized to perform certain functions, among which targeted transport is important in a broad range of real systems, such as the Internet, social networks, or transportation networks. In reality, networks are not isolated entities but instead form interacting parts of larger and more complex systems. These systems are not a random combination of single networks, but instead are organized in a certain way. We investigate the geometric organization of multilayer networks and its implications. We find significant metric correlations between different layers. These correlations are key to answer many important questions concerning real multilayer systems. Metric correlations allow for inter-layer link prediction and the definition and detection of multidimensional communities. Metric correlations improve mutual greedy routing, that is targeted navigation in the whole multilayer system. Interestingly, only in the presence of

metric correlations does the whole system outperform its single layers. We find that optimal correlations make multilayer systems perfectly navigable. Finally, we show how correlations present in the real Internet multiplex help navigating the digital world. Our findings have important implications for the design of real multilayer systems.

BP 35.3 Tue 15:30 H36
Interplay of shape and degree distribution in complex networks — •Robin de Regt and Christian von Ferber — Applied Mathematics Research Centre, Coventry University, UK

Complex networks are often described without geometry. Here, we explore possibilities of how an embedding of such networks in real space (e.g. 2D or 3D) may reveal interesting correlations between standard measures such as degree distributions and the shapes these structures may attain when embedded in a given space.

BP 36: Molecular Dynamics (Focus Session)

Focus session organized by Bert de Groot, Max Planck Institute for Biophysical Chemistry, Göttingen

Time: Wednesday 9:30–11:00 Location: H43

Invited Talk BP 36.1 Wed 9:30 H43
Molecular simulation of protein dynamics and function — •Gerhard Hummer — Max Planck Institute of Biophysics, Frankfurt am Main, Germany

We use molecular simulations to study functional protein dynamics over a broad range of temporal and spatial scales. A hybrid quantum-mechanics/molecular-mechanics (QM/MM) description allows us to follow fast, photoexcitation-driven protein motions. The resulting simulation trajectories are compared directly to femtosecond time-resolved protein crystallography experiments at X-ray free electron lasers. By contrast, to study large-amplitude functional motions in molecular motors on slower timescales, we use equilibrium and nonequilibrium classical simulations. The simulations help us elucidate the mechanisms underlying the efficient operation of biomolecular machines.

BP 36.2 Wed 10:00 H43
In Silico Reduction of Conformational Variance in Cryo-EM Imaging — •Gunnar Schröder — Forschungszentrum Jülich, Jülich, Germany

One of the biggest challenges in the analysis of cryo-EM images is the heterogeneity and flexibility of the molecules, which on the one hand severely limits the achievable resolution but on the other hand reports on conformational dynamics. A computational approach will be presented to reduce the conformational variance of a set of single-particle images with the goal of increasing the resolution. First the conformational variance of a molecule is reconstructed from the variance of the density. The information on conformational variance is then used to extensively classify the images into a number of different classes. In a next step, the individual 3D density reconstructions from all classes are recombined into one single (higher resolution) reconstruction by a novel flexible averaging procedure. In the flexible averaging the density grids of two maps are elastically deformed to account for large scale conformational differences thereby reducing the conformational variance of a data set. The goal is to improve the resolution and at the same time to gain a complete picture of the conformational variance of a macromolecule.

BP 36.3 Wed 10:15 H43
Robust Density-Based Clustering to Identify Metastable Conformational States of Proteins — •Florian Sittel and Gerhard Stock — Biomolekulare Dynamik, Physik, Uni Freiburg

Molecular dynamics (MD) simulations of proteins nowadays deliver an extensive amount of data describing dynamics up to millisecond timescales. Recently, Markov state models (MSM) have been recognized as a concise yet valid manner, to describe the relevant dynamics of proteins.

Here, we provide a novel, self-consistent and robust workflow to construct MSMs from the raw data of MD trajectories. This workflow

involves (I) the reduction of dimensionality with suitable methods like Dihedral angle Principal Component Analysis, (II) the construction of geometrically defined microstates by a newly developed density-based clustering algorithm, (III) and the construction of the final MSM employing a dynamic clustering algorithm.

Additionally, we introduce a novel type of diagram to easily compare metastable protein states by their respective dihedral angle content.

BP 36.4 Wed 10:30 H43
Force probe MD simulations of peptidic foldamers — Lalita Uribe, Jürgen Gauss, and •Gregor Diezemann — Institut für Physikalische Chemie, Universität Mainz, Duesbergweg 10-14, 55128 Mainz, Germany

Foldamers are small oligomers of molecular entities that fold into ordered structures. In the recent past, interest has particularly grown in the thermal and mechanical properties of peptidic foldamers due to their possible peptide-mimetic applications. Here, we present a simulation study of the mechanical unfolding pathway of different natural and artificial peptidic foldamers presenting different folded motifs. Using force probe molecular dynamics we show the importance of the rigidity of the backbone and the strength of the intra-molecular hydrogen bonds in the stabilization of the folded conformations. We analyze the statistical behavior of the unfolding pathway of the peptidic foldamers and identify the main structural properties that shape the free energy profile.

BP 36.5 Wed 10:45 H43
High-throughput thermodynamics of drug-membrane interactions from multiscale simulations — •Tristan Bereau and Kurt Kremer — Max Planck Institute for Polymer Research, Mainz

The number of small organic molecules is overwhelmingly large–so large, that most of it remains unexplored. Computer simulations offer an appealing framework to probe many of these compounds without the need to synthesize them in the laboratory. The main hurdles preventing a high-throughput characterization of many small molecules relies on the time investment to parametrize the force field—a process that typically requires significant human intervention—and extensive sampling requirements. We address these issues by first sampling from the coarse-grained Martini model, for which we developed an automated parametrization protocol for small molecules. The resulting potential-of-mean-force (PMF) curves for the insertion of small molecules in lipid membranes show excellent agreement for a number of benchmark cases. We further use the coarse-grained trajectory as an enhanced-sampling strategy to efficiently estimate the corresponding atomistic PMF. To illustrate the method, we rationalize experimental observations of lipid-domain formation in bacterial membranes after the insertion of a small alcohol compound. This framework enables a fast and efficient strategy to gain insight in the thermodynamic properties of drug-membrane interactions.

BP 37: Cell Mechanics and Migration

Time: Wednesday 9:30–12:45   Location: H44

Invited Talk   BP 37.1   Wed 9:30   H44
Reconstituting basic mitotic spindles in artificial confinement
— •Marileen Dogterom — Department of Bionanoscience, Kavli
Institute of Nanoscience, Delft University of Technology, The Nether-
lands

Microtubules are stiff dynamic polymers that can generate pushing and
pulling forces by growing and shrinking. To fulfill their function, micro-
tubules adopt specific spatial patterns, like the mitotic spindle during
cell division. To understand the basic principles of mitotic spindle
organization, we reconstitute a dynamic microtubule cytoskeleton in-
side three-dimensional water-in-oil emulsion droplets, using lipids that
can be functionalized with dynein molecular motors. We then study
the positioning of centrosomes, from which microtubules are nucleated
that exert pushing and/or dynein-mediated pulling forces when reach-
ing the boundary. We find that two centrosomes adopt an equilibrium
position balancing a dynein-mediated centering effect with a repulsion
force between the two centrosomes, thereby already reproducing a ba-
sic mitotic spindle like organization. We are now using this system as
a platform to study how other essential spindle components affect the
force balance of basic mitotic spindles.

BP 37.2   Wed 10:00   H44
Microglia mechanics: From traction forces to durotaxis —
•David Koser[1,2], Lars Bollmann[1], and Kristian Franze[1] —
[1]University of Cambridge, Cambridge, United Kingdom — [2]German
Cancer Research Center, Heidelberg, Germany

Microglial cells are key players in the primary immune response of the
central nervous system. Their functionality in healthy and pathological
conditions highly depends on their chemical as well as their mechani-
cal environment. While the impact of chemical signaling on microglial
behavior has been studied thoroughly, the current understanding of
mechanical signaling in controlling the cells' behavior is very limited.
Here we investigated the dependency of microglial traction forces on
substrate stiffness and the cells' migratory behavior on substrates in-
corporating stiffness gradients. Primary microglia adapted their actin
cytoskeleton and morphology to the stiffness of the culturing substrate.
Traction force microscopy revealed that stresses exerted by the cells
initially increase with substrate stiffness until reaching a plateau. On
substrates incorporating a stiffness gradient microglial cells preferen-
tially migrated towards stiff in a process termed durotaxis. Immune-
activation of microglia through lipopolysaccharide led to a modulation
of traction forces, increased migration velocities, and an enhancement
of durotaxis. Finally, the experimental findings can be reproduced
by combining a phenomenological stress fluctuation and a biased ran-
dom walk model. Our results clearly demonstrate that microglia are
mechanosensitive, which might be essential in central nervous system
development and pathologies.

BP 37.3   Wed 10:15   H44
**Gating mechanosensitive channels in bacteria with an atomic
force microscope** — •Renata Garces[1], Samantha Miller[2], and
Christoph F. Schmidt[1] — [1]Third Institute of Physics-Biophysics,
Georg August University, Göttingen, Germany — [2]School of Medical
Sciences, University of Aberdeen, Aberdeen, United Kingdom

The regulation of growth and integrity of bacteria is critically linked
to mechanical stress. Bacteria typically maintain a high difference of
osmotic pressure (turgor pressure) with respect to the environment.
This pressure difference (on the order of 1 atm) is supported by the
cell envelope, a composite of lipid membranes and a rigid cell wall.

Turgor pressure is controlled by the ratio of osmolytes inside and
outside bacteria and thus, can abruptly increase upon osmotic down-
shock. For structural integrity bacteria rely on the mechanical stability
of the cell wall and on the action of mechanosensitive (MS) channels:
membrane proteins that release solutes in response to stress in the cell
envelope.

We here present experimental data on MS channels gating. We ac-
tivate channels by indenting living bacteria with the cantilever of an
atomic force microscope (AFM). We compare responses of wild-type
and mutant bacteria in which some or all MS channels have been elim-
inated.

BP 37.4   Wed 10:30   H44

**Using photonic force microscopy to investigate filopodia
mediated phagocytosis** — •Rebecca Michiels and Alexan-
der Rohrbach — Lab for Bio- and Nano-Photonics, University of
Freiburg, Georges-Koehler-Allee 102, 79110 Freiburg, Germany

Macrophage cells are immune cells which internalize and digest for-
eign matter, cell debris and bacteria in the body. This process is
called phagocytosis and is often initiated by filopodia which pull par-
ticles to the cell body where they are taken up by reorganization of
the membrane. Filopodia contain tight bundles of filamentous actin
that protrude from the actin cortex and are connected with the cell
membrane via linker molecules. Retraction towards the cell body is
driven by molecular motors which work in ensembles. The underlying
physical principles that allow macrophages to tune their actions dur-
ing phagocytosis are only little understood. We use a Photonic Force
Microscope in which we combine DIC microscopy with optical tweez-
ers and interferometric particle tracking. Polystyrene beads are held
in an optical trap to enable controlled placement in the vicinity of the
cells. The motion of the bead in the trap can be tracked in 3D with
nanometer precision at a microsecond timescale using back focal plane
interferometry. By changing the optical forces spatially or temporally,
we investigate how the cell reacts to external forces and which mecha-
nisms determine success or failure when attempting to bind and digest
particles. We present novel experiments, which reveal binding, pulling
and unbinding events of macrophage filopodia on a molecular scale.

BP 37.5   Wed 10:45   H44
**Elastic Resonator Stress Microscopy (ERISM) – A Novel
Tool for Cell-Mechanical Investigations** — •Philipp Liehm, Nils
M. Kronenberg, Anja Steude, Andrew Morton, and Malte C.
Gather — School of Physics & Astronomy, University of St Andrews,
St Andrews, Scotland, UK

We present a novel cell force sensing technique based on an elastic
optical micro-cavity. By measuring the spatially resolved interference
pattern of a deformed micro-cavity, we are able to accurately detect
vertical displacements with resolution in the nm range. Integrated
into a conventional inverted fluorescence microscope, our technique
can easily be combined with phase contrast and fluorescence imag-
ing. The low light intensity required for readout, enables long-term
measurements — over periods as long as several days — without any
photo-toxic effects on the cells. ERISM does not require detaching the
cells after a measurement, thus allowing continuous data acquisition
for hundreds of cells at different positions on one sensor (substrate).
The wide-field character of the measurement permits high frame rates
($< 2\,\text{s}$ per frame) and thus enables tracking fast cell movement. The
local deformations are evaluated with a Finite Element Method (FEM)
to obtain local stress information.

In this presentation we will give an introduction to this new micro-
cavity based sensor concept. Furthermore, we show data on the me-
chanical characterization of the elastic micro-cavity with an Atomic
Force Microscope (AFM). Finally, we apply our technique to a wide
range of different cell types including neuroglia.

30 min break

BP 37.6   Wed 11:30   H44
Fibroblast mechanics: a story of history — •Mathias Sander
and Albrecht Ott — Universität des Saarlandes, Saarbrücken, Ger-
many

Cell mechanics is a key player in development, disease and many other
biological processes. Living cells exhibit a complex nonlinear response
to mechanical cues, which is not understood yet. A stiffening as well as
softening is observed, depending on the stimulus and the experimental
technique. Here, we apply large amplitude oscillatory shear (LAOS)
to a monolayer of fibroblast cells using the cell monolayer rheology
technique. We find that the nonlinear cell response not only depends
on the amplitude and the frequency of oscillations. Moreover, it is
highly susceptible to a mechanical preconditioning. Cell response can
exhibit hallmarks of nonlinear viscoelasticity, elastoplastic kinematic
hardening or inelastic fluidization for the same steady state oscilla-
tions. Experimental results indicate that a preconditioning changes
cytoskeletal network structure in a rate dependent way. Network al-
terations can be driven by passive filament reorganisations, filament

rupture and the binding/unbinding of crosslinking proteins. We speculate that the pronounced strain path dependence of nonlinear cell response might obscure the underlying universality of nonlinear cell mechanics on a microscopic scale. Our results highlight the interplay between viscoelastic and inelastic contributions to the cell mechanical response.

BP 37.7   Wed 11:45   H44

Transfer of mechanical stimuli along single microtubules and small networks — •Alexander Rohrbach and Matthias Koch — Universität Freiburg, IMTEK, Georges-Köhler-Allee 102, 79100 Freiburg

Mechanic stimulation allows integrating different parts of a cell nearly instantaneously and is relevant for the response to pressure, gravity, osmotic changes, but also to organize different regions of a dynamic cell into one entity. To explain how a stimulus can propagate across a few tens of micrometers within milliseconds inside a crowded cell is far from trivial. Using time multiplexed optical tweezers and 3D interferometric tracking, we investigate how mechanical stimuli travel along single filaments or through small networks of deforming microtubules. We find that the transduction of signals depends on frequency with faster oscillations being transmitted more efficiently due to microtubule stiffening. Surprisingly, the observed elastic behavior can also be transferred to small networks, which are mechanically different. The dependency on both the frequency and the network geometry, i.e. direction-dependent signal transport are important for biological self-organization based on tensegrity.

BP 37.8   Wed 12:00   H44

The mechano-response of flagellar oscillators — •Gary Klindt[1], Benjamin Friedrich[1], Christian Ruloff[2], and Christian Wagner[2] — [1]MPI PKS, Dresden — [2]Universität des Saarlandes, Saarbrücken

Motile cilia and flagella are slender cell appendages that beat rhythmically, powered by the collective dynamics of thousands of molecular motors inside. The beat of flagella transports fluids in airways and the brain of mammals.

Cellular microswimmers use beating flagella for self-propulsion, such as the green alga 'Chlamydomonas' that swims like a breast-swimmer with two flagella.

We characterize the load characteristic and dynamic force-velocity relationship of beating flagella using controlled microfluidic flows. We obtain a description in terms of a limit-cycle oscillator [1] with force-dependent phase and amplitude dynamics.

We incorporate this flagellar mechano-response into hydrodynamic simulations of flagellar swimming based on a fast boundary element method [2]. With this we computationally assess the role of the active waveform compliance of flagellar beating on swimming and synchronization.

[1] 1. Ma, R., Klindt, G. S., Riedel-Kruse, I. H., Jülicher, F. & Friedrich, B. M. Active Phase and Amplitude Fluctuations of Flagellar Beating. Phys. Rev. Lett. 113, 048101 (2014). [2] Klindt, G.

S., Friedrich, B. M., Flagellar swimmers oscillate between Pusher- and Puller-type swimming, Phys. Rev. E, submitted and accepted.

BP 37.9   Wed 12:15   H44

Actin structural dynamics under geometrical and biomechanical control — •Julia Strübig, Erik Bernitt, and Hans-Günther Döbereiner — Institut für Biophysik, Uni Bremen, Deutschland

The morphology of cells is a crucial effector for the overall spatiotemporal dynamics of protein densities. The complexity and randomness of morphologies of adherent cells comprise a considerable challenge for the comparability of data obtained on individual cells. Further, the comparison of experimental data to theoretical studies is severely compromised. This is especially true for the dynamics of actin, as this protein has the outstanding capability to deform the spatial domain in which it resides.

Here we introduce an experimental system with which we overcome the aforementioned issues. We utilize micro-contact printing to force cells into disc-like morphologies for the study of two different actin-based structures, namely (i) waves of polymerizing actin at the dorsal cell side (CDRs) and (ii) lamellipodia-embedded moving filopodia. Due to the simplified cell edge geometry and periodic boundary conditions in lateral direction, both structures exhibit remarkably regular dynamics facilitating quantitative analysis.

On that basis we test the response of the actin machinery to biochemical interference with drugs targeting actin and myosin systems, which reveals fundamental insight into the mechanisms underlying the dynamics of actin waves and filopodia motion. We demonstrate that our data is explained very well by theoretical models for both systems.

BP 37.10   Wed 12:30   H44

Membrane tension feedback on shape and motility in a phase field model for crawling cells — •Benjamin Winkler[1], Igor Aranson[2,3], and Falko Ziebert[1] — [1]Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Materials Science Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439, USA — [3]Engineering Sciences and Applied Mathematics, Northwestern University, 2145 Sheridan Road, Evanston, IL 60202, USA

In the framework of a 2D phase field model of a single cell crawling on a substrate, we investigate how specific properties of the cell membrane affect the shape and motility of the cell. The membrane influences the cell dynamics on multiple levels and we take into account: (i) the reduction of the actin polymerization rate by membrane tension; (ii) area conservation of the cell's two-dimensional cross-section vs. conservation of the circumference (related to membrane inextensibility); and (iii) the contribution from the membrane's bending energy to the shape and integrity of the cell. We find that the most important effect for freely moving cells is the feedback of membrane tension on the actin polymerization. Bending rigidity induces only minor effects, which can be made visible in dynamic reshaping events, as exemplified by modeling cells encountering obstacles and squeezing through channels.

BP 38: Neurosciences

Time: Wednesday 9:30–11:15   Location: H45

Invited Talk   BP 38.1   Wed 9:30   H45

Optogenetics: Basics, Applications and Chances — •Ernst Bamberg — Max Planck Institute of Biophysics Frankfurt

Optogenetics: Basics, Applications and Chances Ernst Bamberg Max-Planck Institute of Biophysics Frankfurt Abstract Optogenetics is the use of genetically encoded light activated proteins for manipulation of cells in an almost noninvasive way by light. The most prominent example is Channelrhodopsin2(ChR2), which allows the activation of electrical excitable cells via the light dependent depolarization. The combination of ChR2 with hyperpolarizing light driven ion pumps as the Cl- pump halorhodopsin (NphR) enables the multimodal remote control of neural cells in culture, tissue and living animals. Optogenetics has revolutionized neuroscience and is applied by more than 1000 Neurobiology oriented groups. Very soon it became obvious that this method will offer also the chance for a gene therapy for some neurodegenerative diseases. The basics of optogenetics and some applications are presented. Possible biomedical applications with the focus

on blindness are discussed as well.

Invited Talk   BP 38.2   Wed 10:00   H45

The mechanical control of CNS development and functioning — •Kristian Franze — University of Cambridge, Cambridge, UK

Throughout life, central nervous system (CNS) cells migrate and grow over large distances. During development and pathological processes, they are exposed to a multitude of signals determining where to move. Despite the fact that forces are involved in any kind of cell motion, our current understanding of the mechanical interactions of CNS cells and their environment is very limited. We used compliant cell culture substrates, traction force microscopy and calcium imaging to investigate how neurons and glial cells interact with their mechanical environment. Growth and migration velocities, directionality, cellular forces as well as neuronal fasciculation and maturation all significantly depended on substrate stiffness. Moreover, when grown on substrates incorporating linear stiffness gradients, axon bundles turned towards soft substrates while glial cells migrated in the opposite direction. In vivo atomic

force microscopy measurements revealed stiffness gradients in developing brain tissue, which axons followed as well towards soft. Interfering with brain stiffness and mechanosensitive ion channels in vivo both led to similar aberrant neuronal growth patterns with reduced fasciculation and pathfinding errors, strongly suggesting that neuronal growth is not only controlled by chemical signals, as it is currently assumed, but also by the tissue's local mechanical properties.

BP 38.3 Wed 10:30 H45

Single-channel current of calcium channels in rat neocortical layer 5 pyramidal neurons at physiological calcium concentration: fluctuation analysis with voltage ramps — •Christian Scheppach[1,2] and Hugh P.C. Robinson[1] — [1]Physiological Laboratory, Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, U.K. — [2]Institute of Physics, University of Freiburg, Freiburg, Germany

Voltage-gated Ca^{2+} channels are present in many neuronal membranes, playing important roles in presynaptic transmitter release, and in postsynaptic integration of inputs, e.g. by dendritic Ca^{2+} action potentials. Their single-channel current in physiological extracellular Ca^{2+} concentrations (1-2 mM) is not well known, and is too small to be resolved directly with standard patch-clamp. Yet it is a key parameter e.g. for stochastic effects arising from the random opening and closing of single Ca^{2+} channels. We recorded Ca^{2+} channel currents from neocortical L5 pyramidal neurons and used fluctuation analysis to obtain a single-channel current of 0.07 pA at -25 mV membrane voltage and 2 mM extracellular Ca^{2+}. A novel fluctuation analysis protocol was developed, whereby channel currents are recorded during voltage ramps. The presented technique is robust with respect to unstable experimental conditions like rapid run-down of the channel current. The data on the single Ca^{2+} channel current are relevant to a quantitative understanding of dendritic Ca^{2+} action potentials, especially their stochastic aspects.

Reference: C. Scheppach, H.P.C. Robinson (in preparation).

BP 38.4 Wed 10:45 H45

Emulation of the hippocampal circuit with memristive Hebbian Plasticity — •Nick Diederich[1,2], Annika Hanert[2], Thorsten Bartsch[2], Martin Ziegler[1], and Hermann Kohlstedt[1] — [1]Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Germany — [2]Neurologie, Universitätsklinik Schleswig-Holstein, Germany

The hippocampus is one of the crucial brain areas for learning and consolidation of memory in human brains. In particular, it serves as a classical model for neuroplasticity. Therefore, important plasticity mechanisms such as long-term potentiation and depression have been identified and demonstrated in the hippocampal field. For the description of the working principles of the hippocampus a circuit model has been proposed which is based on auto- and heteroassociative networks. In this talk, a computational neural-network model of the hippocampal circuit is presented. Spiking neurons and memristive Hebbian synapses are employed into Hopfield- and feedforward network structures. The obtained network performance is discussed in the framework of pattern completion and recognition and recent studies of mnemonic processing.

Finanical support by the German Research Foundation through FOR 2093 is gratefully acknowledged.

BP 38.5 Wed 11:00 H45

Correlated activity of periodically driven binary networks — •Tobias Kühn[1], Michael Denker[1], Sonja Grün[1,2], and Moritz Helias[1,3] — [1]Inst. of Neuroscience and Medicine (INM-6), Inst. for Advanced Simulation (IAS-6) and JARA BRAIN Inst. 1, Jülich Research Centre, Germany — [2]Theoretical Systems Neurobiology — [3]Dept. of Physics, both Faculty I, RWTH Aachen University, Germany

Experiments showed that excess synchronous spike events are locked to the phase of LFP beta-oscillations more strongly than spikes not part of such events [Denker et al. 2011, Cereb. Cortex]. To identify the mechanisms by which correlations depend on the phase of the LFP, which primarily reflects input activity, we examine a balanced network of homogeneously connected binary model neurons [Ginzburg et al. 1994, PRE] receiving input from a sinusoidal perturbation. The Glauber dynamics of the network is simulated and approximated by mean-field theory. Treating the periodic input in linear response theory, the cyclostationary first two moments are analytically computed. They agree with their simulated counterparts over a wide parameter range. The zero-time lag correlations consist of two terms, one due to the modulated susceptibility (via the external input and network feedback) and one due to the time-varying autocorrelations. For some parameters, this leads to resonant correlations and non-resonant mean activities. Our results can help to answer the salient question how oscillations in mesoscopic signals and spike correlations interact.

Supported by the Helmholtz foundation (VH-NG-1028, SMHB); EU Grant 604102 (HBP). Simulations with NEST (nest-simulator.org).

BP 39: Active Matter (Joint Session with DY)

Time: Wednesday 9:30–12:45   Location: H46

Invited Talk   BP 39.1 Wed 9:30 H46

Nonreciprocal forces in soft matter systems: passive particles become active — •Hartmut Löwen — Institute of Theoretical Physics: Soft Matter, Heinrich-Heine University Duesseldorf,

There is a variety of situations in which Newton's third law is violated. Generally, the action-reaction symmetry can be broken for mesoscopic colloidal particles, when their effective interactions are mediated by a nonequilibrium environment. Here, we investigate different classes of nonreciprocal interactions relevant to real experimental situations and present their basic statistical mechanics analysis verify the principal theoretical predictions in experimental tests performed with two-dimensional binary complex plasmas [1]. For underlying Brownian dynamics [2], nonreciprocal forces result in active particle pairs thus linking nonreciprocal interactions to the field of microswimmers.

References:

[1] A. V. Ivlev, J. Bartnick, M. Heinen, C.-R. Du, V. Nosenko, H. Löwen, Physical Review X **5**, 011035 (2015).

[2] J. Bartnick, M. Heinen, A. V. Ivlev, H. Löwen, J. Phys.: Condensed Matter **28**, 025102 (2016).

BP 39.2 Wed 10:00 H46

Kinetic theory of self-driven particles: Invasion waves and correlation effects — •Thomas Ihle — Institute for Physics, Ernst-Moritz-Arndt University Greifswald, Germany

Models of self-driven agents similar to the Vicsek model are studied by means of kinetic theory. In these models, particles try to align their travel directions with the average direction of their neighbors. At strong alignment a globally ordered state of collective motion forms. An Enskog-like kinetic theory is derived from the exact equation for a Markov chain in phase space using Boltzmann's mean-field approximation of molecular chaos. The kinetic equation is solved numerically by a nonlocal Lattice-Boltzmann-like algorithm. Steep soliton-like waves are observed that lead to an abrupt jump of the global order parameter if the noise level is changed. The shape of the wave is shown to quantitatively agree within 3% with agent-based simulations at large particle speeds. This provides a mean-field mechanism to change the second-order character of the flocking transition to first order. At small densities and realistic particle speeds, the mean-field assumption of Molecular Chaos is invalid near the onset of collective motion, and correlation effects become relevant.

I will show how to self-consistently include correlation effects at the level of ring-kinetic theory. Instead of just one kinetic equation, an additional equation for the time evolution of two-particle correlations will be derived. This equation is solved numerically for a homogeneous system and shown to be in excellent agreement with agent-based simulations in certain parameter ranges.

BP 39.3 Wed 10:15 H46

Model of aerotactic bands — •Marco Giacomo Mazza — Max Planck Institute for Dynamics and Self-Organization, Göttingen

Some bacteria exhibit surprising behavior in the presence of an oxygen concentration. They perform an aerotactic motion along the gradient until they reach their optimal oxygen concentration. And they often organize collectively by forming dense regions, called 'bands', that travel towards the oxygen source. We have developed a model of

swimmers with stochastic interaction rules moving in proximity of an air bubble. We perform MD simulations that reproduce the aerotactic behavior of bacteria. If the oxygen concentration in the system sinks locally below a threshold value, the formation of a migrating aerotactic band toward the bubble can be observed. We reproduce quantitatively the experimental observations on the aerotactic band.

BP 39.4   Wed 10:30   H46

Phase Behavior of Active Particles — •Jonathan Tammo Siebert[1], Janina Carmen Letz[1,2], and Peter Virnau[1] — [1]Johannes Gutenberg University Mainz, Department of Physics, Staudingerweg 7, 55128 Mainz, Germany — [2]University of Utah, Department of Mathematics, Salt Lake City, UT 84112-0090, USA

We have studied the phase behavior of active colloidal particles. Such systems undergo phase separation into a dense liquid-like and a dilute gas-like phase due to self trapping when a certain critical activity is exceeded both in experiment and simulation (Buttinoni et al., Phys. Rev. Lett., 110 (2013)). Starting point of our studies are the well known two dimensional active brownian particles. Further investigations were done on three dimensional as well as systems of active dimers. For all systems the phase diagrams were computed by extensive brownian dynamics simulations. Employing methods from equilibrium statistical physics we have aimed for an accurate estimate of the binodal line in a bulk system. Starting from a simple model system has allowed us to separate the influence of dimensionality and bonding of particles. In agreement with earlier studies we have found that active velocities needed for phase separation are much larger in the three dimensional system. Also active dimers only phase separate at higher activities than active disks.

BP 39.5   Wed 10:45   H46

Active Brownian particles at interfaces: An effective equilibrium approach — •René Wittmann and Joseph Brader — Departement für Physik, Universität Fribourg, 1700 Fribourg, Schweiz

Understanding self-organization in active Brownian systems is a subject of increasing theoretical interest. Recently, a microscopic equilibrium theory was developed from first principles [1], which accounts for the motility-induced phase separation (MIPS) observed in numerous experiments. This is achieved by mapping the active system onto an effective (static) interaction potential.

So far, experimental studies of active systems have focused on bulk properties. We apply our effective equilibrium theory [1] to inhomogeneous systems using density functional theory (DFT) with a simple perturbative treatment of the (effective) attractive interaction. In this case, the activity induces an effective external (wall) potential [2,3].

For a passively repulsive active fluid at a passively repulsive wall, the theory predicts motility-induced wetting as the MIPS transition is approached. For a Lennard-Jones interparticle potential the wall first dries with increasing activity, followed by a re-entrant wetting phenomenon. In a slit pore we observe motility-induced capillary condensation or evaporation, depending on the passive potential. These findings [3] constitute a compelling motivation to study such systems experimentally or using Brownian dynamics simulations.

[1] T. F. F. Farage, P. Krinninger and J. M. Brader, Phys. Rev. E **91**, 042310 (2015). [2] A. Pototsky and H. Stark, Europhys. Lett. **98** 50004 (2012). [3] R. Wittmann and J. M. Brader, in preparation.

15 min. break

BP 39.6   Wed 11:15   H46

Using motility patterns to manipulate self-propelled particles — •Celia Lozano[1,2], Borge ten Hagen[3], Hartmut Löwen[3], and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [3]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany.

Active colloidal particles capture many aspects of motile microorganisms and are therefore considered to provide a suitable model system to understand self-organization and pattern formation in living and non-equilibrium systems. Contrary to most experimental situations where the particle motility is position-independent, here we investigate a system where the self-propulsion velocity is spatially modulated. This is achieved by a light-induced propulsion mechanism and a spatially modulated light field [1]. By subjecting a dilute active colloidal

suspension to an asymmetric and periodic light field, we demonstrate directed particle motion. In addition, we show, that particle transport is highly sensitive to the particle size and thus acts also as a filtering device for active suspensions [2].

[1] VOLPE G, BUTTINONI I, VOGT D, KÜMMERER H J AND BECHINGER C 2011 MICROSWIMMERS IN PATTERNED ENVIRONMENTS SOFT MATTER 7, 8810 (2011) [2] C. Lozano, B. ten Hagen, H. Löwen, and C. Bechinger. In preparation

BP 39.7   Wed 11:30   H46

Dynamics of self-propelled Janus particles in viscoelastic fluids — •Juan Ruben Gomez-Solano[1] and Clemens Bechinger[1,2] — [1]2. Physikalisches Institut, Universitaet Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

The motion of many natural micro-swimmers, such as bacteria and spermatozoa, commonly takes place in viscoelastic media. The understanding of their swimming mechanisms has triggered a lot of experimental and theoretical work in recent years as well as the development of artificial self-propelled particles. Although the motion of microswimmers in Newtonian fluids has been extensively studied, so far only few investigations have focused on the swimming of microorganisms in viscoelastic fluids. In this work, we experimentally investigate the dynamics of spherical Janus colloidal particles in a viscoelastic fluid. The particles are self-propelled by local demixing of a critical binary polymer mixture induced by laser illumination. We observe a dramatic enhancement of both translational and rotational diffusion with increasing particle velocity, even at low Weissenberg number, where the drag force on the particle exerted by the fluid obeys the Stokes law. We observe a similar enhancement for passive particles driven by an external constant force, e.g. gravity. Our results suggest that these effects originate from the coupling between the thermal fluctuations of the particle and the surrounding flow field, which displays large relaxation times of several seconds.

BP 39.8   Wed 11:45   H46

Hydrodynamicaly-Tuned Phase Separation of Spherical Micro-Swimmers — •Johannes Blaschke, Karthik Menon, Maurice Maurer, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Active motion of microorganisms and artificial micro-swimmers is relevant both to real world applications, as well as for posing fundamental questions in non-equilibrium statistical physics. A striking feature of their collective behaviour is that, for sufficiently strong self-propulsion dense clusters coexists with a low-density disordered surrounding. Due to the required computational effort, active particles are often modelled by neglecting the full hydrodynamic interactions.

However, real micro-swimmers, such as ciliated microorganisms, catalytic janus particles, or emulsions of active droplets, employ propulsion mechanisms reliant on hydrodynamics.

Here we examine the influence of the full hydrodynamic interactions on the motility-induced phase separation of spherical micro-swimmers in quasi-2D confinement. We follow up on previous work [1] by increasing the total system size allowing us to quantitatively resolve the phase-coexistence regime.

[1] A. Zöttl and H. Stark, PRL **112**, 118101 (2014)

BP 39.9   Wed 12:00   H46

Comparison of external control strategies for optimized payload delivery — •Tobias Bäuerle[1], Jakob Steiner[1], Lena Bremicker[2], Daniel Häufle[2], and Clemens Bechinger[1] — [1]2. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Institut für Sport- und Bewegungswissenschaft, Universität Stuttgart, 70569 Stuttgart, Germany

Synthetic microswimmers, i.e. self-propelled particles, constitute an interesting class of non-equilibrium systems which exhibit structural and dynamical features similar to those observed in assemblies of motile organisms like bacteria or cells. In addition, they may find applications as microrobots which will deliver payloads to specific sites in liquid environments.

In our studies, we addressed the question how the delivery process can be optimized by the choice of the control strategy. Experimentally, this was achieved by light-activated microswimmers, where the propulsion velocity was controlled by the light intensity. Depending on the particle orientation and its distance from the target, the illumination was turned on and off, resulting in an intermittent change

between Brownian and active motion. Even for slight variations of control strategies, we find large changes e.g. in the ratio of the delivery time and the total propulsion energy. Our results are in excellent agreement with numerical simulations.

BP 39.10   Wed 12:15   H46

Self-propelled janus droplets for gene extraction and controlled cargo delivery — •Menglin Li[1], Martin Brinkmann[1,2], Ralf Seemann[1,2], and Jean-Baptiste Fleury[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

We report the existence of a new type of self-propelled Janus droplets, that are obtained from the spontaneous phase separation between two fully miscible fluids (water/solvent) in the presence of surfactants which are preferentially soluble in the solvent phase. At start, the related self-propulsion mechanism is generated by a Marangoni flow mediated by the solvent dissolution into the oily phase. During this motion, the droplets are absorbing a large amount of surfactant. This dynamic surfactant adsorption leads to spontaneous water/solvent demixing and the formation of Janus droplet. We characterize the hydrodynamics properties of these microwimmers during their different stages of evolution. Interestingly, the squirmer properties evolve in time from a weak pusher to a neutral squirmer and potentially to a dimer of neutral squirmers. Finally, we used this active system as a smart carrier to extract genes in situ and delivering them at a target location. (Submitted)

BP 39.11   Wed 12:30   H46

Pattern Formation and Clustering in Chemorepulsive Active Colloids — •Benno Liebchen[1], Davide Marenduzzo[1], Ignacio Pagonabarraga[2], and Michael E Cates[3] — [1]SUPA, School of Physics and Astronomy, University of Edinburgh, Edinburgh EH9 3FD, United Kingdom — [2]Departament de Fisica Fonamental, Universitat de Barcelona-Carrer Marti i Franques 1, 08028-Barcelona, Spain — [3]DAMTP, 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. This can, in the case of chemoattraction where particles migrate up chemical gradients, induce a clustering-instability of the uniform state. This instability currently attracts renewed attention in artificial Janus colloids that swim by catalysing reactions in a chemical bath and show a similar signalling behaviour as micro-organisms.

Here, we demonstrate that also the previously underappreciated case of chemorepulsion (where particles migrate away from high chemical density) can induce clustering. The underlying instability may either rely on anisotropy in the chemical production at the particle surface or on delay effects. In contrast to chemoattractive clustering our chemorepulsive route predicts clusters of self-limiting size. This size increases with self-propulsion velocity which agrees qualitatively with recent experimental observations of dynamic clustering in active Janus colloids.

BP 40: Statistical Physics of Biological Systems II (Joint Session with DY)

Joint session with DY organized by BP.

Time: Wednesday 11:30–12:30   Location: H43

BP 40.1   Wed 11:30   H43

Receptor arrays optimized for sensing natural odors — •David Zwicker[1], Arvind Murugan[1,2], and Michael P. Brenner[1] — [1]School of Engineering and Applied Sciences, Harvard University — [2]Department of Physics and the James Franck Institute, University of Chicago

Natural odors typically consist of many molecules at different concentrations, which together determine the odor identity. This information is encoded in the collective response of olfactory receptors and subsequently interpreted by the brain. However, it is unclear how the receptors can measure both the composition of the odor and the concentrations of its constituents. I will discuss a theoretical model of receptor arrays from which we derive design principles for optimally communicating the odor information. These principles can be summarized as two possibly conflicting goals: (i) each receptor should respond to half of all odor mixtures; (ii) activity patterns of different receptors should be orthogonal. We show that there is a family of receptor arrays that satisfy these conditions and thus transfer the odor information near-optimally. Within this family, we can then discuss additional optimization goals, like the accuracy of concentration measurements and the capability for discriminating mixtures. Taken together, we can predict the performance and properties of receptor arrays based on a few, measurable quantities. Our work can thus be used to infer information about the receptors from physiological measurements. Moreover, we can use our results to improve artificial sensor arrays.

BP 40.2   Wed 11:45   H43

Making a loop - from polymer conformation to single file diffusion and back — •Wenwen Huang[1], Yen Ting Lin[1,2], Daniela Frömberg[1], Frank Jülicher[1], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]School of Physics and Astronomy, University of Manchester, M139PL, Manchester, United Kingdom.

In this contribution, we show that the conformations of a pinned polymer loop embedded in a heat bath with a constant external force field can be modeled by an asymmetric exclusion process (ASEP) with reflecting boundary conditions. This correspondence allows us to find the exact solution for both systems' equilibrium statistics, which is well approximated by the Fermi–Dirac distribution. Moreover, we can quantify not only the behavior of average positions of the particles of the ASEP and the corresponding monomers of the polymer loop,

but also their fluctuations. The condition of forming a loop and the corresponding constraint in the ASEP model lead to explicit dependence of the fluctuations on the position of the particles in ASEP and the monomers of the polymer. To close the loop of analogies we show that the kinetic Monte Carlo simulations, which can be performed for the ASEP with a well defined physical time, can be related to the non-equilibrium dynamics of polymer loops.

BP 40.3   Wed 12:00   H43

Evolutionary emergence of phenotype switching — Pintu Patra[1,2] and •Stefan Klumpp[1,3] — [1]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Potsdam, Germany — [2]Rice University, Houston, Texas, USA — [3]Institut für Nichtlineare Dynamik, Universität Göttingen, Göttingen, Germany

Bacterial persistence (phenotypic tolerance to antibiotics) provides a prime example of bet-hedging, where normally growing cells generate slow-growing but antibiotic-tolerant persister cells to survive through periods of exposure to antibiotics. The population dynamics of persistence is explained by a phenotype switching mechanism that allows individual cells to switch between these different cellular states with different environmental sensitivities. We report a theoretical study based on an exact solution for the case of a periodic variation of the environment to address how phenotype switching emerges and under what conditions switching is or is not beneficial for long-time growth [1]. Specifically we report a bifurcation through which a fitness maximum and minimum emerge above a threshold in the duration of exposure to the antibiotic. Only above this threshold, the optimal phenotype switching rates are adjusted to the time scales of the environment, as emphasized by previous theoretical studies, while below the threshold a non-switching population is fitter than a switching one. Whether the transition is continuous or discontinuous depends on how the phenotype switching rates are allowed to vary. [1] P. Patra and S. Klumpp, Phys. Biol. 12, 046004.

BP 40.4   Wed 12:15   H43

The statistical physics of hematopoiesis: from stem cell engraftment to ageing and disease — •Peter Ashcroft[1], Sebastian Bonhoeffer[1], Philipp Rauch[2], and Markus Manz[2] — [1]ETH Zurich, Zurich, Switzerland — [2]University Hospital Zurich, Zurich, Switzerland

Hematopoietic stem cells (HSCs) maintain blood production. The

hematopoietic system has the highest turnover and proliferation rate of cells in the body, however, hematologic malignancies are not the most frequent forms of human cancer. A fine tuned system with many layers of control has evolved that limits and eliminates potentially malignant clones. The overall aim of our research is to obtain a clear, quantitative understanding of the hematopoietic system and the emergence of disease through combined theoretical and experimental work. Here we will describe the theoretical approach. We use techniques from statistical physics and probability theory to analyse the structure of the hematopoietic system at different scales. Experimental investigations of HSCs often involve the transplantation of low numbers of stem cells into a host. We construct and analyse an individual-based model of this process, and determine the probability that donor cells successfully engraft in the host. These donor cells could also represent the invasion of malignant cells and the initiation of blood-based diseases. We also investigate the structure of the hematopoietic tree and the influence this has on the proliferation of diseased cells. Finally, we describe the impact that stem cell ageing has on the hematopoietic system's ability to maintain a healthy supply of blood to the body.

BP 41: Microswimmers II (Joint Session with DY)

Joint Session with DY organized by BP.

Time: Wednesday 11:30–13:00   Location: H45

BP 41.1   Wed 11:30   H45
Interactions of self-thermophoretic swimmers — •Santiago Muiños Landin, Andreas Bregulla, and Frank Cichos — Molecular Nanophotonics, Universität Leipzig, Institut for Experimental Physics I, Linnéstrasse 5, 04103 Leipzig, Germany

Propulsive mechanisms and collective behavior of self propelled microswimmers are interesting and challenging topics which had been studied in different natural and artificial systems during last years. Given that the collective behavior depends on how do these swimmers interact, and the fact that the aspects of these interactions are directly related to their propulsive mechanisms, we can say that these both aspects are coupled. Here we present an experimental method, based on previous own related work[1,2]. The developed Photon Nudging technique allows us to collect a well defined number of self-thermophoretic Janus particles in a small sample volume. Based on this we show results of a free expansion study of an active particle gas in solution which provides information in the mutual interactions between these photophoretic swimmers

[1] B.Qian, D. Montiel, A. Bregulla, F. Cichos, Chem. Science 4, 1420 (2013) [2] A. Bregulla, H. Yang, and F. Cichos, ACS Nano 8(7), 6542 (2014)

BP 41.2   Wed 11:45   H45
Escaping turbulence? Phytoplankton use active shape control to rapidly adapt swimming strategies — •Anupam Sengupta[1,2], Francesco Carrara[1], and Roman Stocker[2] — [1]Massachusetts Institute of Technology, 15 Vassar Street, Cambridge MA 02139, USA — [2]ETH Zurich, Institute for Environmental Engineering, Stefano-Franscini-Platz 5, 8093 Zurich, Switzerland

Turbulence has long been known to affect phytoplankton fitness and species succession, yet, a mechanistic view of how turbulence affects phytoplankton migration has been lacking. Here we report on the first observations demonstrating that phytoplankton can actively respond to turbulence-like cues. Using the red-tide producing species Heterosigma akashiwo as a model system, we show that hydrodynamic cues mimicking overturning by Kolmogorov-scale turbulent eddies trigger a diversification in the migration behavior. Upon exposure to repeated overturning, an originally upward swimming population robustly splits in two equi-abundant subpopulations, one swimming upward and one swimming downward. Quantitative image analysis at the single-cell level showed that the behavioral switch was accompanied by a rapid morphological change at the sub-micrometer scale, and a mathematical model of the cell's mechanical stability confirms that this shape change can flip the swimming direction and ultimately induce downward migration. The results indicate that certain phytoplankton species may have evolved subtle strategies to actively change their migratory behavior in response to turbulent cues, possibly a bet-hedging strategy to escape from turbulent microzones in the ocean.

BP 41.3   Wed 12:00   H45
Run-reverse-flick strategy of interacting bacteria — •Fabian Schwarzendahl, Stephan Herminghaus, and Marco Giacomo Mazza — Max Planck Institute for Dynamics and Self-Organization, Göttingen Am Fassberg 17, 37077 Göttingen, Germany

Bacteria have different swimming strategies for finding nutrition. *Escherichia coli* follow a run and tumble strategy whereas *Vibrio alginolyticus* have a run-reverse-flick pattern [1]. We simulate the latter using molecular dynamics to integrate the underlying stochastic equations. Without interactions between the bacteria, the analytical result by Theves [2] is recovered. Furthermore, hard-core interactions are used. Here, we study the effect of particle interactions by varying the filling fraction as well as the ratio of mean forward-to-backward run time (biased run). We find that the diffusion-density coupling parameter has a minimum at a forward to backward runtime ratio of 0.6, which is the value that was measured for *Vibrio alginolyticus* by Xie et. al. [1]. Furthermore we present an analytical model based on a Fokker-Planck approach.

[1] Li Xie et. al., Proc. Natl. Acad. Sci. USA **108**, 2246 - 2251 (2010)
[2] Matthias Theves et. al., Biophys. J. **105**, 1915 - 1924 (2013)

BP 41.4   Wed 12:15   H45
Swimming dynamics of a polar multi-flagellated bacterium — •Marius Hintsche[1], Matthias Theves[1], Marco Kühn[2], Kai Thormann[2], and Carsten Beta[1] — [1]Universität Potsdam, Germany — [2]Justus-Liebig-Universität Giessen, Germany

Bacterial motility patterns and chemotaxis strategies are very diverse and depend on factors such as flagellation as well as the typical environment the species encounters. For some bacteria the motility pattern and the underlying flagellar dynamics have already been elucidated – as in the paradigmatic run-and-tumble behavior of *E. coli*. We study the swimming motility and chemotactic behavior of the polar multi-flagellated soil dwelling bacterium *Pseudomonas putida*. Its run-and-reverse motility pattern with many sharp reversal events is reminiscent of the behavior of some monoflagellated species. However, upon a reversal, *P. putida* changes its swimming speed by a factor of two on average. We also analyze the swimming pattern in the presence of chemical gradients. Using benzoate as a chemoattractant, we measure key motility parameters in gradients of different strength in order to quantify the directional bias these conditions introduce in this swimmer's random walk. Our results indicate a change in the reversal frequency depending on changes in the chemoattractant concentration consistent with earlier qualitative reports. Using high-speed fluorescence microscopy, we examine the dynamics of the polar bundle of flagella during smooth swimming and turning and discuss some recent hypotheses concerning the bundle dynamics of these bacteria in the light of our new observations.

BP 41.5   Wed 12:30   H45
Sperm navigation along helical paths in 3D chemoattractant landscapes — •Jan F. Jikeli[1], Luis Alvarez[1], Benjamin Friedrich[2], Laurence G. Wilson[3], and U.Benjamin Kaupp[1] — [1]research center caesar; Ludwig-Erhard-Allee 2; 53175 Bonn Germany — [2]Biological Physics, Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [3]Department of Physics, University of York, YO10 5DD Heslington, York, UK

Sperm require a sense of direction to locate the egg for fertilization. They follow gradients of chemical and physical cues provided by the egg or the oviduct. However, the principles underlying three-dimensional (3D) navigation in chemical landscapes are unknown. Here using holographic microscopy and optochemical techniques, we track sea urchin sperm navigating in 3D chemoattractant gradients. Sperm sense gradients on two timescales, which produces two different steering responses. A periodic component, resulting from the helical swimming, gradually

aligns the helix towards the gradient. When incremental path corrections fail and sperm get off course, a sharp turning manoeuvre puts sperm back on track. Turning results from an "off" Ca2+ response signifying a chemoattractant stimulation decrease and, thereby, a drop in cyclic GMP concentration and membrane voltage. These findings highlight the computational sophistication by which sperm sample gradients for deterministic klinotaxis. We provide a conceptual and technical framework for studying microswimmers in 3D chemical landscapes.

BP 41.6   Wed 12:45   H45

Elastic microswimmers in confined spaces — •Jayant Pande[1], Timm Krüger[2], Jens Harting[3,4], and Ana-Sunčana Smith[1,5] — [1]PULS group, Dept. of Phys. and EAM Cluster of Excellence, Friedrich-Alexander Univ., Erlangen, Germany — [2]School of Engg., Univ. of Edinburgh, Edinburgh, U.K. — [3]Dept. of Appl. Phys., Eindhoven Univ. of Technology, Eindhoven, The Netherlands — [4]Research Centre Jülich, Helmholtz-Inst. Erlangen-Nuremberg, Nuremberg, Germany — [5]Div. of Phys. Chem., Ruđer Bošković Inst., Zagreb, Croatia

Both natural microswimmers such as bacteria and artificial ones such as microscopic drug delivery systems (as currently foreseen) commonly move through constrained spaces such as thin films or biological channels. This constrainment alters their conditions of motion, relative to swimming in an infinite expanse of fluid, due to effects such as fluid reflection from channel walls, heightened drag forces, etc., and is manifested in fundamentally different fluid flow fields. We study these effects by employing the LB3D simulation system, based on the lattice-Boltzmann and immersed boundary methods, to simulate the three-sphere swimmer of Najafi and Golestanian as it moves through narrow and wide channels. We modify the original three-sphere model to allow different degrees of elasticity in the swimmer, and investigate the interplay of these degrees of elasticity with the channel shapes and dimensions in determining the swimming efficiency. We present ways to take the swimmer elasticity into consideration analytically, and show that motion within channels may be understood in terms of the swimming regimes that depend on the drag force faced by the swimmer.

BP 42: Biomaterials and Biopolymers I (Joint Session CPP/MM/BP)

Time: Wednesday 15:00–18:15   Location: H40

BP 42.1   Wed 15:00   H40

Self-assembled plasma protein nanofibers — •Christian Helbing[1], Tanja Deckert-Gaudig[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science, Department of Materials Science and Technology, Otto Schott Institute of Materials Research (OSIM), Faculty of Physics and Astronomy, Friedrich Schiller University Jena, Jena, Germany — [2]Institute for Photonic Technology, Jena, Germany

Protein nanofibers (PNFs) are promising materials for numerous applications in the field of biomedical engineering. Especially, self-assembled PNFs based on plasma proteins have a high importance due their easy fabrication and high biocompatibility. However, knowledge about the self-assembly mechanism of such PNFs is limited. The aim of the current study is to deepen the understanding of the formation mechanism. We tested the hypotheses that morphology and inner structure of PNF depends on environmental conditions. In this work, we present results of self-assembled PNF structures formed in solution from a plasma protein combination. The observed morphology of the formed PNFs depended strongly on the formation conditions. The structural analysis suggest that a partial denaturation, i.e. a change in the secondary structure, of the plasma proteins is a necessary requirement for the formation of PNFs. The comparison of the secondary structure of the PNFs and the native proteins helps to improve the understanding of the self-assembly mechanism. The current results leads to a better control during the PNF formation.

BP 42.2   Wed 15:15   H40

Automatically recognizing structural patterns in (bio)polymers — •Michele Ceriotti — École Polytechnique Fédérale de Lausanne

Atomistic simulations have been constantly increasing in accuracy and predictive power over the past decade, and materials and molecules of growing complexity are now amenable to modelling. There is however a dire need for algorithms to analyze the outcome of such simulations, to infer the elementary building blocks and the design principles that link atomic-scale structure and the emergence of meso-scale complex behavior. Here I will show how a probabilistic analysis of molecular motifs (PAMM) algorithm can be used to automatically recognize secondary structure patterns in proteins, and discuss how this approach could be used to identify new hydrogen-bond patterns in situations in which biopolymers are encountered in unusual conditions, such as in non-aqueous mediums or at inorganic interfaces.

Invited Talk   BP 42.3   Wed 15:30   H40

Competing oligonucleotide macromolecules: binding preferences instead of a ménage a trois — •Albrecht Ott — Biologische Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany

The description of macromolecular recognition is usually reduced to the consideration of molecular pairs. In the simplest descriptions the receptor pairs exhibit a lock and key interaction, which mainly depends on the shape of the molecular recognizers, and this is supposed

to lead to a highly specific recognition process. Much more refined and quantitative physical descriptions have been proposed, however, they are again based on pairwise interaction, and we remain far from understanding molecular binding in competition as it occurs in a biological organism. Here we present experiments on DNA macromolecular binding in competition. We identify situations where the binding constant of one DNA strand is highly dependent on the presence of another, very similar competitor. We interpret our findings as the result of an interaction term that leads to a formal equivalent of a Landau phase transition. We present experimental results from in vitro transcription assays that highlight the existence of other non-trivial competitive situations that may act along similar lines.

BP 42.4   Wed 16:00   H40

Poly(ethylene glycol) films and nanomembranes as flexible platform for humidity sensors and bioengineering — Musammir Khan and •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

We discuss possible applications of novel poly(ethylene glycol) (PEG) hydrogel films and membranes (PHFs and PHMs). They were fabricated by thermally activated crosslinking of amine- and epoxy-terminated, star-branched PEG oligomers and characterized by tunable thicknesses of 4 - 200 nm. As demonstrated, PHFs and PHMs can be used as highly sensitive elements in humidity sensors and moisture-responsive nanoelectronic devices, relying on resistive transduction technique. Their resistance change by ca. 5.5 orders of the magnitude upon relative humidity variation from 0 to 100%, which is unprecedented response for homogeneous materials. As another representative example, we show that PHFs and PHMs are able to host protein-specific receptors, providing, at the same time, protein-repelling and humidity-responsive matrix with a characteristic mesh size up to 8.4 nm. A noticeable grafting density of the test avidin protein, specifically attached to the biotin moieties coupled to the free amine groups in the PHMs, was achieved, whereas the analogous values for non-specifically adsorbed proteins were lower by a factor of 4-5. The engineering of PHMs with biomolecule-specific receptors and their loading with biomolecules are of potential interest for sensor fabrication and biomedical applications, including tissue engineering and regenerative therapy.

BP 42.5   Wed 16:15   H40

Dynamic biointerfaces: new generation of cell instructive materials — •Chiara Fedele, Ravichandran H. Kollarigowda, Silvia Cavalli, and Paolo A. Netti — Center for Advanced Biomaterials for Healthcare, Istituto Italiano di Tecnologia, Neaples, Italy

Nowadays the growing interest in tissue engineering and biology for the in vitro control of cell fate has led to the design of dynamically actuable platforms through the implementation of stimuli-responsive materials in order to mimic the continuous remodeling of the extracellular matrix in living systems. Dynamic biointerfaces are conceived in order to be able to modify in a predictable spatiotemporal manner the cell-material crosstalk, overcoming the limitations of static conven-

tional biomaterials. In our work, azobenzene-containing photosensitive polymers (e. g. polymer brushes, thin films, crosslinked free standing polymers) are designed as biomaterials to obtain patterned or reshaping substrates using photolithographic techniques or single laser beam instruments, in some cases even in presence of cells, allowing for a real-time modification of cell behavior.

15 min. break

BP 42.6   Wed 16:45   H40

Tuning the Morphology of Langmuir Polymer Films through Controlled Relaxations of Non-Equilibrium States — •Renate Reiter, Sivasurender Chandran, and Günter Reiter — University of Freiburg, Experimental Polymer Physics, Freiburg, Germany

In general it is difficult to reproduce well defined morphologies of Langmuir polymer films (LPFs) because they have a high propensity to form non-equilibrium states. When these films are allowed to relax, a decay of the surface pressure with time might be observed indicating that the system is not equilibrated. Monitoring the temporal evolution of these relaxations and correlating them with snapshots of the corresponding morphologies sheds light on the associated structural reorganisation processes.

We present a systematic study based on different compression protocols designed to allow for relaxations of LPFs under well defined conditions. The homo peptide poly-γ-benzyl-L-glutamate (PBLG) was chosen for this study because it is a well investigated system that represents the relaxational behaviour of rod-like molecules which is expected to show less complexity than coiled polymer molecules. Our results demonstrate that experimentally manipulating the course of relaxations in LPFs has tremendous impact on the ordering of the molecules. Therefore various macroscopic properties of these biological relevant thin films are accessible.

BP 42.7   Wed 17:00   H40

Impact of Silver Nanoparticles on the mechanical properties of Aquabacterium biofilms — •Yvonne Schmitt[1], Alexandra Grün[1], Dimitri Demeshko[2], Werner Manz[1], and Silke Rathgeber[1,2] — [1]Institute for Natural Sciences, University of Koblenz-Landau, Koblenz, Germany. — [2]Technology Institute for Functional Polymers and Surfaces (tifko) GmbH, Neuwied, Germany.

The antimicrobial properties of silver nanoparticles (AgNP) led to a wide range of applications in consumer products. As a consequence, there is an increasing release of AgNP into aquatic environments. Biofilms, a conglomerate of extracellular DNA, polysaccharides and proteins, play an important role in sediment stabilization in riverine systems. AgNP are supposed to be a continuous source for silver ions (Ag^+) which can bind to functional groups of the biofilm constituents. This might lead to a decrease in the number of possible intermolecular interactions and, thus, reduced stability of the network. An impairment of the sediment stabilization due to enrichment of the AgNP in the biofilms might be detrimental to the whole ecosystem. In this work we studied the mechanical properties of an *A. citratiphilum* biofilm by means of rheology. The bacterium chosen is representative for a numerically dominant group of bacteria in different freshwater habitats. The biofilm was exposed to environmentally relevant concentrations of AgNP. In order to distinguish physical effects, resulting from the presence of the nanoparticles in the biofilms, from chemical effects, due to the activity of Ag^+, we studied biofilms exposed to Ag^+ as reference. We discuss our results in respect to their environmental implications.

BP 42.8   Wed 17:15   H40

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

The process of crystal growth controlled by biomolecules is known as biomineralization. This type of controlled growth results in crystals with a myriad of interesting properties, useful in a variety of applications. Therefore it is of great importance to gain deeper insights into the mechanistic details of interactions on the bioinorganic interface. For this purpose we present a systematic study of a set of amino acids, the elementary building blocks of peptides and proteins. Our

methodology includes fully atomistic molecular dynamics simulations of the interface made of amino acids, water and slabs of calcite. Two different calcite slabs were taken into account, one with the stable (104) face and one with the unstable (001) face, which is associated with crystal growth. Free energies of binding to both surfaces for all the individual amino acids were determined using a series of sampling simulations with biasing potentials. These in turn reveal the importance of charged and polar groups in the interaction with calcite. This work provides reference data which can be helpful in further theoretical and experimental studies of calcite/peptide interfaces.

BP 42.9   Wed 17:30   H40

Biomimetic Surface Templating of Silica Nanoparticles by Lysine-Leucine Peptide on Au Substrate — •Hao Lu[1], Yeneneh Yimer[2], Rüdiger Berger[1], Mischa Bonn[1], Jim Pfaendtner[2], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Chemical Engineering University of Washington, Seattle, USA

Fabrication of silica thin films and architectures has led to many applications in electronic and optical devices, cosmetics, and catalysis; recently, bioinspired silica fabrication approaches have attracted great attention because of low production cost and mild, sustainable fabrication methods. We are the first to demonstrate that the biomimetic molecules can also exert control over silica mineralization when bounded to inorganic surfaces. We use amphiphilic helical peptides based on leucine and lysine side chains (LKa14) carrying cysteine terminal groups as linkers, providing stable covalent bond to gold surfaces. Using XPS, VSFG, and AFM, complemented by molecular dynamic simulation, we have investigated the silica mineralization process at the molecular level directly at the surface: In analogy to solution mineralization, the LKa14 peptides on Au tend to assemble into ordered lateral structures, maintain their solution state helical folding and are oriented upright on the surface. The LKa14 peptides nucleate silica nanoparticles at the surface, which then grow into larger, globular structures. This surface mineralization process serves as a well defined model system for lateral protein assembly and biomineralization and is of potential interest for the design of silica-based biomimetic coatings.

BP 42.10   Wed 17:45   H40

Reaction kinetics and diffusion in cell-free protein synthesis altered in polymer hydrogels — •Julian Thiele[1], Maike M. K. Hansen[2], David Foschepoth[2], Hans A. Heus[2], and Wilhelm T. S. Huck[2] — [1]Leibniz Institute of Polymer Research Dresden (IPF), Leibniz Research Cluster (LRC) and Department of Nanostructured Materials, Hohe Straße 6, 01069 Dresden, Germany — [2]Radboud University, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, NL

Despite the viscous and highly crowded interior of a cell and its influence on diffusion and reaction kinetics, in vitro studies on protein synthesis often fail to take into account the density and spatial organization of the cytoplasm.

We mimic the complex cellular environment using a porous hydrogel matrix, and study the effects of macromolecular crowding on gene expression. While gene expression is strongly decreased by macromolecular crowding in conventional dilute bulk solutions, both gene transcription and translation are significantly enhanced 5x and 4x, respectively, when performed in a microscopic hydrogel environment.

These results highlight the need to consider the influence of the physical environment on complex biochemical reactions including macromolecular crowding as well as microscale confinement and spatial organization.

BP 42.11   Wed 18:00   H40

Protein-protein interactions in crowded lysozyme solutions — •Karin Julius[1], Michael Paulus[1], Julian Schulze[1], Stefanie Roese[1], Metin Tolan[1], and Roland Winter[2] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund — [2]Fakultät Chemie, Technische Universität Dortmund, 44221 Dortmund, Germany

Inside cells, proteins are surrounded by different macromolecules, including proteins themselves, which cover approximately 30% of the available volume. It has been shown that this reduction of free space by macromolecules, the so called crowding effect, has a significant impact on the stability of proteins, rendering them more resistant to temperature or pressure denaturation. However, the influence of crowding on the protein-protein interaction potential that is mediated by the solvent is still unknown. The final goal of this project is the investiga-

tion of the pressure dependent interaction potential between proteins in aqueous protein solution as a function of the crowder concentration, mimicking intracellular solution conditions. For this purpose, small-angle x-ray scattering (SAXS) under high hydrostatic pressure will be applied. As we will focus on the effect of crowding, the well characterized model protein lysozyme is used at a concentration of 5 - 10 wt.-% in combination with the macromolecular crowder Ficoll PM 70 and its monomeric subunit sucrose.

BP 43: Cell Adhesion

Time: Wednesday 15:00–17:00 — Location: H43

Invited Talk — BP 43.1 — Wed 15:00 — H43
Cellular Mechanosensing — ●RUDOLF MERKEL — Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Throughout the organism almost all tissues experience mechanical strain of sizeable magnitude that often is important to their organization and development. To unravel the underlying signal sensing and processing an in vitro model consisting of cells cultivated on stretchable substrates was introduced. Here, I will show how this system can be used as quantitative tool to unravel the contributions of the different cytoskeletal systems and to quantify the "mechanosensing potential" of individual molecules.

BP 43.2 — Wed 15:30 — H43
Adhesion of the eukaryotic microalga *Chlamydomonas* to model surfaces — ●CHRISTIAN KREIS, MARCIN MAKOWSKI, and OLIVER BÄUMCHEN — Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

Microorganisms are often found in aqueous environments and complex geometries, where they are likely to come into contact with interfaces. Therefore, their survival and behaviour in confinement depends upon their interaction with and adhesion to surfaces. In these processes, flagella and cilia play a crucial role since they are the source of locomotion and may come into direct contact with an interface. However, their interactions with interfaces are not yet understood. Microalgae represent microorganisms that are omnipresent in bioengineering. Their adhesion to surfaces, however, may obstruct the fluid flow and performance output of, e.g., alga farms and microfluidic devices. The unicellular alga *Chlamydomonas* serves as a biological model organism that entails a high technological relevance in terms of the production of biofuel and drugs. We perform adhesion experiments to study the interaction of *Chlamydomonas* and its flagella to interfaces, as a model for eukaryotic cells, flagella and cilia. We employ a micropipette force sensor technique that enables us to probe dynamic interfacial forces of microscale objects down to the pN range. The optical control enables us to track the adhesion of the cell body and the adhesion of the flagella. We observe that only the flagella and not the cell body adhere to our test substrates and provide precise adhesion force measurements of eukaryotic flagella to different model substrates.

BP 43.3 — Wed 15:45 — H43
Cytoskeletal dynamics in blood platelets during spreading on fibrinogen — ●INGMAR SCHÖN, SEBASTIAN LICKERT, and VIOLA VOGEL — Laboratory of Applied Mechanobiology, ETH Zurich, Switzerland

Blood platelets are small anucleate cells that form a thrombus during blood coagulation. The most abundant platelet integrin $\alpha_{\mathrm{IIb}}\beta_3$ specifically binds fibrinogen and thereby enables platelet aggregation. Patients with Glanzmann Thrombasthenia (GT) carry a genetic mutation in integrin $\alpha_{\mathrm{IIb}}\beta_3$ and suffer from defective platelet aggregation and excessive bleeding. Here we investigated the spreading of healthy or GT platelets on fibrinogen-coated surfaces by time-lapse fluorescence imaging, confocal microscopy, and super-resolution microscopy (dSTORM). Healthy platelets re-arranged their cytoskeleton and adhesion complexes during spreading from an early "stellar" arrangement into pronounced bundles spanning the whole cell. GT platelets also adhered and spread on fibrinogen but exclusively exhibited a stellar cytoskeletal arrangement. Based on these findings we hypothesize that cytoskeletal dynamics of GT platelets gets stalled at an early stage of the spreading process. We will present results from experiments with specific inhibitors, knock-out cells, different ligand proteins, and other means that aimed at identifying the crucial step where things went awry.

In general, we suggest that platelets are an interesting biophysical model system to study the autonomous, acto-myosin-driven cytoskeletal dynamics during adhesion formation.

BP 43.4 — Wed 16:00 — H43
Modelling the adhesion of malaria-infected red blood cells — ●ANIL KUMAR DASANNA[1,2] and ULRICH S. SCHWARZ[1,2] — [1]Institute for Theoretical Physics, Heidelberg University — [2]BioQuant, Heidelberg University

Clinical symptoms of the malaria disease appear when healthy red blood cells are invaded by the parasites during the blood stage of the malaria lifecylce. An infected red blood cell (iRBC) starts to develop adhesive protrusions, so-called knobs, on its surface. The parasite takes about two days to rebuild the iRBC and during this time, the density of knobs increases whereas their typical size decreases. The knobs cause iRBCs to adhere to endothelial cells in the microvasculature, preventing their clearance by spleen and liver, but also leading to capillary obstruction. To better understand the adhesion of iRBCs under capillary flow, we studied the adhesion of iRBC in shear flow using Stokesian dynamics simulations. The iRBC is assumed to have a spherical shape and the knobs are modelled as cluster of receptors on the spherical surface. The ligands are distributed on the substrate to which receptors on iRBC can make bonds that then can rupture under force. We investigate mainly how the spatial organisation of the receptors on the surface of the iRBC changes its adhesive behavior in shear flow. We discuss the different dynamical states of infected RBC, such as rolling adhesion, transient adhesion, firm adhesion and free motion, as a function of knob density and size. We also will discuss the role of heterogeneous receptor distributions and the role of cell elasticity.

BP 43.5 — Wed 16:15 — H43
Morpho-dynamics and Mechanics of T lymphocytes — PIERRE DILLARD[1,2], ASTRID WAHL[1], FUWEI PI[1], RANIME ALLAMEDDINE[1], EMMANUELLE BENARD[1], PIERRE-HENRI PUECH[2], ANNE CHARRIER[1], LAURENT LIMOZIN[2], and ●KHEYA SENGUPTA[1] — [1]CINaM/AMU-CNRS UMR 7325, Marseille, France. — [2]LAI/INSERM UMR 1067 AMU-CNRS UMR 7333, Marseille, France.

We investigate adhesion and membrane organization of T lymphocytes interacting with surrogate antigen presenting cells (sAPCs) carrying the ligand anti-CD3 against the T cell receptor (TCR) complex. The sAPCs comprise supported bilayers with mobile/immobilized ligands (BiophysJ 2014), or ordered arrays of ligand nano-dots in a non-adhesive matrix (NanoLett 2013,2015), or soft elastomers. We show that ligand mobility is an important control parameter in cell spreading: cells adhere but fail to spread on mobile ligands, spreading can be rescued by suppressing myosin activity. We also demonstrate a dual scale of T cell response: locally, the cell responds at the nano-scale and restructures its membrane according to local cues; globally, it integrates the signal and responds to an average dose. Finally, the mechano-response of T cells is very different from connective tissue cells: unlike most previously reported cell types, T-cells spread more on soft than on hard elastomers. These results taken together point to original aspects of TCR-mediated response to mechanical cues which are should be relevant for understanding lymphocyte mechanotransduction.

BP 43.6 — Wed 16:30 — H43
The membrane as a matchmaker in the cell adhesion process — TIMO BIHR[1,2], SUSANNE FENZ[3,4], ●DANIEL SCHMIDT[1,2], RUDOLF MERKEL[4], KHEYA SENGUPTA[5], UDO SEIFERT[2], and ANA-SUNČANA SMITH[1,6] — [1]PULS Group, Inst. f. Theor. Physik and Excellence Cluster "Engineering of Advanced Materials", Universität Erlangen-Nürnberg — [2]II. Inst. f. Theor. Physik, Universität Stuttgart — [3]Department of Cell and Developmental Biology, Universität Würzburg — [4]ICS 7: Biomechanics, Forschungszentrum Jülich — [5]CNRS UPR 3118, CINaM, Aix-Marseille Université — [6]Division of Physical Chemistry, Institute Ruđer Bošković, Zagreb

The integrity of living tissues is maintained by cadherin rich domains. Cadherin molecules form *trans*-dimers bridges between neighbouring

cells. The formation of domains of *trans*-bonds is controlled by lateral, /in-plane/*cis*-interactions. The origin of these interactions are still debated. In this presentation, we show that the formation of *cis*-domains is regulated by the membrane via its elasticity and fluctuations. Observations from a cell free system consisting of cadherin-decorated model membranes show that the membrane regulates the *trans*-binding, and is itself a source of *cis*-interactions. We develop a theoretical framework to explicitly show that membrane fluctuations introduce complex cooperative effects that modulate the rates of binding and unbinding of the *trans*-dimers. The regulatory activity of the membrane, quantified here in the context of cadherins, relies purely on physical principles and therefore may be a generic player in the context of formation of any adhesion structures on the plasma membrane and in the cell interior.

BP 43.7   Wed 16:45   H43
Cytoskeletal organization in cells on micropatterns — •Marco Linke[1,2], Felix Frey[1,2], Vytaute Starkuviene-Erfle[2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg

University, Germany — [2]BioQuant, Heidelberg University, Germany

Mammalian cells show large variability in cell shape and cytoskeletal organization when grown on planar cell culture substrates with homogenous protein coating. Therefore micropatterns are increasingly used to normalize their shape and structure, but a quantitative understanding of the resulting intracellular organization is missing. Here we analyze the cytoskeleton of cells growing on a micropatterned substrate by measuring the local orientation of the microtubule network and calculate a typical orientation field for various micropattern geometries. We then model the microtubule cytoskeleton with two different approaches. First, we simulate individual filaments and take the interaction between the actin and microtubule networks into account by using an effective persistence length of the microtubules. Secondly, we use a continuum model based on the theory of liquid crystals in which we minimize the nematic free energy functional. By considering biologically plausible boundary conditions and the influence of the centrosome and the cell nucleus, in both cases we get predictions for global cell organization that agree well with experimental results.

BP 44: Biotechnology & Bioengineering

Time: Wednesday 15:00–16:45   Location: H45

Invited Talk   BP 44.1   Wed 15:00   H45
Physics for the Origins of Life — •Dieter Braun — Systems Biophysics and Center for NanoScience, LMU Muenchen, Amalienstr. 54, D-80799 Munich

The origin of life is located between the astronomy, geology and chemistry of early Earth and biology. Can concepts from physics help to bridge the gap between dead and living matter? Our experiments show that phase transitions, cooperative binding and non-equilibrium couplings can make headway towards understanding a stable replication and selection of the first living genetic molecules.

1. A phase transition of DNA or RNA oligomers into hydrogels is found under non-equilibrium driving. Only molecules with matching gene sequences form one hydrogel. This highly nonlinear phase transition can allow for an unusual, yet robust sequence replicator.

2. The cooperative of joining of three DNA strands implement hypercycle dynamics in sequence space. Besides providing replication under serial dilution and feeding, the hyperexponential growth make majority sequences outcompete minority sequences. By this, diversity is stabilized even under diffusional mixing.

3. Thermal gradients in porous rock implement the thermal cycling required in above experiments. Such a setting can accumulate genetic molecules, enhance their polymerization, encapsulate them by vesicle formation and drive their replication dynamics by thermal convection. The fluid interaction with a continuous feeding flow allow longer strands to outcompete faster growing short strands and drive evolution towards increasing complexity.

BP 44.2   Wed 15:30   H45
Investigation of light harvesting complex LHCBM6 for dye-sensitized solar cells — •Fabian Schmid-Michels[1], Nina Lämmermann[2], Olaf Kruse[2], and Andreas Hütten[1] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Faculty of Biology, Algae Biotechnology & Bioenergy, Bielefeld University, Germany

Light harvesting complexes (LHC) or antenna complexes participate in photosynthesis by harvesting sunlight and transferring the excitation energy to the reaction centre. By channelling this energy elsewhere it is possible to use LHC either as a dye for dye-sensitized solar cells or as energy harvesters for artificial photosynthesis (AP). Solving this challenge could lead to a more efficient regenerative fuel production. To investigate LHCBM6, dye sensitized solar cells were prepared on ITO glass with the LCHs bound to TiO2 nanoparticles. Different binding types were evaluated by electrical measurements and microscopy (AFM, SEM).

BP 44.3   Wed 15:45   H45
Microscale Thermophoresis to Diagnose alpha1-Antitrypsin Deficiency Disorder in Plasma — •Evgeniia V. Edeleva[1,2], Therese Dau[3], Susanne A.I. Seidel[1], Dieter Jenne[3], and Dieter Braun[1,2] — [1]Systems Biophysics, LMU, Munich, Germany — [2]Quantitative Biosciences Munich (QBM), Munich, Germany —

[3]Comprehensive Pneumology Center (CPC), Munich, Germany

Conventional diagnostics of deficiency disorders is often limited to the measurement of concentration, not the affinity of the deficient component. In case of alpha1-antitrypsin (AAT) deficiency disorder, AAT plasma level is low in patients due to the genetic mutation. However, measured concentration of AAT does not correlate with the manifestation of symptoms. We hypothesized that AAT affinity to its target neutrophil elastase is different in plasma of different patients.

We developed a competition assay based on the physical phenomenon of thermophoresis. Our assay assesses the affinity of AAT in addition to its concentration. The measurement is performed directly in the natural milieu of blood plasma. The three-body binding problem is used to fit the experimental data.

The amplitude of thermophoresis correlates with symptoms manifestation in patients. Further measurements suggest a previously unknown component in plasma, capable of modulating the affinity of AAT to the target. Our work highlights the possibility of assay development in the natural environment of blood plasma with thermophoresis with the promise to significantly improve the management of AAT deficiency.

BP 44.4   Wed 16:00   H45
Study of Reaction Networks with High-Throughput Nanoliter Thermophoresis — •Ferdinand Greiss[1], Franziska Kriegel[2], and Dieter Braun[1] — [1]Systems Biophysics, Quantitative Biosciences Munich (QBM), LMU, Munich, Germany — [2]Molecular Biophysics, LMU, Munich, Germany

Quantifying the cooperative effect of protein binding is important and a well-established field in biochemistry. For instance, the binding of oxygen to hemoglobin is a widely known and thoroughly studied case of a positive homotropic binding reaction. This means that oxygen together with other oxygen molecules is binding in a positive cooperative manner. Many biological relevant reaction networks, e.g. transcription factors binding to DNA, include heterotropic binding interactions, both being negative or positive as well as with weak or strong cooperative effects.

We use synthetic DNA constructs as a simplified testbed to study the cooperative effects in heterotropic reaction networks with microscale thermophoresis (MST). All three DNA species have two different binding sites that can only access one partner. The advantage of the assay is that only one species needs to be labeled. The binding reaction network can be studied by independent single-point mutations, both in experiment and by theory.

With a newly designed high-throughput micro-scale thermophoresis setup, we are able to sample the large concentration space in a rapid, robust and user-friendly way.

BP 44.5   Wed 16:15   H45
GALA - A cell penetrating peptide with a trigger — Johannes Franz[1], Denise Schach[1], Will Rock[1], Christoph Globisch[2], Steven Roeters[3], Sander Woutersen[3], Christine Peter[2], Mis-

cha Bonn[1], Sapun Parekh[1], and •Tobias Weidner[1] — [1]MPI für Polyforschung, Mainz, Germany — [2]Universität Konstanz, Germany — [3]University of Amsterdam, The Netherlands

Cell-penetrating peptides are promising for drug delivery into cells. Since the cell uptake mainly involves endocytic mechanisms, the enclosure of peptides within endosomes is still an unresolved challenge for biomedical applications * the peptide and its cargo are trapped in the *recycling bin* of the cell. The peptide GALA, a viral fusion mimic is triggered by pH, and takes advantage of the decreasing pH during endosome maturation to selectively attack endosomal membranes. Below pH 6, the sequence folds into a helix and disrupts biomembranes. We used surface specific sum frequency generation (SFG) spectroscopy jointly with fluorescence imaging and molecular dynamics simulations to study GALA in action at interfaces. We show that the lipid bilayer radius-of-curvature has a negligible effect on GALA-induced membrane leakage and that GALA remains pH responsive after inserting into a lipid membrane. The peptide can be reversibly *switched* between its inactive and active states after incorporation into the hydrophobic environment of lipid membranes, even after substantially interacting with lipid chains. GALA-based delivery is a potentially safe, effective route towards effective endosomal escape strategies. JACS 137, 12199*12202 (2015); ChemComm 51, 273-275 (2015); JCP 141, 22D517 (2014).

BP 44.6   Wed 16:30   H45
Compact helical antenna for smart implant applications

— •Dmitriy Karnaushenko, Daniil Karnaushenko, Denys Makarov, and Oliver G. Schmidt — Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, Dresden, 01069 Germany

Smart implants are envisioned to monitor bioprocesses in the human body. Hence, their compactness is highly desirable to minimize discomfort during and after the implantation. If the length of the device is about 5 mm and the diameter less than 0.5 mm, it can be implanted using standard medical syringes. In this spirit, electronic devices self-assembled into compact tubular architectures[1] possess the desired dimensions and reveal biosensory capabilities[2] or can be used as neuro-interfaces[3]. Integration of antennas into self-assembled devices will allow remote implant monitoring, drug release or stimulation of biological tissues. In this work, a self-assembled helical antenna operating in the ISM radio band is presented[4]. Our novel material platform permits fabrication of antennas with operation frequencies at 2.4 GHz with a total length of only 5.5 mm. To tune the resonance frequency, the helical antenna is encapsulated with a dielectric material. Moreover, the revealed communication between the helical antenna and a smartphone highlights the potential of this technology for medical applications. [1] O. G. Schmidt et al., Nature 2001, 410, 168. [2] C. S. Martinez-Cisneros et al., Nano Lett. 2014, 14, 2219. [3] D. Karnaushenko et al., Adv. Mater. 2015, DOI 10.1002/adma.201503696. [4] D. D. Karnaushenko et al., NPG Asia Mater. 2015, 7, e188.

BP 45: Statistical Physics in Biological Systems III (Joint Session with DY)

Time: Wednesday 15:30–16:15   Location: H46

BP 45.1   Wed 15:30   H46
Bursting noise in gene regulation networks: exact and numerical results for stationary distributions and first passage times — •Yen Ting Lin[1], Charles Doering[2], and Tobias Galla[1] — [1]The University of Manchester, Manchester, UK — [2]University of Michigan, Ann Arbor, USA

Understanding how effects of noise propagate from one level of modelling to another is key in a number of applications in physiological or biological systems. Including short-lived mRNA populations in models of gene regulation networks introduces bursting noise, and understanding the effects of this in higher-level models is an open task. In this talk, I will present a coarse-graining method to construct mesoscopic models for such type of dynamical systems, which fully accounts for the bursting noise. We systematically compare different levels of modeling, ranging from individual-molecule-based models including mRNA populations, over protein-only individual-based models to mesoscopic models such as diffusion-type models and our proposed model. We show that the proposed mesoscopic model outperforms conventional diffusion-type models. In a one-dimensional autoregulated network, we present closed-form analytic solutions for both the stationary distribution of protein expression as well as first-passage times of the dynamical system. We present numerical solutions for higher-dimensional gene regulation networks, in which case we also carry out analysis in the weak-noise limit. References: arXiv:1508.02945, arXiv:1508.00608 (*J. R. Soc. Interface* in press)

BP 45.2   Wed 15:45   H46
Population dynamics in switching environments — •Peter Hufton, Yen Ting Lin, Tobias Galla, and Alan McKane — School of Physics and Astronomy, The University of Manchester, Manchester, UK

In gene regulatory networks, the binary state of a single gene can have drastic effects on the dynamics of a population of proteins. Similarly, switches between environmental states are important in bacterial populations and in models of epidemic spread. The mathematical treatment of problems of this type—populations in switching environments—is an open challenge. We present a systematic approach to computing stationary states of these problems. We identify two sources of randomness: the stochasticity from environmental switches, and the intrinsic noise from fluctuations in the population. By extending the linear-noise approximation and utilising a piecewise-deterministic Markov process, we develop a method which incorporates both these effects.

BP 45.3   Wed 16:00   H46
Geometry Dependence of the Diffusion Coefficient in Molecular Dynamics Simulations with Periodic Boundary Conditions — •Martin Vögele and Gerhard Hummer — Max-Planck-Institut für Biophysik, Frankfurt am Main

We investigate the dependence of the diffusion coefficient on the box geometry and its application to lipid membrane simulations.

For this purpose, we compare predictions from a simple analytic correction based on hydrodynamic arguments to molecular dynamics simulations of liquid argon. Increasing the box size in two dimensions, we find a logarithmic dependence on the system size. Increasing the box size in only one dimension, we find a linear dependence. In both cases, diffusion is anisotropic. Additionally, we observe an upper limit for the diffusion coefficient in the limit of infinite systems.

We also test the effect of box geometry on the diffusion in lipid membranes, which are usually simulated in very flat periodic boxes. There we find the predicted logarithmic increase with growing edge lengths.

BP 46: Posters - Biomaterials and Biopolymers

Time: Wednesday 17:00–19:00   Location: Poster C

BP 46.1   Wed 17:00   Poster C
Neutron Reflectometry Yields Structural Insight into Protein Adsorption from Blood Serum onto Polymer Brushes — Ignacio Rodriguez Loureiro[1], •Victoria Latza[1], Avraham Halperin[2], Giovanna Fragneto[3], and Emanuel Schneck[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Université Joseph Fourier, Grenoble, France — [3]Institut Laue-

Langevin, Grenoble, France

The density profiles of proteins adsorbed from human blood serum onto poly(ethylene glycol) (PEG) brushes grafted to phospholipid surfaces are characterized by neutron reflectometry (NR). PEG brushes are commonly used to suppress undesired protein adsorption to biotechnological surfaces but brush failure is often reported. In contrast to

conventional methods, NR with contrast variation allows directly distinguishing among primary protein adsorption at the grafting surface, secondary adsorption at the brush outer edge, and ternary adsorption to the polymer chains. We find significant primary protein adsorption into the lipid headgroup region. At the same time our results exclude pronounced ternary adsorption. Interestingly, the total amount of protein adsorbed to the brush-decorated surfaces is comparable to that adsorbed to the bare lipid surfaces.

BP 46.2   Wed 17:00   Poster C
Novel hybrid hydrogel substrates elicit differential responses from human mesenchymal stem cells — •Christina Jayachandran[1] and Florian Rehfeldt[2] — [1]Drittes Physikalisches Institut, Georg- August -Universität, Göttingen, Germany — [2]Drittes Physikalisches Institut, Georg- August -Universität, Göttingen, Germany

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 elasticity.

In this study, we prepared hybrid hydrogels by incorporating collagen fibrils into the linearly elastic (PA) hydrogel. We tuned these gels in their physical stiffness from the soft to the stiff regime and investigated the responses of adult human mesenchymal stem cells (hMSC). On soft hybrid gels, hMSCs behave significantly different than on collagen coated gels, as they show classical morphologies resembling a stiff environment. Fluorescence imaging of hybrid gels revealed that stem cells locally re-organize the underlying collagen fibrils. These findings imply that stem cells behaviour is dependent on the non-linear elasticity of collagen and can show 3D network like behaviour even on a 2D hydrogel.

BP 46.3   Wed 17:00   Poster C
Stochastic binding of Staphylococcus aureus — •Nicolas Thewes[1], Alexander Thewes[2], Friederike Nolle[1], Ludger Santen[2], and Karin Jacobs[1] — [1]Saarland University, Dept. of Experimental Physics, 66041 Saarbrücken — [2]Saarland University, Dept. of Theoretical Physics, 66041 Saarbrücken

Bacteria exhibit an outstanding ability to adhere to various kinds of surfaces. The Hydrophobic interaction plays a crucial role for the adhesion of bacteria [1]. Hence, we studied the contact formation process of Staphylococcus aureus to hydrophobic surfaces by combining AFM single cell force spectroscopy and computer simulations of a simple model for bacterial adhesion [2]. We found 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, S. aureus is able to attach to surfaces over distances far beyond the range of classic surface forces.

In our model the bacterial surface biopolymers are represented by elastic springs that interact with a surface via a square potential. The model is analyzed using Monte-Carlo Simulations and the results suggest that the bacterial adhesion process in general, can be described by solely taking into account the tethered biopolymers between a bacterium and a surface.

[1] N. Thewes et al, Beilstein J. Nanotechnol. 2014, 5, 1501 - 1512
[2] N. Thewes et al, Soft Matter 2015, 11, 8913 - 8919

BP 46.4   Wed 17:00   Poster C
DNA-based molecular force sensors in reconstituted actin networks — •Christina Jayachandran[1], Florian Rehfeldt[2], and Christoph Schmidt[3] — [1]Drittes Physikalisches Institut, Georg- August -Universität, Göttingen, Germany — [2]Drittes Physikalisches Institut, Georg- August -Universität, Göttingen, Germany — [3]Drittes

Physikalisches Institut, Georg- August -Universität, Göttingen, Germany

Actin is the main structural component of the cytoskeleton among the other bio-polymers responsible for cellular shape and mechanical stability. The actin cytoskeleton which self-assembles into networks of crosslinked filaments and bundles is responsible for a myriad of cellular processes, ranging from migration, division, intracellular transport to cell morphogenesis. Stresses and stress propagation in these networks are crucial for function.

We utilize dsDNA constructs as stress sensors in order to understand network mechanics. We studied the macro- and micro-rheological properties of in vitro actin networks to test the sensors and to analyze network failure mechanisms beyond the non-linear response.

BP 46.5   Wed 17:00   Poster C
Programming mechanics in semiflexible DNA tube networks — •Carsten Schuldt[1,2], Tina Händler[1,2], Martin Glaser[1,2], Tom Golde[1,2], Jessica Lorenz[2], Jörg Schnauss[1,2], Josef A. Käs[1,2], and David M. Smith[2] — [1]Soft Matter Physics Division, Institute for Experimental Physics I, University of Leipzig, Germany — [2]Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany

Biologically evolved materials are often used as inspiration in the both the development of new materials as well as examinations into the underlying physical principles governing their general behavior. One prominent example is the semiflexible polymer actin and its set of modulatory proteins and motors. Here, a major goal is to understand the emergent viscoelastic properties of networks assembled from individual filaments. Impossible with actin, we assess the impact of the filamentous rigidity (persistence length l_p) on network mechanics in *in vitro* experiments. We employ programmable DNA tubes comparable to actin but tunable in their circumference and therefore their l_p.

According to the well established tube model, network elasticity G_0 should drop with increasing l_p. Here, we show that networks made of DNA tubes resemble many of the characteristics of actin. However, we find that network elasticity increases linearly with filaments stiffness $G_0 \sim l_p$. Since our observations are in strong contrast to the theoretical predictions, we conclude that the current tube model describes the bulk elasticity inadequately and demands theoretical revision.

BP 46.6   Wed 17:00   Poster C
Mesh size of semiflexible polymer networks — •Tina Händler[1,2], Martin Glaser[1,2], Tom Golde[1], Carsten Schuldt[1,2], Jörg Schnauss[1,2], Josef Käs[1], and David Smith[2] — [1]University of Leipzig, Soft Matter Physics Division, Leipzig — [2]Fraunhofer Institute for Cell Therapy and Immunology, Leipzig

Studying the mechanics and dynamics of biopolymers has inspired many ideas and theories in polymer physics. One prominent example is actin, being the best-studied semiflexible polymer. Unfortunately, naturally occurring protein-based biopolymers are limited in their properties such as length, stiffness and interaction strengths. This highlights the advantage of having "programmable" model polymers at hand, which give the opportunity to experimentally test parameters otherwise unavailable in natural systems. Nanotubes formed from synthetic DNA strands are an ideal match to this need: they are semiflexible over their typical length scale and can be hybridized to have characteristics such as persistence length which are similar to actin filaments or can be varied in a controllable way. We use this model system to measure the mesh size of entangled networks by observing the reptation of single filaments. The results show a concentration scaling similar to the theoretically predicted scaling for flexible polymers, as opposed to the stiff rod approximation. These findings point towards a more complex description of semiflexible polymer reptation and demonstrate the applicability of this method.

BP 47: Posters - Active Matter

Time: Wednesday 17:00–19:00   Location: Poster C

BP 47.1   Wed 17:00   Poster C
Emergent Vortex Patterns in Systems of Self-Propelled, Chiral Particles — •Lorenz Huber, Jonas Denk, Emanuel Reithmann, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of

Physics, Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München, Germany

Self-organization of FtsZ polymers is vital for Z-ring assembly during bacterial cell division, and has been studied using reconstituted in vitro model systems. Employing Brownian dynamics simulations and

a Boltzmann approach, we model FtsZ polymers as active particles moving along chiral circular paths. With both methods we find self-organization into vortex structures and characterize different states in parameter states. Our work demonstrates that these patterns are robust and are generic for active chiral matter. Moreover, we show that the dynamics at the onset of pattern formation is described by a generalized complex Ginzburg-Landau equation.

BP 47.2   Wed 17:00   Poster C
Dynamical density functional theory for hard, active disks — •Josua Grawitter and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

We study a collection of self-propelled, active particles using a modi-fied dynamical density functional theory (DDFT) in two dimensions. DDFT provides an ensemble description of hard-sphere interactions in colloidal systems. It therefore gives insight into statistical properties which would otherwise require extensive Brownian dynamics simulation.

When active particles are placed in a harmonic trapping potential, we observe nonequilibrium steady states, which were previously noted by Pototsky and Stark using different methods [1]. Switching to the co-moving and -rotating reference frame of a single particle produces the radial-orientational distribution function of the liquid. Using this model, we can statistically predict the relative orientations and positions of active particles close to each other.

[1] A. Pototsky and H. Stark, Europhys. Lett. **98**, 50004 (2012).

BP 48: Posters - Bioimaging and Spectroscopy

Time: Wednesday 17:00–19:00   Location: Poster C

BP 48.1   Wed 17:00   Poster C
NET- the Network Extraction Tool — •Jana Lasser — MPI for Dynamics and Self-Organization, Göttingen, Germany

We present the Network Extraction Tool (NET). The tool is especially designed for high-throughput semi-automated analysis of biological datasets containing networks of very large sizes. Applied to a network, NET extracts information about its geometry (node positions and edge radii) as well as information about the topology (neighbourhood relations). The information NET collects provides a basis for quantitative research of the networks in question. The framework starts with the segmentation of the image and then proceeds to vectorization using methodologies from optical character recognition. After a series of steps to clean and improve the quality of the extracted data the framework produces a graph in which the network is represented only by its nodes and edges. The networks extracted by NET are comparable to manually extracted networks with regards to their quality but take significantly less time to generate. Additionally, the extracted networks are very easy to handle computationally. Several projects researching biological networks such as leaf veins, insect trachea and blood vessels already use NET for their data acquisition. As it is an open source tool based on a collection of python scripts feel free to find and try out the software at https://github.com/JanaLasser/network_extraction.

BP 48.2   Wed 17:00   Poster C
Aggregation of mono-stained proteins visualized ex vivo by two-dimensional polarization microscopy — •Daniela Täuber[1], Rafael Camacho[1], Christian Hansen[2], Jia-Yi Li[2], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]Biomedical Center, Lund University, Lund, Sweden

Neurodegenerative diseases are linked to aggregation of particular proteins. The investigation of pathologic pathways and the development of suitable medication demand for methods to visualize protein aggregation ex vivo. Sophisticated microscopy often requires two color labelling, while conventional fluorescence microscopy can reveal the expression of such proteins in brain tissue, but not their aggregation. Here we apply 2-dimensional polarization imaging [1] to visualize aggregation of human α-synuclein expressed in brain tissue from transgenic mice. We employ Förster Resonance Energy Transfer (FRET) between identical (single color) green fluorescent protein (GFP) tags linked to α-synuclein. We obtain information on aggregation, which cannot be seen from fluorescence intensity [3]. Our finding of α-synuclein aggregation in olfactory bulbs of old mice correlates with results from a behavioral study on that mice [2]. The aggregation pattern was not found in young mice.

D.T. acknowledges funding from the german science foundation DFG-TA 1049/1-1.

[1] Camacho, R. et al., Chem. Phys. 406, 30, 2012. [2] Hansen, C. et al., Neurobiol. Dis. 56, 145, 2013. [3] Camacho, R. et al., in preparation

BP 48.3   Wed 17:00   Poster C
Fluorescence-Lifetime Imaging Microscopy of the Specific Uptake of Gold Nanoparticles into Cells — •Marina Mutas, Tim Hadler, Christian Strelow, Tobias Kipp, and Alf Mews — Institute of Physical Chemistry, University Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Small gold nanoparticles (AuNPs) with a thiol-functionalized surface show strong emission attributed to Au-S-hybrid states on the particle surface. AuNPs with a diameter of 2 nm functionalized with Mercaptoundecanoic acid (MUA-AuNPs) exhibit fluorescence lifetimes longer than 100 ns. In comparison, the autofluorescence of biological cells exhibit lifetimes of just a few ns. We use the different fluorescence lifetimes to investigate the specific uptake of these biofunctionalized MUA-AuNPs into cells by means of fluorescence-lifetime imaging microscopy (FLIM). We show that the biofunctionalized MUA-AuNPs specifically bind to their receptors on the cells' membrane. To distinguish between bound and uptaken MUA-AuNPs we are using cross-sectional FLIM scans of individual layers at different heights through the cells. With these scans we are able to image the whole cell with the bound/uptaken MUA-AuNPs based on their different lifetimes.

BP 48.4   Wed 17:00   Poster C
Probing the heterogeneity of cellular fluids — Olivia Stiehl, •Claudia Donth, and Matthias Weiss — Universität Bayreuth, Experimentalphysik 1

Cellular fluids, e.g. the cytoplasm, are crowded with macromolecules at concentrations up to 400g/l. Such crowded fluids may feature not only a considerable environmental heterogeneity on the scale of proteins but also diffusive transport on the mesoscale can be expected to exhibit remarkable spatiotemporal fluctuations.

To explore the heterogeneity of cellular and biomimetic fluids on the nano- and mesoscale, we have used fluoresecence lifetime imaging (FLIM), fluorescence correlation spectroscopy (FCS), and high-resolution imaging.

Imaging and FCS on mitotic cells suggests a significant heterogeneity of the contiguous nucleo-cytoplasmic fluid on length scales of some micrometers [1,2]. Our FCS results on interphase cells suggest that mesoscale heterogeneities in cytoplasm and nucleoplasm are comparable to those in highly concentrated solutions of established crowding agents such as dextran or PEG.

FLIM experiments on an environment-sensitive molecular rotor indicate a similar heterogeneity of cytoplasm and nucleoplasm on the nanoscale while artificial crowded fluids appear to be somewhat less heterogeneous.

[1] Pawar, Donth & Weiss, Curr. Biol. 24, 1905 (2014).
[2] Schweizer, Pawar, Weiss & Maiato, J. Cell Biol. 210, 695 (2015).

BP 48.5   Wed 17:00   Poster C
Optical setup and algorithms for a fast synchronized dual image acquisition — •Jonas Pfeil[1], Tobias Neckernuss[1], Christoph Koch[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Germany — [2]Department of Physics, Humboldt University Berlin, Germany

For thickness measurements and 3D reconstruction of microscope images, the most-common approach is using a z-stack of pictures. As this requires a sequential image acquisition of the sample with different focal heights, it is not feasible in time resolved experiments. Therefore we use two synchronized cameras to get a minimal z-stack at well defined time points. To image at two different focal heights, we split the light path with a beam splitter and mount the cameras at different distances from the objective. For adjustment and recording of the images it is necessary to develop a software which is able to capture two cameras at the same time.

The software for the camera control is written in Matlab and C++ for easy maintenance and high flexibility and extensibility. Only documented features of Matlab and only standard C++ methods are used to retain highest possible compatibility across different computation systems and versions. We demonstrate a live asynchronous picture display with two different cameras at the same time for alignment purposes and a blocking synchronous method for a short burst capturing of as many frames as possible.

BP 48.6   Wed 17:00   Poster C
Functionalization of Nanodiamond for the Use in Biophysics — •Frederike Erb[1], Patrick Paul[1], Fedor Jelezko[2], and Kay-E. Gottschalk[1] — [1]Institute of Experimental Physics, Ulm University, Germany — [2]Intstiute of Quantum Optics, Ulm University, Germany

Synthetic nanoparticles offer various new imaging and metrology approaches [3]. Of particular interest is the use of fluorescent nanodiamonds (FND) as markers for cell labeling. They contain negatively charged nitrogen-vacancy centers as fluorophores, whose emission lies in the near-infrared window of bioimaging and is dependent on the environment. Those nanodiamond markers are biocompatible and in contrast to dyes do neither blink nor bleach.

In order to prevent agglomeration and to offer specific binding the FNDs need to be functionalized [1], [2]. Here, we present preliminary results for our functionalization.

References: [1] Martin, R., Alvaro, M., Herance, J. R., Garcia, H. (2010). Fenton-treated functionalized diamond nanoparticles as gene delivery system. ACS Nano, 4(1), 65-74.
[2] Liang, Y., Ozawa, M., Krueger, A. (2009). A general procedure to functionalize agglomerating nanoparticles demonstrated on nanodiamond. ACS Nano, 3(8), 2288-2296.
[3] Chang, B. M., Lin, H. H., Su, L. J., Lin, W. D., Lin, R. J., Tzeng, Y. K., Lee, R. T., Yu, A. L., Chang, H. C. (2013). Highly fluorescent nanodiamonds protein-functionalized for cell labeling and targeting. Advanced Functional Materials, 23(46), 5737-5745.

BP 48.7   Wed 17:00   Poster C
Measurement of the height of living cells via an optimized phase-shifting interferometer. — •Shuaishuai Li[1], Xia Wang[2], and Othmar Marti[1] — [1]Institute for Experimental Physics, University of Ulm, 89069 Ulm, Germany — [2]School of Optoelectronics, Beijing Institute of Technology, 100081, China

Phase-Shifting Interference Microscopy is a real-time observation technique. It is widely used for observing the growth process of monolayer cells and has many advantages, such as high precision, non-contact measurement etc. According to the principle of phase-shifting interferometry measuring method, a dual-angle incident interferometer is designed in our lab. Using a CCD digital imaging device to record the vision field, we can get a serial of cell interference patterns with certain phase changes. Phase unwrapping is the step that we extract the phase of an interference pattern. Afterward, we could reductive the Wavefront Pattern which can reflect the microscopic appearance and calculate the height value of living cells. We synthesize the advantages of the branch-cut method and the quality guide method. Experimental results show that this fusion phase unwrapping method is effective and practical in the processing of cell interferograms.Finally, through the experiment setup we designed, we measured the height value of one Styrene particles, which had been accurately measured by ZYGO measure instrument. The relative error is 0.023.

BP 48.8   Wed 17:00   Poster C
Application of Rotational Dark-Field Microscopy in Biology — •Daniela Beck, Daniel Geiger, Tobias Neckernuss, and Othmar Marti — Institute of Experimental Physics, Ulm University

It has been published recently, that rayleigh's criterion can be beaten by total internal reflection dark-field imaging [1]. This is based on the incoherent summation of images that are obtained by coherent scattering at different angles of incidence. The original setup is altered in order to increase the maximum possible frame rate.

Our new measurement technique sets the path for high temporal and increased spatial resolution. This makes the observation of biological processes on the millisecond timescale with increased resolution compared to Abbe's limit feasible. Preliminary measurements on biological samples show the prospects of this measurement setup that is also capable of simultaneous fluorescence and bright-field imaging.
[1] P. von Olshausen and A. Rohrbach, Opt. Lett. 38, 4066-4069 (2013)

BP 48.9   Wed 17:00   Poster C
Experimental Setup for THz-Time-Domain-Spectroscopy on Complex Biological Samples — •Lisa Schneiderwind, Andreas Garz, Heiko Lokstein, and Maria Krikunova — Institut for Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin

The goal of this project is a free space setup for THz time-domain spectroscopy (THz-TDS) on samples containing water and biomolecules, for example molecules involved in the processes of photosynthesis. The generation and detection of the THz radiation to investigate such molecules is based on a photo-conductive antennae equipped with a focusing aspheric silicon lens. In this setup a femtosecond fiber laser is used to pump the antennae. With this configuration, it is possible to perform THz-TDS experiments by either measuring the amplitude of the THz-field at a fixed time-delay or fully characterizing the THz-field at all time delays. The setup can be further extended by replacing the detection antenna by electro-optical sampling. To produce THz radiation with higher field strength the generation antenna can also be replaced by non-linear crystals. The setup allows to perform time-resolved experiments to investigate the behavior of complex molecules after excitation.

BP 48.10   Wed 17:00   Poster C
Confocal Light-Sheet Microscopy: Separation of ballistic and diffusive fluorescence photons — •Tobias Meinert and Alexander Rohrbach — Laboratory for Bio-and Nano-Photonics, University of Freiburg, Germany

In the last ten years light-sheet microscopy has got more and more attention in biological research and is on its way to become the standard technology for long time observation of thick samples. However, the observation of strongly scattering objects suffers from strong imaging artefacts. In particular, the scattering of coherent illumination light generates strong image artifacts. Microscopy with Self-Reconstructing Beams (MISERB), such as Bessel beams, has proven to be a powerful tool to reduce scattering artifacts. By imaging 150 μm thick Arabidopsis root tips, these effects become well visible.

Reduced contrast due to strong side loops in the Bessel beam profile can be compensated effectively by confocal line detection. Independently of the illumination beam, a general source of reduced contrast is the scattering of fluorescent photons emitted from layers deep inside the object. This effect usually becomes very dominant at an imaging depth of a few 10 μm. In this presentation a so-called object point spread function (PSFobj) is introduced, which describes the blurring of images due to the object itself. By estimating this function, it is possible to separate the influence of ballistic (unscattered) and diffusive (multiply scattered) photons on the imaging process. Removing the influences of the diffusive photons, a so far unreached image quality in strongly scattering media is obtained.

BP 48.11   Wed 17:00   Poster C
Single Shot Quantitative Phase Microscopy Technique — •Tobias Neckernuss[1], Xiaoming Jiang[1,2], Jonas Pfeil[1], Christoph Koch[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Germany — [2]Department of Physics, Humboldt University Berlin, Germany

The thickness of adherent cells is an important parameter in various biological and biophysical applications. However it is a difficult task to measure cell thickness with a microscope when using conventional microscopy techniques. There are several commercial systems around, measuring the optical path length through the cell with an interferometric approach. However, most of these systems use a compact Mach-Zehnder interferometer which is difficult to customize for special needs and additional instrumentation. To overcome this, we designed a setup that allows us to measure the optical path length through a transparent phase object with an inline holographic approach. We use a two camera system with two slightly different focus points. The sample is illuminated by a LED light source with sufficient spatial coherence. For reconstruction of the phase image the "Transport of Intensity Equation" is used for a first guess and an iterative algorithm for phase retrieval refines the reconstruction by forward and backward propagation of the reconstructed images and comparison to the captured ones. With this method we are able to determine the phase shift during transmission through a phase object. The main advantage of this compared to conventional z-stack techniques is the potential for high acquisition speeds.

BP 48.12   Wed 17:00   Poster C

Rotational Dark-Field Microscope for Fast Image Acquisition
— •Daniel Geiger, Tobias Neckernuss, and Othmar Marti —
Institute of Experimental Physics, Ulm University

The technique to obtain label-free optical images beyond the diffraction limit has been published recently [1]. Incoherent addition of coherent scattering images illuminated from different directions leads to an increase in contrast between two adjacent objects. However, this original setup is, due to the implementation with a spatial light modulator, only able to take images at rates around 1 Hz.

We replaced the spatial light modulator with a rotating double prism setup that can rotate with much higher frequencies. Our setup is designed to operate at 100 Hz that is the maximum image capturing rate of the used camera. Furthermore the illumination angle can be dynamically adjusted between zero and maximum angle given by the used objective's NA by variation of the prism separation. In principle, this setup can be enhanced to rotation rates in the kHz regime by using a hollow shaft electromotor that contains the prisms. This allows the label-free observation of fast biological processes on a length scale that was so far not accessible by conventional light microscopy.

[1] P. von Olshausen and A. Rohrbach, Opt. Lett. 38, 4066-4069 (2013)

BP 48.13   Wed 17:00   Poster C
Light sheet microscopy using Bessel beams and the STED principle — •Luis Köbele, Cristian Gohn-Kreuz, and Alexander Rohrbach — University of Freiburg, Laboratory for Bio- and Nano-Photonics, 79110 Freiburg, Germany

Light sheet microscopy is an imaging technique which features enhanced optical sectioning by using a thin, sheet-like illumination of only that part of the object, which is in the plane of focus. By the use of computer-generated holograms, we generate self-reconstructing Bessel beams, which showed enhanced propagation stability and penetration depth in scattering media and are thus superior, particularly for imaging in dense biological specimen. However, the pronounced ring system, which facilitates the self-reconstructing property of the scanned Bessel beams, produces a significant image background by exciting out-of-focus fluorophores. By superposing a concentrically aligned, doughnut shaped Bessel beam, stimulated emission depletion (STED) is used to improve the light sheet quality, generating effectively thinner light sheets with reduced background. We present first results of such an imaging setup and discuss advantages and challenges.

BP 48.14   Wed 17:00   Poster C
Photothermal detection of single gold nanoparticles in living fibroblasts — •Alice Abend, Romy Schachoff, and Frank Cichos — Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

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. Our method to transfer nanoscopic objects into the cytoplasm of live mammalian cells is called mechanodelivery [1]. This approach is based on mechanical damage of the cell membrane to deliver nano objects into the intracellular space. In contrast to passive delivery strategies allows the mechanodelivery approach for deposition of nano objects without them being engulfed in vesicles. We deliver gold nanoparticles (AuNPs) to the cells 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 and metabolism processes.

[1] Nanoscale, 2014, 6, 4538

BP 48.15   Wed 17:00   Poster C
Combined AFM/SPR ellipsometry study of protein adsorption at liquid/solid interface — •Peter Basa[1], Peter Petrik[2], and Nils Anspach[1] — [1]Semilab Semiconductor Physics Laboratory Co. Ltd., Budapest, Hungary — [2]Institute for Technical Physics and Materials Science, Budapest, Hungary

The deeper understanding of interaction of biomaterials with solid surfaces is crucial in case of microfluidic devices applied to biosensorics. In this study, surfactant molecules mixed with protein species were adsorbed on gold nanofilm coated solid surfaces. Surface plasmon resonance (SPR) enhanced spectroscopic ellipsometry (SE) utilizing special adapted liquid cell, and atomic force microscopy (AFM) were used to study the adsorption dynamics, the resulting composition ratio of adsorbed species, and the biomolecule surface coverage depending on initial gold thin film surface structure/morphology.

In the poster, the performance of Semilab's combined SE and AFM measurement platform will be described using real experiment examples, with correlations pointed out in between different metrology results on the measured samples.

BP 48.16   Wed 17:00   Poster C
Time Modulated Stimulated Emission Depletion (STED) Based Fluorescence Correlation Spectroscopy (FCS) —
•Benedikt Prunsche[1], Peng Gao[1,2], Karin Nienhaus[1], and Gerd Ulrich Nienhaus[1,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [3]Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801, USA

Fluorescence correlation spectroscopy (FCS) is a powerful tool to study bio-molecular dynamics, such as protein diffusion or receptor-ligand interactions inside living cells. It is based on the correlation analysis of fluorescence intensity fluctuations in a small observation volume. These fluctuations arise due to Brownian motion of fluorescent particles in and out of the volume. Because of the diffraction-limited size of the focus volume, conventional FCS is only sensitive to fluorescence fluctuations induced by fluorophores at nanomolar concentrations, which is typically not realized in biological samples. To overcome this limitation, we have reduced the focal volume in all three dimensions by stimulated emission depletion. Background noise, which is inherent in conventional STED based FCS, has been reduced by time-gated detection, and further compensated by using an auxiliary Gaussian depletion beam. As a result, the dynamics of biomolecules at ~10-fold higher concentrations can be quantified with 3D STED based FCS.

BP 48.17   Wed 17:00   Poster C
Acto-myosin in cardiac muscle cells by scanning x-ray nanodiffraction — •Jan-David Nicolas, Marten Bernhard, and Tim Salditt — Institut für Röntgenphysik, Göttingen, Deutschland

Owing to the highly oriented molecular structure of the actin-myosin cortex in muscle cells, diffraction techniques are well-suited to study the geometry of this filament assembly down to nanometer resolution. In particular, classical x-ray diffraction studies on muscular tissue were the first to unravel the detailled structure of the sarcomere. In these experiments, however, structural information is averaged over macroscopically large volumes of the tissue, with diffraction volumes containing a vast ensemble of muscle cells. Contrarily, recent progress in x-ray optics has enabled diffraction experiments with spot sizes in the sub-micron range, well-suited to illuminate only selected organelles of a single cell.

We report on recent experiments analyzing the micro-structure of acto-myosin complexes in individual cardiomyocytes which make up the striated muscular tissue of the heart. We performed experiments on (initially) alive, chemically fixed as well as freeze-dried cell preparations. Scanning the sample through the nano-focused beam, SAXS data were recorded and analysed to generate mappings of different structural parameters. Scanning SAXS mappings are complemented by holographic reconstructions, extending the covered frequency range by two orders of magnitude. By means of x-ray holography, samples could also be immediately checked for radiation damage.

BP 48.18   Wed 17:00   Poster C
Photothermal Excitation for Reliable and Quantitative High-resolution AFM imaging and force spectroscopy — •Florian Johann, Aleksander Labuda, Deron Walters, Maarten Rudgers, Jason Cleveland, and Roger Proksch — Asylum Research, an Oxford Instruments Company, Wiesbaden, Germany

Photothermal excitation is an alternative method for exciting a cantilever by heating/cooling the base of the cantilever to drive the cantilever. Photothermal excitation results in repeatable, accurate and time-stable cantilever tunes. Therefore, the setpoint remains truly

constant while imaging, preventing tip crashes, or unwanted tip retractions. True atomic resolution images of calcite in water were made for hours with no user intervention, testifying to the stability of photothermal excitation. Unlike other specialized drive methods, photothermal excitation is compatible with almost any cantilever and with all AFM techniques. Furthermore, because the photothermal tune represents the true cantilever transfer function, existing AFM theories can be applied to accurately recover conservative and dissipative forces between the tip and the sample. This is especially important for force spectroscopy, dissipation studies, as well as the frequency modulation AFM techniques.

BP 48.19   Wed 17:00   Poster C

Signatures of correlated noise and disorder in 2D electronic spectroscopy — ●David J. Ing[1,2], James Lim[2], Jan Jeske[1], Jared H. Cole[1], Susana F. Huelga[2], and Martin B. Plenio[2] — [1]Chemical and Quantum Physics, School of Applied Sciences, RMIT University, Melbourne, Victoria 3001, Australia — [2]Institut für Theoretische Physik, Albert-Einstein-Allee 11, Universität Ulm, D-89069 Ulm, Germany

Two-dimensional electronic spectroscopy has revealed the presence of long-lived quantum coherences in photosynthetic systems. To explain the microscopic origin of the long-lived coherences in these biological systems, several hypotheses have been formulated theoretically, including correlated noise and vibronic coupling. However the complexity of photosynthetic systems and their 2D spectra make the identification of the microscopic origin a challenging task. Here, we investigate a correlated noise model to study how the correlations in noise and disorder affect the features in 2D spectra. By employing the Bloch-Redfield equation, where the degree of spatial correlation can be quantified continuously, we show that the amount of correlation affects both the lineshapes and lifetimes of oscillatory 2D signals. We also show how non-secular effects in the noise, that yield to coupling between populations and coherences, influence the 2D signals.

BP 48.20   Wed 17:00   Poster C

Nonlinear optical properties and photochemical polymerization of monomer crystals — ●Oktay Aktas[1], Max Jonathan Kory[2], Carsten Becher[1], Arnulf Dieter Schlüter[2], and Manfred Fiebig[1] — [1]The Laboratory for Multifunctional Ferroic Materials, Department of Materials, ETH Zurich, Switzerland — [2]Polymer Chemistry, Department of Materials, ETH Zurich, Switzerland

Organic materials have been used in a variety of applications for a century. With the advances in their synthesis, their potential applications are also rapidly increasing. In recent years there has been a growing interest in organic crystals for applications in electronics and photonics since some of them exhibit large optical nonlinearities. To possibly find such functional optical properties, we performed second harmonic generation spectroscopy on a polar and chiral monomer crystal, which can be polymerized by a photochemical reaction and confined to two dimensions (2D polymer) [1]. Measurements performed with 10 ns pulses have revealed that the monomer is strongly nonlinear in a large spectral range. In addition, the light-induced polymerization of monomers leads to differences in SHG intensities. As the depolymerization of polymer crystals can be achieved through heating, the monomer and polymer represent two switchable states with different nonlinear optical properties, which may find applications in integrated optics. [1] Max J. Kory, Michael Wöle, Thomas Weber, Payam Payamyar, Stan W. van de Poll, Julia Dshemuchadse, Nils Trapp and A. Dieter Schlüter, Nat. Chem. 6, 779 (2014)

BP 49: Posters - Cell Mechanics and Migration & Physics of Cancer

Time: Wednesday 17:00–19:00   Location: Poster C

BP 49.1   Wed 17:00   Poster C

Investigation of Mechanical Properties of the Cytoskeleton Using FEM Simulations — ●Ralf Schuster, Tobias Neckernuss, Tobias Paust, Kay Gottschalk, and Othmar Marti — Institute of Experimental Physics, Ulm University, D-89081 Ulm

We show the implementation of structure-bearing parameters in a numerical finite element model of a cell. The point of interest is the interplay between intermediate filament network and mechanical properties. The cytoskeleton is 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. Metastasizing cells can have a softer cytoskeleton through changes in the network. This leads to a reduced resistance against forces.

There are numerical models, concerning cell deformation, but they are either considering the cytoplasm as a continuum, or limit the simulations to microtubules and actin filaments. In contrast we have a closer look at the behavior of intermediate filaments and we implement a 3D-model of the cell, with the intermediate filament network as main component, regarding force transmission and stiffness, to simulate laboratory experiments. Therefore displacements of beads captured in the filament network, caused by an applied force, are simulated and compared to experimental microrheology data. The geometry, material parameters and boundary conditions are varied to find a model reflecting the real behavior of the inside of a cell in an acceptable manner.

BP 49.2   Wed 17:00   Poster C

Force Generation of Blood Platelets — ●Jana Hanke and Sarah Köster — Universität Göttingen, Göttingen, Deutschland

Blood platelets play a crucial role in wound closure by attaching to the wounded site and spreading over it to form a temporary seal. During this process, the platelets contract after attachment to the extracellular matrix. Given the heterogeneity of tissues in the body, platelets encounter areas of varying stiffness to which they must adapt. To examine the influence of these environments on the force generated by the platelets, we perform live cell experiments on soft and stiff substrates. We use time-resolved Traction Force Microscopy (TFM) by seeding the cells on polyacrylamide gels of varying physiological stiffness containing fluorescent beads. Given the small size of blood platelets compared to other cells previously studied by TFM, it is important to adjust the experimental set-up as well as the analysis procedures. Here, the evaluation process is performed by a combination of Particle Image Velocimetry (PIV), Lagrangian marker tracking and Fourier Transform Traction Cytometry (FTTC). So far, the manner of contraction leads us to observe three contraction behaviours: One group of platelets show one single contraction towards a maximum force plateau, another group contracts before relaxing again whereas the last group shows oscillations of contraction. A relaxation is mostly observed in gels of lower stiffness while platelets on stiffer gels tend towards a force plateau. Platelets exerting oscillatory forces could so far be observed on various gel stiffness.

BP 49.3   Wed 17:00   Poster C

Phagosomes of different size show qualitatively different transport characteristics — ●Steve Keller, Konrad Berghoff, and Holger Kress — Department of Physics, University of Bayreuth, Germany

Phagocytosis is one of the key processes of the mammalian immune system. The uptake of pathogens is typically followed by a transport of the phagosomes towards the perinuclear region as part of their maturation process. This process shows high phagosome-to-phagosome variations that are not fully understood. We hypothesize that the phagosome size has an influence on the maturation process by directly influencing the transport characteristics. We test this hypothesis by tracking the transport of phagosomes with different diameters ranging from 1 μm to 3 μm inside macrophages. We show that larger phagosomes are transported more persistently towards the nucleus and that they exhibit less backwards motion. We furthermore found that the effective transport velocity towards the nucleus increases with the phagosome size despite nearly equal instantaneous velocities for the different sizes. In addition, we investigated the microtubule density distribution in macrophages. We found that density differences between the nucleus-facing side of phagosomes and the opposite side can explain part of the observed transport characteristics. Our findings suggest that a simple size-dependent cellular sorting mechanism might exist that supports inward transport of large phagocytosed bacteria for facilitating their digestion and that simultaneously supports outward transport of small bacterial fragments for example for antigen presentation.

BP 49.4   Wed 17:00   Poster C

Fibroblast mechanics: a story of history — •Mathias Sander and Albrecht Ott — Universität des Saarlandes, Saarbrücken, Germany

Cell mechanics is a key player in development, disease and many other biological processes. Living cells exhibit a complex nonlinear response to mechanical cues, which is not understood yet. A stiffening as well as softening is observed, depending on the stimulus and the experimental technique. Here, we apply large amplitude oscillatory shear (LAOS) to a monolayer of fibroblast cells using the cell monolayer rheology technique. We find that the nonlinear cell response not only depends on the amplitude and the frequency of oscillations. Moreover, it is highly susceptible to a mechanical preconditioning. Cell response can exhibit hallmarks of nonlinear viscoelasticity, elastoplastic kinematic hardening or inelastic fluidization for the same steady state oscillations. Experimental results indicate that a preconditioning changes cytoskeletal network structure in a rate dependent way. Network alterations can be driven by passive filament reorganisations, filament rupture and the binding/unbinding of crosslinking proteins. We speculate that the pronounced strain path dependence of nonlinear cell response might obscure the underlying universality of nonlinear cell mechanics on a molecular/microscopic scale. Our results highlight the interplay between viscoelastic and inelastic contributions to the cell mechanical response.

BP 49.5   Wed 17:00   Poster C
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

The importance of cell mechanics on different physiological or pathophysiological conditions like stem cell differentiation [1] or cancer [2] is increasingly being recognized. Hence the knowledge of the mechanical properties of cells under varying conditions is crucial for understanding the underlying mechano-chemical feedback cycles. Importantly, the effect of strain on cell mechanics is of great relevance for a variety of cell types like endothelial cells in the lung, in arteries or on the bladder, but is not well understood on the cellular and subcellular level. For the detailed analysis of the cellular mechano-response to stretch, we present here a self developed cell stretching device combined with an atomic force microscope.

[1] Engler, A. J., Sen, S., Sweeney, H. L., and Discher, D. E. (2006). Matrix Elasticity Directs Stem Cell Lineage Specification. Cell, 126(4), 677-689.
[2] Suresh, S., Spatz, J., Mills, J. P., Micoulet, A., Dao, M., Lim, C. T., Seufferlein, T. (2005). Connections between single-cell biomechanics and human disease states: gastrointestinal cancer and malaria. Acta Biomaterialia, 1(1), 15-30.

BP 49.6   Wed 17:00   Poster C
Measuring cell clasticity in PXE- and TMEM43-cells using an Optical Stretcher — •Daniel Helling[1], Jialiang Yu[1], Roland Stange[4], Jennifer Petersmeyer[2], Bettina Ibold[3], Doris Hendig[3], Volker Walhorn[1], Hendrik Milting[2], and Dario Anselmetti[1] — [1]Experimental Biophysics & Applied Nanoscience, Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [2]Herz- und Diabeteszentrum Nordrhein-Westfalen (HDZ NRW) - Universitätsklinikum der Ruhr-Universität Bochum, Erich und Hanna Klessmann-Institut für Kardiovaskuläre Forschung und Entwicklung, 32545 Bad Oeynhausen, Germany — [3]Herz- und Diabeteszentrum Nordrhein-Westfalen (HDZ NRW) - Universitätsklinikum der Ruhr-Universität Bochum, Institut für Laboratoriums- und Transfusionsmedizin, 32545 Bad Oeynhausen, Germany — [4]RS Zelltechnik GmbH, 04103 Leipzig, Germany

We compared the cellular elasticity of fibroblasts provided by patients suffering from PXE (Pseudoxanthoma elasticum) and ARVC (Arrhythmogenic right ventricular cardiomyopathy), respectively. We used an optical stretcher setup with edge detection and automated data analysis, which allows for high cell throughput experiments (>1000 cells per measurement, setup provided by RS Zelltechnik GmbH, Leipzig, Germany). The differences in cell elasticity will be discussed in detail and related to the pathological findings.

BP 49.7   Wed 17:00   Poster C
Mechano-sensitivity is cell type specific — •Galina Kudryasheva and Florian Rehfeldt — Georg-August-Universität Göttingen Fakultät für Physik III. Physikalisches Institut

Nowadays it is widely acknowledged that cellular function, morphology and fate are dependent on the mechanical properties of their microenvironment. Human mesenchymal stem cells (hMSCs) are a striking example that stem cell differentiation into various cell types can be guided by tuning the extracellular matrix stiffness. 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 modeled using classical mechanics with an active spring model. We use this approach to analyze the mechanical cell-matrix interactions of hMSCs and several types of differentiated cells, such as C2C12 myoblasts , SAOS-2 osteoblasts, human primary osteoblasts and 3T3 fibroblasts. We plate hMSCs and differentiated cells on elastic poly-acrylamide hydrogels covering the whole physiological range of stiffness given by Young's moduli E from 1 to 130 kPa. Applying immunofluorescence approach we label stress fibers and analyze cytoskeletal morphology by fluorescence microscopy. We analyze cell shape and extract corresponding material constants that show distinct differences during the differentiation process in different cell types. Our experiments showed that cellular susceptibility to the substrate elasticity is highly cell type specific.

BP 49.8   Wed 17:00   Poster C
Mechanical properties of young and senescence dermal fibroblast cells using passive microrheology. — •Samira Khalaji[1], Fenneke KleinJan[1], Eugenia Makrantonaki[2], Vida Farsam[2], Ulla Nolte[1], Karin Scharffetter-Kochanek[2], and Kay-E Gottschalk[1] — [1]Institut für Experimentelle Physik, Universität Ulm — [2]Klinik für Dermatologie und Allergologie, Universitätsklinikum Ulm

Biological aging is a multi-dimensional process that takes place over a whole range of scales from the nanoscopic alterations within cells, over transformations in tissues and oragans. On the single cell level, aging involves in gene mutations, altered gene expression and post translational modifications of proteins. A variety of proteins are affected, including proteins of the cell cytoskeleton. Previous work quantified the gene and protein expression of cytoskeleton proteins in senescent and young fibroblasts. Their results show that senescent skin fibroblasts have an upregulated expression of the intermediate filament (IF) protein vimentin in contrast to actin and tubulin which are downregulated. IFs play an important role in providing mechanical stability of cells. However the mechanical properties of IFs depending on cellular senescence or age of the donor has not been studied so far. Hence, we employed passive microrheology on young and senescence human dermal fibroblasts from donors with different age and different population doubling level. In contrast to the expectations, our primary results show no significant differences in the viscoelastic properties of fibroblasts depending on age of the donor or cellular replicative senescence.

BP 49.9   Wed 17:00   Poster C
Transport of micro-objects by amoeboid cells — •Manuel Frey, Oliver Nagel, Matthias Gerhardt, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

The transport and positioning of micron-sized objects in complex geometries is often accomplished by fluid flow. However, under geometric constrains, like dead end structures, this is difficult to achieve. An alternative approach would be the use of magnetic or optical tweezers. Yet these techniques require a lot of time to rearrange many objects, since it has to be done one by one. Here, we propose a novel approach to move micron-sized objects in confined geometries, exploiting the chemotactic behavior of single cells. We use cells of the social amoeba Dictyostelium discoideum to transport objects of different sizes and shapes. Both chemotactic movement in artificial gradients as well as the endogenous aggregation of this microorganism can be exploited to achieve different transport tasks. In particular, cells may act individually on small particles but they can also transport larger objects in a collective effort.

BP 49.10   Wed 17:00   Poster C
Mechanical coupling between the cytoskeleton and the nucleus — •Gabriele Straass and Florian Rehfeldt — Third Physical Institute - Biophysics, Georg-August University, Göttingen

It is nowadays widely acknowledged that mechanical cues are as important for cellular behavior as traditional biochemical ones. Strikingly, adult stem cells can be guided to differentiate towards various cell types when cultured on elastic hydrogels with appropriate Young's modulus E. Here, the acto-myosin cytoskeleton organization shows significant

differences within the first 24 hours after plating. We investigate the mechanical properties of the nucleus by atomic force microscopy and fluorescence microscopy and demonstrate the impact of substrate elasticity E on nuclear morphology and elasticity via acto-myosin stress fibers and other cytoskeletal filaments. Elucidating the mechanical coupling of the cytoskeleton and the nucleus might reveal a direct mechanical pathway that alters gene transcription and might impact adult stem cell differentiation.

BP 49.11   Wed 17:00   Poster C

Cell adhesion and cell sorting across the EMT —
•Steve Pawlizak[1], Anatol Fritsch[1], Steffen Grosser[1], Linda Oswald[1], Dave Ahrens[1], Tobias Thalheim[1], M. Lisa Manning[2], and Josef A. Käs[1] — [1]University of Leipzig, Institute of Experimental Physics I, 04103 Leipzig, Germany — [2]Syracuse University, Department of Physics, Syracuse, NY 13244, USA

The spatial segregation of different cell populations in distinct compartments and the formation of well-defined lineage boundaries in-between is a fundamental process during the embryonic development. While normal cells will, in general, never cross these boundaries, metastatic cancer cells undergoing an epithelial-mesenchymal transition (EMT) may eventually acquire the ability to do so. To evaluate the role of cell cohesion in cell sorting and compartmentalization across the EMT, we analyze the mechanical properties of three cell lines exhibiting a shift in cadherin levels characteristic of an EMT. We apply a diverse set of methods to measure cell-cell adhesiveness, cell stiffness, and cell shapes, and compare the results to predictions from cell sorting in mixtures of the cell types. Although the final sorted state is extremely robust among all three cell lines, suggesting that cell sorting may play an important role in organization and boundary formation in tumors, we surprisingly find that the differential adhesion hypothesis (DAH) does not correctly predict the final sorted state. This indicates that these tissues do not behave like immiscible fluids, and that dynamical effects such as directional motility, friction, and jamming may play a much more important role than previously expected.

BP 49.12   Wed 17:00   Poster C

Mechanical properties of non-adhering cells — •Samaneh
Rezvani[1], Tod M. Squires[2], and Christoph F. Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität, Göttingen, Germany — [2]Department of Chemical Engineering, University of California, Santa Barbara, USA

Cells sense their micro-environment through biochemical and mechanical interactions. They can respond to stimuli by undergoing shape- and possibly volume changes. Key components in determining the mechanical response of a cell are the viscoelastic properties of the actomyosin cortex, effective surface tension, and the osmotic pressure. We use custom-designed microfluidic chambers with integrated hydrogel micro windows to be able to rapidly change solution conditions for cells without any hydrodynamic flow. We use biochemical inhibitors and different osmolytes and investigate the immediate response of individual cells. Using a dual optical trap makes it possible to probe suspended rounded-up cells by active and passive microrheology to quantify the response to the various stimuli.

BP 49.13   Wed 17:00   Poster C

Regulation of muscle contraction by Drebrin-like protein 1 probed by atomic force microscopy — •Renata Garces, Eu-
genia Butkevich, Mitja Platen, and Christoph F. Schmidt — Third Institute of Physics-Biophysics, Georg August University, 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 coordinated force generation in striated muscles.

Recently, we have identified a C. elegans drebrin-like protein 1 (DBN-1) as a novel sarcomere component, which stabilizes actin filaments during muscle contraction. To further characterize the function of DBN-1 in muscle cells, we generated a new dbn-1 loss-of-function allele. Absence of DBN-1 resulted in a unique worm movement phenotype, characterized by hyper-bending.

It is not clear yet if DBN-1 acts to enhance or reduce the capacity for contraction. We present here an experimental mechanical study on C. elegans muscle mechanics. We measured the stiffness of the worm by indenting living C. elegans with a micron-sized sphere adhered to the cantilever of an atomic force microscope (AFM). Modeling the worm as a pressurized elastic shell allows us to monitor the axial tension in the muscle through the measured stiffness. We compared responses of wild-type and mutant C. elegans in which DBN-1 is not expressed.

BP 49.14   Wed 17:00   Poster C

Macrophages are sensitive to substrate elasticity during Fcγ receptor-mediated phagocytosis — •Wolfgang Gross,
Kathrin Weidner-Hertrampf, and Holger Kress — Department of Physics, University of Bayreuth, Germany

Phagocytosis, the internalization of micrometer-sized objects like bacteria and dead cells by macrophages is a main function of the innate immune system. After the detection of foreign particles by membrane receptors, this process is driven by the reorganization of the actin cytoskeleton, which leads to a protrusion of the membrane around the target. Although many molecular players have been identified in the past, there is still little known about the mechanics of this process and in particular about the role of the mechanical cellular environment.

In this work we investigate the influence of the underlying substrate rigidity on uptake efficiency. We cultured murine J774 macrophages on PDMS-substrates with elastic moduli ranging from 1.5 to 28kPa. The uptake efficiency of IgG-coated microparticles was quantified with secondary antibody staining. We found that the uptake efficiency depends on the rigidity of the substrate. Furthermore, we observed that cells were able to adapt to the various substrate stiffnesses and showed comparable uptake efficiencies after several weeks of adaptation. Our results support the hypothesis that phagocytosis is a mechanosensitive process. In addition, our results might contribute to understand the complex interplay between the immune system and disease states that come along with changes in tissue rigidity such as cancer, atherosclerosis and fibrotic tuberculosis.

BP 49.15   Wed 17:00   Poster C

Non-equilibrium mechanics of suspended cells probed by dual optical traps — •Florian Schlosser, Christoph F. Schmidt, and
Florian Rehfeldt — Drittes Physikalisches Institut - Biophysik, Georg-August Universität Göttingen

Cells sense and respond to their mechanical environment. Besides their well characterized biochemical interactions, they also communicate through mechanical interactions. They actively probe the mechanical properties of their surroundings with contractile forces. Key player in the generation of those forces is the actomyosin cytoskeleton.

We use a dual optical trap to suspend cells between two fibronectin-coated polystyrene beads. Analyzing the correlated motion of the beads allows us to dissect the non-equilibrium fluctuations that the cell generates. By applying oscillatory forces, we are able to simultaneously probe the viscoelastic properties of the cell. Using a force-feedback allows us to apply constant forces to a cell and monitor its response. With biochemical perturbation experiments using blebbistatin and nocodazole to interfere with the actomyosin cytoskeleton or microtubules we show that myosin motors are the key element for contractile force generation. We combine our optical trap with a confocal microscope to directly image LifeAct and non-muscle Myosin-II transfected cells to monitor the distribution of the actomyosin cortex during the trapping experiments.

BP 49.16   Wed 17:00   Poster C

Mechanically tunable biomimetic hyaluronic acid based hydrogels — Frederike Derksen, Gevin von Witte, and •Florian
Rehfeldt — Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany

Mechanical properties of the microenvironment of cells, e.g. matrix elasticity, influence many aspects of cell behavior including morphology, motility and even more complex processes such as differentiation. Therefore, it is important to design and characterize hydrogels for cell culture that resemble the in vivo environment of cells.

Cross-linked hyaluronic acid (HA) matrices offer an alternative to conventionally used polyacrylamide hydrogels as HA is biocompatible and therefore not toxic for cells. Using different thiol modifications of HA, we prepare hydrogels with a well-defined elasticity in the physiologically relevant range of E = 0.1 kPa to 100 kPa, which is much softer than glass or tissue culture plastic. Coatings with RGD peptide allow cell adhesion leaving hydrogel mechanics independently tunable. Hybrid gels with thiol modified recombinant human gelatin enable the preparation of 3D culture environments by embedding cells during hydrogel polymerization. Gelation kinetics of the hydrogels were investigated by rheology using oscillatory deformation tests. Both the storage modulus G' as well as the loss modulus G" were measured in order to analyze the viscoelastic properties of the cross-linked hydrogels. The

morphological and cytoskeletal responses of human mesenchymal stem cells (hMSCs) to different elasticities and hydrogel compositions were investigated both in 2D and 3D cultures.

BP 49.17   Wed 17:00   Poster C

Controlling and multiscale modelling of contractility in adherent cells — •Dimitri Probst[1], Christoph A. Brand[1], Marco Linke[1], Patrick W. Oakes[2], Elizabeth Wagner[3], Michael Glotzer[3], Margaret L. Gardel[2], and Ulrich S. Schwarz[1] — [1]Institute for Theoretical Physics and BioQuant, Heidelberg University, Heidelberg, Germany — [2]Institute for Biophysical Dynamics, James Franck Institute and the Department of Physics, University of Chicago, Chicago, USA — [3]Department of Molecular Genetics and Cell Biology, University of Chicago, Chicago, USA

Cell contractility is coordinated inside the cell mainly by the spatial regulation of RhoA activity, a protein which in its active form is known to promote both growth of actin filaments and their contraction through myosin II molecular motors. For adherent cells, this usually leads to the formation of so-called stress fibers, which are condensed bundles of actin filaments contracted by myosin II minifilaments. In order to attain a theoretical understanding of the cytoskeletal reorganization during phases of RhoA-activity, we have developed a discrete viscoelastic cable network model which can well reproduce the spatiotemporal properties of the actomyosin system. We show how the addition of stress fibers, represented as additional elastic links in the network, changes the overall behaviour of the simulated cytoskeleton from Maxwell-type to Kelvin-Voigt-type. We show that, by means of discrete homogenization, the parameters of the discrete cytoskeleton model can be directly mapped to the macroscopic quantities of a viscoelastic continuum model.

BP 49.18   Wed 17:00   Poster C

Contractility of human induced pluripotent stem cell-derived cardiomyocytes on micropatterned substrates of different stiffnesses — •Til Driehorst[1,2], Malte Tiburcy[2], Wolfram Hubertus Zimmermann[2], and Christoph Friedrich Schmidt[1] — [1]Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen — [2]Institut für Pharmakologie und Toxikologie, Universitätsmedizin Göttingen, Göttingen

Human induced pluripotent stem cells can be differentiated into cardiomyocytes (hiPSC-CM). This method can be used for high-throughput generation of cardiomyocytes for basic research. hiPSC-CM also hold great promise for in-vitro pharmacologic testing and studies of different illnesses such as arrhythmias. However, these cells remain in a somewhat immature, embryo-like state. This lack of maturity is thought to be partly due to missing biochemical and physical stimuli in currently used culture formats. Here, we have studied the basic sarcomeric contractility of hiPSC-CM in order to gain insight into the behavior of isolated CMs, and to also understand the intercellular mechanical coupling between myocytes. We applied methods of microcontact printing to shape the CMs to physiological aspect ratios (~7:1) on elastic substrates of various stiffnesses. We then transfected the cells with an ACTN2-Citrine construct to visualize the z-bands in the living mycoytes. Exploiting high-speed confocal microscopy, we recorded the sarcomeric motion of hiPSC-CM at high frame rates and applied statistical algorithms to characterize this motion and investigate the coupling between cells in close proximity.

BP 49.19   Wed 17:00   Poster C

Cell motility generated by actin polymerization waves — •Nicolas Ecker and Karsten Kruse — Theoretical Physics, Saarland University, PO Box 151150, 66041 Saarbruecken, Germany

A cell's ability to move is one of its greatest merits. It enables the cell to efficiently search for nutrients and drives complex processes in tissues.

Cell motility is often driven by the actin cytoskeleton. Although many important factors involved in actin-driven cell crawling have been identified and characterized in amazing detail, it is still poorly understood how the actin filament network is organized in this process. Spontaneous actin waves have been observed in a large number of different cell types. They present an attractive concept to understand actin-network organization during crawling. We introduce a mean-field description for actin assembly by nucleating promoting factors, negative feedback of actin filaments on the nucleators' activity, and active stress generation by molecular motors. The system can spontaneously generate traveling waves. We study confinement of this system to a cellular domain by means of a phase field and calculate the corresponding phase diagram. In particular, we find erratic motion due to the formation of spiral waves.

BP 49.20   Wed 17:00   Poster C

Investigations on Single Squamous Cell Carcinoma Cells — •Susanne Steeger[1], Julia Kristin[2], Marcel Glaas[2], Jörg Schipper[2], and Mathias Getzlaff[1] — [1]Heinrich-Heine-Universität Düsseldorf, Deutschland — [2]Univ.-HNO-Klinik Düsseldorf, Deutschland

In this contribution we report on measurements of the mechanoelastic properties of ENT squamous cell carcinoma cells. The study of these single cancer cells in culture medium is carried out by Atomic Force Microscopy. Our main interest is the determination oft the Youngs Modulus calculated by the Hertzian Model. We identify the elasticity of cancer cells in order to compare it with that of similar benign cells. Because Live Cell Imaging is a challenging task we first focus on testing different cantilevers and various strategies to treat the cells carefully. Just recently we apply our new AFM with QI-Mode (JPK NanoWizard 3) which allows for a more detailed investigation of living cells. In order to determine the individual properties of the cancer cells we additionally analyse their cytoskeleton (actin and tubulin) by using a confocal fluorescence microscope. Cancer cells are known for their modified cytosekelton which is reflected in the different elasticities of both cancer and comparable benign cells.

BP 49.21   Wed 17:00   Poster C

Corellation of Adhesive and Viscoelastic Tumor Markers — •Erik W. Morawetz[1], Lars Christian Horn[2], Michael Höckel[3], and Josef A. Käs[1] — [1]Universität Leipzig, Physik der weichen Materie, Fakultät für Physik und Geowissenschaften, Leipzig, Deutschland — [2]Universitätsklinikum Leipzig, Institut für Pathologie, Leipzig, Deutschland — [3]Universitätsklinikum Leipzig, Klinik für Frauenheilkunde, Leipzig, Deutschland

Compartmentalization is a developmental process, functioning independently from the generation of organ structures. Metastasizing cancer cells are able to pass organ boundaries, but seem to be restricted by compartmental ones, as impressively shown by the success of the Leipzig School of Radical Pelvic Surgery. A transition to different cellular phenotypes is necessary to surpass compartment boundaries, including changes in protein expression, e.g. levels of the Cadherin (Cad) family of adhesion molecules, as well as altered physical properties of the cell body. Cancer cells become softer, providing possibilities for migration and cellular streaming and Cad expression is shifted from E- to P- and N-Cad, what is linked to the epithelial-mesenchymal transition. We conduct clinical studies to directly correlate this two fundamental markers. By the means of optical rheology, coupled with fluorescence microscopy, we are able to link E-Cad levels to viscoelastic properties in the case of tumor samples. Control experiments show no correlations, hinting at the basic change in developmental levels of cancer cells. This interplay of tumor markers in combination with theoretical models may shed new light on mechanisms and development of cancer.

BP 50: Posters - Cell Adhesion

Time: Wednesday 17:00–19:00   Location: Poster C

BP 50.1   Wed 17:00   Poster C

Adhesion of oral bacteria to titanium surfaces of different roughness measured by single-cell force spectroscopy — •Kordula Schellnhuber, Christian Spengler, Nicolas Thewes, and Karin Jacobs — Department of Experimental Physics, Saarland

University, 66041 Saarbrücken

Bacteria adhere to virtually all surfaces and promote the formation of biofilms. In the oral cavity, these initial biofilms may lead to plaque and consequently to severe health problems. Therefore, understanding and controlling the process of bacterial adhesion to oral implants is of

great importance for material science and medicine. A common material for dental prostheses is titanium due to its robustness and high biocompatibility with various tissues. We use single-cell force spectroscopy to study the adhesion of Streptococcus mutans to titanium surfaces of different roughness. In addition, we compare the bacterial adhesion to titanium with the adhesion to very smooth samples of hydroxyapatite, the mineral component of teeth. Furthermore, we investigate the adhesion of Streptococcus mutans to real oral biofilms of different ages.

BP 50.2   Wed 17:00   Poster C

Single cell force spectroscopy and initial cell adhesion — ●Hendrik Brehme, Philipp Wysotzki, Marco Stubbe und Jan Gimsa — Universität Rostock, Lehrstuhl für Biophysik, Gertrudenstraße 11a, D-18057 Rostock, Deutschland

For medical implants, there is a general risk for so-called "implant-associated infections". The starting point for a possible infection is the "race for the surface", in which bacteria and body cells compete in making initial contacts to the implant's surface. Bacteria which may successfully colonize the surface tend to form biofilms, which can hardly be fought by the immune system of the patient. In the experiments, the individual behavior of single cells during their initial adhesion was investigated using single cell force spectroscopy. For this, cells of the bone cell line MC3T3 or bacteria were attached to the cantilever and their initial adhesion behavior to different surfaces was measured using a NanoWizard II atomic force microscope (JPK, Berlin).

The setpoint and adhesion forces were correlated with the electric impedance of a microelectrode structure for single cell detection (single cell-interdigitating electrode structure; SC-IDES).

BP 50.3   Wed 17:00   Poster C

Substrate elasticity and ligand affinity affect traction force evolution — ●Christina Müller and Tilo Pompe — Institute of Biochemistry, Universität Leipzig, Germany

Mechanotransduction is known as one control mechanism for several basic cell functions, like proliferation, differentiation and cell death. We investigated early cell adhesion on hydrogels with an independent variation of substrate stiffness and affinity of the adhesion ligand fibronectin to the hydrogel surface. Thin film coatings of maleic acid copolymers on top of polyacrylamide hydrogel layers were fabricated to tune protein binding. The Young's modulus of the hydrogel was modulated between 2.5 kPa and 9 kPa. Human umbilical vein endothelial cells were monitored during the first two hours of cell adhesion by time-resolved cell traction force microscopy. Three different regimes of traction force generation were found. In the first regime (R0) cells spread fast, but traction forces were negligibly small. Regime R1 is characterized by a decelerated spreading and a succeeding force increase. After completion of spreading cells enter regime R2 with saturated forces. Substrate stiffness ligand and affinity were both found to affect the kinetics and absolute levels of traction force quantities. A faster increase and a higher saturation level of traction forces were observed for a higher substrate stiffness and a higher ligand affinity. The results show that cells perform varying proportions of work against conservative and dissipative forces. Finally, our findings complement recent modeling approaches and contribute to a better understanding of the dynamics of cell adhesion on viscoelastic substrates.

BP 50.4   Wed 17:00   Poster C

Size, kinetics and free energy of clusters formed by ultra-weak bonds between glycolipids — ●Hannes Witt[1], Marieelen Oelkers[1], Filip Savic[1], Shahid I. Awan[2], Daniel B. Werz[2], Burkhard Geil[2], and Andreas Janshoff[2] — [1]Georg-August-Universität Göttingen — [2]Technische Universität Braunschweig

Many biological processes, like cell motility or immunological recognition, rely on transient binding, which demands the use of weak, non-covalent bonds with fast binding and unbinding kinetics, characteristics ideally met by carbohydrate-carbohydrate-interactions (CCI). Here we employ atomic force microscopy (AFM) to study the trans-interaction of the trisaccharide Lewis X bound to a fluid lipid membrane. We show how even this ultra-weak interaction leads to the formation of binding clusters resulting in biologically relevant adhesion forces and describe this process with a simple diffusion-reaction-scheme, which allows us to access the bond number, reaction kinetics and free binding energies.

BP 50.5   Wed 17:00   Poster C

Dynamics of actin stress fiber patterns in laterally constrained cells — ●Andreas Müller and Tilo Pompe — Univer-

sität Leipzig, Institute of Biochemistry, Johannisallee 21-23, 04109 Leipzig, Germany

Living cells are subjected to many physical cues, such as viscoelasticity of the environment and spatial constraints. The latter holds especially true for cells in multicellular, compartmentalized organisms, like us. In previous work we found a bimodal behavior with regard to the formation of exterior and interior stress fibers and their spacing for human umbilical vein endothelial cells under lateral constraints [1].

We now observed a high robustness of this bimodal behavior against changes in biophysical and biochemical parameters, including substrate stiffness, also within cell types of higher contractility. We found that inhibition of myosin activity with blebbistatin or inhibition of ROCK with Y-27632 only lead to minor perturbations in the bimodal behavior. Furthermore, traction forces and strain energies of laterally confined cells were only slightly attenuated with increasing constraint and showed no apparent correlation to the two distinct actin cytoskeleton morphologies. Live cell imaging of stress fiber patterns revealed a fast switching between different stress fiber states within minutes, indicating that cells under lateral constraints permanently adapt to their surroundings.

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

BP 50.6   Wed 17:00   Poster C

Microbial adhesion on nanorough titanium: Insight into the nanostructure of the microbe-material-interface — ●Claudia Lüdecke-Beyer[1,3], Martin Roth[2,3], Jörg Bossert[1,3], and Klaus D. Jandt[1,3] — [1]Otto Schott Institute of Materials Research, Chair of Materials Science, Friedrich Schiller University, Jena, Germany — [2]Leibniz Institute for Natural Product Research and Infection Biology, Bio Pilot Plant, Hans Knöll Institute, Jena, Germany — [3]Jena School for Microbial Communication (JSMC), Excellence Graduate School, Friedrich Schiller University, Jena, Germany

Implant-associated infections are primarily initiated by the adhesion of microorganisms on the implants' surfaces. Recently, materials with surface roughnesses in the nanometer range gained interest to reduce microbial adhesion, however, the mechanisms remained so far unclear. The aim of this study was to explore the unknown nanostructure of the microbe-titanium-interface to gain understanding of the physical mechanism of microbial adhesion as a function of nanoroughness. Microbial adhesion was investigated using physical vapor deposited titanium thin films as nanorough 2D model surfaces. We found evidence that with decreasing titanium surface peak density and decreasing specific titanium surface area the surface coverage with microbes was reduced. Investigating the structure of the microbe-material-interface indicated that the initial adhesion of the microbes is controlled by the number of nano contact points between the microbial cell and the material's surface. These findings support the development of new antibiotic-free strategies to prevent implant-associated infections.

BP 50.7   Wed 17:00   Poster C

Nano contact points control initial microbial adhesion on biomaterials surfaces — ●Carolin Dewald[1,2,3], Claudia Lüdecke-Beyer[1,3], Martin Roth[2,3], Jörg Bossert[1,3], and Klaus D. Jandt[1,3] — [1]Otto Schott Institute of Materials Research, FSU Jena, Germany — [2]Leibniz Institute for Natural Product Research and Infection Biology, Hans Knöll Institute, Jena, Germany — [3]Jena School for Microbial Communication, FSU Jena, Germany

New antibiotic-free strategies are needed for prevention of biomaterials-associated infections. Our preliminary results indicated that microbial adhesion is controlled by the nano contact points between the microbes and the material's surface. The aim of this study was to use nanoparticles (NPs) for physically structuring materials' surfaces to modulate the number of possible contact points between the microbes and the nanostructured surfaces. 15 nm gold NPs were immobilized in different concentrations to gold surfaces. Microbial adhesion on these surfaces as well as the nanostructure of the microbe-material-interface was investigated to gain understanding of the physical mechanisms of microbial adhesion as function of the material's nanostructure. With decreasing NP density, microbial adhesion was statistically significantly reduced. High resolution SEM revealed that the NPs controlled the initial contact between the microbial cells and the material's surface. We assume that the total adhesion strength is correlated with the NP density i. e. the contact point density. Our new findings suggest that adjusting the nanostructure of biomaterials' surfaces might be a promising antibiotic-free approach for controlling microbial adhesion.

BP 51: Posters - Cytosceletal Filaments

Time: Wednesday 17:00–19:00   Location: Poster C

BP 51.1   Wed 17:00   Poster C
Cytoskeletal reorganization in human platelets during spreading — •Aishwarya Paknikar, Gerrit Brehm, Tim Dullweber, and Sarah Köster — Institute for X-Ray Physics, Georg-August-Universität Göttingen, Germany

To maintain the life-sustaining process of repairing damaged blood vessels, activated platelets change their shape, adhere, spread and contract in a hemostatic plug to seal the injuries. Dynamic and ordered rearrangements of their acto-myosin and microtubule (MT) cytoskeleton are responsible for these processes. We image the actin and MTs while they remodel in platelets in a time-resolved manner by labeling them with the recently introduced SiR-actin/tubulin probes. We demonstrate the ability to directly observe the formation of F-actin structures and coiling of the MTs as the platelets spread. The averaged actin intensity of single platelets reveals an initial steep rise followed by a linear increase that gradually reaches a plateau indicating the formation and increase in content of polymerized actin until the platelet spreads completely. By treatment of the platelets with pharmacological inhibitors we can indirectly show the crosstalk between the acto-myosin and microtubule dynamics. Our real-time cytoskeletal dynamics are all in agreement to post-fixation literature studies. Our results highlight a novel approach for studying real-time platelet cytoskeleton dynamics which is an important step in understanding the structural and mechanical aspects of platelet function better.

BP 51.2   Wed 17:00   Poster C
Molecular assembly studied in microflow by fluorescence correlation spectroscopy — •Viktor Schroeder[1], Eleonora Perego[1], Harald Herrmann[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, Georg-August-Universität Göttingen, Germany — [2]Division of Molecular Genetics, German Cancer Research Center (DKFZ), Heidelberg, Germany

We present a combination of microfluidic diffusive mixing and fluorescence correlation spectroscopy (FCS) to study rapid molecular assembly processes. In FCS, information about diffusing fluorescent particles is retrieved by analyzing the correlation of intensity fluctuations. To overcome the limited temporal resolution of FCS caused by long measuring times on the order of at least ten seconds, we use continuous flow microfluidic tools to map the temporal evolution to a spatial axis. Thus we achieve a temporal resolution of milliseconds with a dead time of only one second. Molecular assembly processes are initiated by the inflow of trigger molecules. The macromolecules of interest then spread over the whole cross section of the channel via diffusion, thus leading to a constant concentration downstream. Data are collected at different positions along the channel. As an example, we employ this method for studying the assembly of vimentin intermediate filament protein.

BP 51.3   Wed 17:00   Poster C
Stochastic Mechanochemical Simulation of Microtubules — •Matthias Schmidt and Jan Kierfeld — Theoretische Physik I, Technische Universität Dortmund

Microtubules are tubular filaments in eukaryotic cells made of α-/β- tubulin heterodimers. They have distinct growth dynamics called dynamic instability which is characterized by catastrophes, i.e. sudden changes from the growing phase to fast shrinkage, and rescues after which the microtubule starts to grow again.

We implement a stochastic simulation which combines the mechanics of the microtubule on tubulin molecule level with the chemical processes like depolymerization into a mechanochemical model. The mechanics of the microtubule are described by longitudinal bonds between tubulin dimers in the same protofilament, lateral interactions between adjacent tubulin molecules via springs and inter- and intra-dimer curling of hydrolyzed tubulin dimers.

BP 51.4   Wed 17:00   Poster C
A diffusion and capture mechanism creates large-scale correlations in the enzyme distribution on biofilaments — •Emanuel Reithmann, Louis Reese, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich, Germany

Diffusive motion on filaments with eventual capture at a reaction site is a common feature of regulating proteins in cell biology. Using a lattice gas model we study the impact of diffusion and capture for two central microtubule regulating proteins, which promote microtubule growth and shrinkage, respectively. We show that the capture mechanism has highly significant implications: It localizes the proteins at the reaction site and creates large-scale spatial correlations in the protein distribution along the filament. The latter finding leads to the failure of standard analytic approximation methods such as mean-field theories. To overcome this limitation, we develop an analytic approximation that globally accounts for relevant correlations and yields results that are in excellent agreement with experimental data. Our results show that diffusion and capture operates most efficiently at cellular enzyme concentrations which points to in vivo relevance.

BP 51.5   Wed 17:00   Poster C
Complex thermorheology of living cells — •Enrico Warmt, Sebastian Schmidt, Tobias Kiessling, and Josef Käs — Universität Leipzig, Soft Matter

Temperature has a reliable and nearly instantaneous influence on mechanical responses of cells. As recently published, MCF-10A normal epithelial breast cells follow time-temperature superposition (TTS) principle. Here, we measured thermorheological behaviour of eight common cell types within physiologically relevant temperatures and applied TTS to creep compliance curves. Our results showed that superposition is not universal and was seen in four of the eight investigated cell types. For the other cell types, transitions of thermorheological responses were observed at 36 °C. Activation energies (EA) were calculated for all cell types and ranged between 50 and 150 kJ/mol. The scaling factors of the superposition of creep curves were used to group the cell lines into three categories. They were dependent on relaxation processes as well as structural composition of the cells in response to mechanical load and temperature increase. This study supports the view that temperature is a vital parameter for comparing cell rheological data and should be precisely controlled when designing experiments.

BP 52: Posters - Multi-Cellular Systems

Time: Wednesday 17:00–19:00   Location: Poster C

BP 52.1   Wed 17:00   Poster C
Signal propagation and summation in *Physarum polycephalum* — •Felix Bäuerle and Karen Alim — Max Planck Institute for Dynamics and Self-Organization, D-37077 Göttingen, Germany

The slime mold *Physarum polycephalum*, among a number of organims growing and sustaining considerably large networks, excels in connecting food sources in a ressource balancing fashion. Furthermore, it was shown that the transport along the tubular body is optimized for dispersing nutrients with a peristaltic wave of contractions matching specimen size. In our research we want to understand the interplay of stimuli reactions, network growth and decision commitment in a context of biochemical and biophysical signals propagating along the network. By stimulation with, i.e., repulsive light illumination or glucose based attractants change in local and global behaviour is studied to gain insight into the slime molds ability to control its own transport mechanism.

BP 52.2   Wed 17:00   Poster C
Morphogenesis Control by Mechanical Stresses — •Jason Khadka and Karen Alim — Max Planck Institute for Dynamics and Self-Organization, D-37077 Göttingen, Germany

A major question in developmental biology is to understand how reproducible shapes arises from the collective behavior of individual cells. Here, we investigate the role of physical forces and mechanical feedback during plant tissue growth. We build a three dimensional vertex model to represent the plant tissue and to simulate its growth including mechanical feedback on individual cell growth. Varying the feedback strength we investigate the role of mechanical feedback on the robustness of tissue shape.

BP 52.3   Wed 17:00   Poster C
Quantifying Cell Volume and Proliferation in MDCK II Model Tissues — ●Simone Gehrer[1], Damir Vurnek[1], Sara Kaliman[1], Florian Rehfeldt[2], Diana Dudziak[3], and Ana-Sunčana Smith[1,4] — [1]PULS Group, Institute of Theoretical Physics I, FAU Erlangen — [2]3rd Institute of Physics/Biophysics, GAU Göttingen — [3]University Hospital Erlangen — [4]Division of Physical Chemistry, IRB Zagreb

Multicellular migration of 2D cell sheets is essential for wound healing and organ development. In-vitro model systems show that cell volume and proliferation are key players in active epithelial rearrangement and tissue expansion. Although studied extensively, precise temporal and spatial quantitative analysis of proliferation still remains a challenge.

To reveal the dependence of cell volume and proliferation on different monolayer compartments we droplet seeded MDCK II cells on collagen I coated glass. Grown from subconfluency to fully compartmentalized clusters they were examined on days 1, 2, 4 and 6. Volume studies were carried out on confocal images of actin and DAPI stained samples. As a part of the testing procedures the analysis was repeated on the stably transfected cell line with GFP histones generated in our lab. To visualize proliferation the monolayers were preincubated with EdU, stained, and imaged with fluorescence microscopy. Cells were counted individually with a home-written Matlab routine and the radial distribution of cell proliferation was obtained. For proliferation an inverse dependence on density was confirmed. Surprisingly, we found a direct correlation between the proliferation and the age of the tissues.

BP 52.4   Wed 17:00   Poster C
Simulating multicellular homeostasis with a cell-based discrete receptor dynamics model: the non-mutational origin of cancer and aging — ●Yuting Lou[1] and Yu Chen[2] — [1]The University of Tokyo, Japan — [2]The University of Tokyo, Japan

The purpose of the study is to investigate the multicellular homeostasis in epithelial tissues over very large timescales. An agent-based model is constructed based on the receptor dynamics of IBCell model proposed by Rejniak, et al. Instead of observing the multicellular architectural morphologies, the diversity of homeostatic states is quantitatively analyzed through a substantial number of simulations by measuring three new order parameters, the phenotypic population structure, the average proliferation age and the relaxation time to stable homeostasis. Nearby the interfaces of distinct homeostatic phases in 3D phase diagrams of the three order parameters, intermediate quasi-stable phases of slow dynamics that features quasi-stability with a large spectrum of relaxation timescales are found. A further exploration on the static and dynamic correlations among the three order parameters reveals that the quasi-stable phases evolve towards two terminations, tumorigenesis and degeneration, which are respectively accompanied by rejuvenation and aging. With the exclusion of the environmental impact and the mutational strategies, the results imply that cancer and aging may share the non-mutational origin in the intrinsic slow dynamics of the multicellular systems and the two processes are probably two absorbing phase transitions with distinct critical exponents.

BP 53: Posters - Statistical Physics of Biological Systems

Time: Wednesday 17:00–19:00   Location: Poster C

BP 53.1   Wed 17:00   Poster C
The stability of predator-prey systems on multiple patches coupled by migration — ●Philipp Gramlich[1], Sebastian Plitzko[1], Lars Rudolf[2], Barbara Drossel[1], and Thilo Gross[2] — [1]Institut für Festkörperphysik, TU Darmstadt, Deutschland — [2]Faculty of Engineering, University of Bristol, United Kingdoms

Dispersal between different habitats influences the dynamics and stability of populations considerably. Furthermore, these effects depend on the local interactions of a population with other species. Using a generalized modelling approach that is based on a linear stability analysis, we perform a comprehensive study of the simplest possible system that includes dispersal and local interactions, namely a 2-patch 2-species system. We evaluate the impact of dispersal on stability and on the occurrence of bifurcations, including pattern forming bifurcations that lead to spatial heterogeneity, in several different classes of models. We find that dispersal often destabilizes equilibria, but it can stabilize them if it increases population losses. If dispersal is nonrandom, i.e. if emigration or immigration rates depend on population densities, the correlation of stability with dispersal rates is positive in part of the models. We then extend the model to include many patches that are connected as a Random Geometric Graph and investigate the effect of the topological features of the patch network on the stability of the system.

BP 53.2   Wed 17:00   Poster C
Stochastic thermodynamics of learning in neural networks — ●Sebastian Goldt and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Over the past decade, stochastic thermodynamics has emerged as a powerful framework to understand the role of information in physical systems and the thermodynamic costs of manipulating it. A particularly intriguing application of these ideas is biology: every organism first gathers information about its noisy environment and then builds models from that data, at the expense of energy dissipation. Here, we focus on the second part of this process: learning.

Biologically, learning is implemented in neural networks where neurons receive and send signals from and to many other neurons via synapses. The strength of these synapses determines whether an incoming signal will make the neuron trigger an action potential, the electric pulse that is the basic token of communication in neural systems. The adaptation of synapses is the physiological mechanism for memory formation, e.g. in Hebbian learning.

Here, we use stochastic thermodynamics to analyse the learning of a classification rule by a feedforward neural network, whose synapses we endow with stochastic dynamics. Starting from the total entropy production of the network, we identify the rate of learning in a thermodynamically consistent way and introduce a measure for the thermodynamic efficiency of learning, which we compute for different learning algorithms.

BP 53.3   Wed 17:00   Poster C
Inference of chemotactic strategies of *E. coli* and *Pseudonomas putida* using Kramers-Moyal coefficients — ●Maximilian Seyrich[1], Oliver Pohl[1], Marius Hintsche[2], Carsten Beta[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut 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 includes rotational Brownian motion and shot noise, which initiates tumbling events with rates based on chemical gradients.

By analyzing experimental data of swimming trajectories, we infer the parameters of our model. For this purpose generalized Kramers-Moyal coefficients are calculated of our shot-noise 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 for E. coli and P. putida, i.e., bacteria adapt their tumble rate to the chemical gradients. Second, we find evidence that a subpopulation of E. coli, unlike P. putida, uses an additional turning bias during tumble events. We provide statistics which distinguish tumble rate chemotaxis and angle bias chemotaxis using scaling arguments for the Kramers-Moyal coefficients.

BP 53.4   Wed 17:00   Poster C
Species diversity in meta-foodwebs consisting of several patches coupled by stochastic migration — •Tatjana Thiel and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Germany

The structure of space has a considerable influence on the stability and diversity of ecosystems. So far, there are only few theoretical studies investigating the population dynamics of systems consisting of many species that can migrate between several patches, and most of these model migration as 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.

To this purpose, we place a foodweb model consisting of many species on a system of several patches and evaluate the stable configurations 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 explore the different ways in which migration rates can depend on population sizes and body masses.

We will discuss how the local and regional species diversity depend on the mode and frequency of migration. Typically, local diversity is largest with intermediate migration rates, since migration is frequent enough that species can be rescued from extinction by immigration but not so frequent that all patches have an identical species composition.

BP 53.5   Wed 17:00   Poster C
Influence of heterogeneous habitat quality on meta-foodweb robustness — •Michaela Hamm and Barbara Drossel — Institut für Festkörperphysik, TU Darmstadt, Deutschland

Anthropogenic changes in ecosystems, e.g. habitat fragmentation due to agricultural land usage, have a large effect on the diversity and stability of ecosystems.

In order to better understand these effects, theoretical investigations are needed that take into account the complex foodweb structure as well as the distribution of the species over several habitats and the different quality of these habitats.

We therefore present a computer simulation study of the influence of the degree of habitat heterogeneity on the robustness (number of persisting species) and on the local and regional biodiversity of meta-foodwebs. Each habitat is randomly assigned a high or low quality (abundance of resources), and the total number of habitats as well as the fraction of high- and low-quality habitats are varied.

Among other results we find that heterogeneity promotes diversity, because predators cannot be supported by low-quality habitats, thus providing refuges for prey.

BP 53.6   Wed 17:00   Poster C
Maze runner: microbial swimming in hexagonal and squared arrays — •Marco Bahrs, Marius Hintsche, Michael Raatz, Matthias Theves, and Carsten Beta — Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

By randomly changing direction, bacteria effectively explore their surroundings. The natural habitat of many microbial swimmers is dominated by interfaces and narrow interstitial spacings. Thus, the organism's movement strategy cannot be understood without reference to its environment and to the close interactions with it. We examined the steric effects of a homogeneously distributed geometrical pattern on bacterial swimming behavior. Experiments were conducted in a microfabricated array of hexagonal and square obstacles. In these environments we recorded the flux of bacteria through the resulting system of channels. Results were compared to an environment comprised of an array of linear channels. Motility parameters like the effective diffusion coefficient and the mean square displacement serve to compare the different experimental surroundings.

BP 53.7   Wed 17:00   Poster C
Geometric hindrance in multi-species transport on microtubules — •Patrick Wilke, Emanuel Reithmann, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich, Germany

Intracellular transport on microtubules is performed by molecular motors which have for a long time been thought to move exclusively longitudinally to the axis of the cylindrically shaped biopolymer. Recent experimental studies have revealed that, opposed to this standard hypothesis, motion on spiraling paths is observed for many kinesin such as kinesin-2 [1] and 8 [2]. Here, we study collective transport of multiple particle species which move along different, periodically intersecting spiraling paths on a cylinder. Based on a lattice gas description we find that these intersections provoke correlations in the exclusion process which significantly influence the particle flux. Opposed to classical transport models, our system is characterized by a vanishing particle current at densities far below full occupation. To account for such effects, we develop an analytic framework which allows us to compute the current reduction due to geometric hindrance and the underlying correlations. Surprisingly, the stationary particle-density profile exhibits spatially oscillating patterns which are unfeasible in classical single-species ore one-dimensional models.
[1] M. Brunnbauer et al. Molecular cell 46.2 (2012): 147-158.
[2] V. Bormuth et al. Biophysical journal 103.1 (2012): L4-L6.

BP 53.8   Wed 17:00   Poster C
Stuttering of Min oscillations is induced by stochastic effects — •Lukas Wettmann and Karsten Kruse — Theoretische Physik, Universität des Saarlandes, Postfach 151150, 66041 Saarbrücken, Germany

The site of cell division in wild type E. coli bacteria is determined through pole-to-pole oscillations of the Min proteins. Although the oscillations are fairly stable across a wide variety of cell shapes and protein concentrations the emerging patterns are subject to molecular noise, due to the small copy number of proteins in a single cell. This causes the oscillations to sometimes "stutter" and remain in the same polar configuration. We used a model based on transient binding of MinE to the cytoplasmic membrane to describe the dynamics of the Min system and analyzed the stochastic dynamics in the limit of weak noise.

BP 53.9   Wed 17:00   Poster C
Micro-swimming with inertia — •Oleg Trosman[1,2], Jayant Pande[1,2], and Ana-Sunčana Smith[1,2,3] — [1]PULS group, Department of Physics, Friedrich-Alexander-University of Erlangen-Nuremberg, Germany — [2]Cluster of Excellence: Engineering of Advanced Materials, Department of Physics, Friedrich-Alexander-University of Erlangen-Nuremberg, Germany — [3]Division of Physical Chemistry, Ruđer Bošković Institute, Zagreb, Croatia

Increased theoretical study in the past few decades has enabled scientists to gain a good understanding of the motion of micro-swimmers, yet this has focused on the world of inertia-free swimming. While this is a good approximation for many micro-swimmers as the Reynolds numbers of their flow are typically negligible, for some micro-swimmers inertia can have observable effects on the motion, such as affecting the swimming gait and the velocity. In this talk we present a theoretical study of a micro-swimmer where inertial effects are taken into account to the lowest non-zero order. For this we employ the popular Golestanian model of the swimmer, with three beads attached in series in a fluid and the motion along the axis of the swimmer. By combining the Oseen-Stokes equations for the coupled motion of distant spheres in a fluid with Newton's force-mass relations, we obtain a coupled system of second-order differential equations for the sphere positions. Solutions of these equations numerically and analytically allow us to discuss interesting deviations from inertia-less swimming.

BP 53.10   Wed 17:00   Poster C
Correlated fluctuations in strongly-coupled binary networks beyond equilibrium — •David Dahmen[1], Hannah Bos[1], and Moritz Helias[1,2] — [1]Inst. of Neurosci. and Medicine (INM-6) and Inst for Advanced Simulation (IAS-6) and JARA BRAIN Institute I, Jülich Research Centre — [2]Dept. of Physics, Faculty 1, RWTH Aachen University

Randomly coupled Ising spins constitute the classical model of collective phenomena in disordered systems. Their phase diagram is obtained by averaging over the quenched random couplings, but many applications require the activity statistics for a single realization of the possibly asymmetric couplings in finite-sized networks: the reconstruction of couplings from the observed dynamics, learning in the central nervous system by correlation-sensitive synaptic plasticity, and representation of probability distributions for sampling-based inference. We present a systematic cumulant expansion for kinetic binary (Ising) threshold units with strong, random and asymmetric couplings that goes beyond mean-field theory and is applicable outside thermodynamic equilibrium; a system of approximate non-linear equations predicts average activities and pairwise covariances in quantitative

agreement with full simulations down to hundreds of units [Dahmen et al. 2015, arXiv]. The linearized theory yields an expansion of the correlation- and response functions in collective eigenmodes, leads to an efficient algorithm solving the inverse problem, and shows that correlations are invariant under scaling of the interaction strengths. Partly supported by Helmholtz association: VH-NG-1028 and SMHB; EU Grant 604102 (HBP).

BP 53.11   Wed 17:00   Poster C
Coarse-Grained Interacting Particle Models for Chromatin Remodeling — •Michael Wolff, Johannes Nübler, and Ulrich Gerland — Physik-Department TU München, James-Franck-Straße 1, 85748 Garching

To explore the action of remodeling mechanisms on nucleosome patterns, we are studying physical models for one-dimensional interacting particle systems under the influence of additional agents actively displacing or evicting the particles. We characterize the connections between the mechanics of remodelers and the arising patterns, including non-equilibrium steady states with non-zero entropy production. We compare our modeling results, for example the formation of clusters, to nucleosome patterns obtained under varying experimental conditions with the aim to identify biologically relevant mechanisms.

BP 54: BP Mitgliederversammlung (Annual General Meeting of the Biological Physics Division)

Time: Wednesday 19:00–20:00   Location: H43

Discussion

BP 55: Symposium - Scientometric Maps and Dynamic Models of Science and Scientific Collaboration Networks (SYSM)

Time: Thursday 9:30–12:15   Location: H1

Invited Talk   BP 55.1   Thu 9:30   H1
Science Forecasts: Measuring, Predicting, and Communicating Scientific Developments — •Katy Börner — Indiana University

In a knowledge-based economy, science and technology are omnipresent and their importance is undisputed. Equally evident is the need to allocate resources, both monetary and human, in an effective way to foster innovation. In the preceding decades, data mining, metrics, and indicators have been embraced to gain insights into the structure and evolution of science; but there have been no significant efforts into mathematical, statistical, and computational models that can predict future developments in science, technology, and innovation (STI). While it may not be possible to predict the nature, essence, or the precise extent of impact of the next scientific or technological innovation, it is often possible to predict the circumstances leading to it, i.e., where it is most likely to happen and under which conditions. See Scharnhorst, Börner, and Besselaar, eds. 2012. Models of Science Dynamics: Encounters Between Complexity Theory and Information Science. Springer Verlag for an overview of major model types.

This talk reviews and demonstrates the power of computational models for simulating and predicting possible STI developments and futures. In addition, it showcases novel means to broadcast moderated STI forecasts to make them accessible and understandable for a general audience.

Invited Talk   BP 55.2   Thu 10:00   H1
Mapping science with variable-order Markov dynamics reveal overlapping fields and multidisciplinary journals — •Martin Rosvall — Umeå University, Sweden

To better understand the parallel human endeavor of science, we need good maps that both simplify and highlight the flows of ideas and underlying research organization. However, current maps of science cannot effectively identify the multilevel and overlapping fields of science with multidisciplinary journals. For example, whereas maps based on citations between journals in first-order Markov models can only assign each journal to a single field, maps based on multi-step citation chains in higher-order Markov models become computationally infeasible already for moderate-sized systems. To overcome these problems, we introduce a method that uses model selection to find the appropriate variable-order Markov model. We also present interactive maps of science that highlights the assignments of multidisciplinary journals and how ideas flow through those journals.

Invited Talk   BP 55.3   Thu 10:30   H1
Network algorithms for reputation and quality in scholarly data — •Matúš Medo, Manuel Mariani, and Yi-Cheng Zhang — University of Fribourg, Fribourg, Switzerland

The ever-increasing quantity and complexity of scientific production have made it difficult for researchers to keep track of advances in their own fields. This, together with growing popularity of online scientific communities, calls for the development of effective information filtering tools. Network theory is an important driving aspect for such algorithms. We will first discuss the case of an online scientific community where users and papers form a bipartite network which can be effectively used to evaluate the reputation of users and fitness of papers. We show that when the input data is extended to a multilayer network including users, papers and authors, the resulting performance improves on multiple levels. In particular, top papers have higher citation count and top authors have higher h-index than top papers and top authors chosen by other algorithms. We will then move to stress the role of time in scholarly data. Most research metrics either ignore time (such as the h index) or consider it in an ad-hoc fashion (such as the m quotient). On the example of PageRank which has been used in the past to assess the quality of papers, we show that a demonstrably better ranking of papers can be obtained by considering time in a principled way.

15 min. break

Invited Talk   BP 55.4   Thu 11:15   H1
Modeling scientific networks in social media — •Cassidy Sugimoto — School of Informatics and Computing, Indiana University Bloomington, USA

This talk will examine the role of social media in constructing new or reinforcing old epistemic communities. In particular, we will analyze the interconnectivity of scientists on social media platforms according to their disciplinary affiliation and the degree to which these networks reinforce or contrast with models constructed through collaboration and citation relations. We will analyze the role of gender and other socio-demographic characteristics where possible.

Invited Talk   BP 55.5   Thu 11:45   H1
Modeling scientific collaboration across multiple scales: from individuals to Europe — •Alexander Petersen — IMT Lucca Institute for Advanced Studies, Lucca, Italy

Quantitative measures are becoming increasingly prevalent at all scales of scientific evaluation, largely due to the advent of large comprehensive publication databases that allow for detailed studies of ideas, people, and institutions, and the vast networks connecting them. As such, there is plenty of room to apply methods from complex systems to address policy-oriented issues relevant to the entire science system. In the first half, I will discuss micro-scale patterns of collaboration from a researcher's local 'ego' perspective, showing that scientific collaboration is characterized by a high turnover rate juxtaposed with frequent 'life partners'. I will show that these extremely strong collaborations have a significant positive impact on productivity and citations – the

apostle effect – representing the measurable advantage of 'super' social ties. In the second half, I will discuss macro-scale collaboration patterns concerning the evolution the European Research Area (ERA), a cross-border labor, funding, and mobility scheme aimed at fostering innovation and growth within Europe. However, despite decades of integration policies, recent analyses have shown there to be little cross-border integration in the EU above global trends – i.e. Europe remains a collection of national innovation systems. I will show that

high-skilled mobility – i.e. brain drain, largely from East to West following the 2004/2007 EU enlargement – can explain why the cross-border integration of R&D within the ERA is lagging.

Right after the symposium, participants are invited to enjoy a guided tour of the Places and Spaces: Mapping Science exhibition (http://scimaps.org) on display in the foyer of the university library.

BP 56: The Physics of Water Interactions with Biological Matter (Joint Focus Session with CPP)

Organizers: Emanuel Schneck (MPIKG Potsdam), Regine von Klitzing (TU Berlin), Tristan Bereau (MPIP Mainz)

The role of water in biological systems is not simply to act as a solute for biomolecules. Water mediates the interaction between biological interfaces and has to be considered an integral component of biomolecular assemblies. These interactions can alter the properties of both water and the biomolecules in significant ways. Recent methodological progress in experimental techniques and computer simulations provides us with improved tools to gain insight into the relevant physics, from quantum-chemical details of individual molecules, to collective behavior at interfaces, to hydration-dependent structures of biomaterials. The purpose of this Focus Session is to bring scientists from various disciplines to search for solutions to integrate hydration phenomena on different length scales.

Time: Thursday 9:30–12:45   Location: H37

Invited Talk   BP 56.1   Thu 9:30   H37
It is water what matters: THz absorption spectroscopy as a new tool to study solvation dynamics — •Martina Havenith — Physikalische Chemie II, Ruhr-Universität Bochum, Bochum, Germany

Terahertz (THz) absorption spectroscopy is a powerful tool to study (bio)molecular hydration. Experimental advances in the development of new THz sources had to go hand in hand with the development of new theoretical concepts which are able to describe the underlying solute-induced sub-picosecond dynamics of the hydration shell.

Recent results show the significance of hydrogen bond dynamics for molecular recognition. We find a gradient of water motion toward functional sites of proteins, the so-called "hydration funnel", which is found to be essential for biomolecular function.

Transient THz spectroscopy can be used to record snapshots of the low frequency spectrum of a solvated proteins during protein folding, thus capturing changes during hydrophobic collapse in real time during biological function. Within the talk I will present examples of low frequency spectra of hydration water around solutes which can be correlated to changes in entropy.

V. Conti Nibali, M. Havenith New insights into the role of water in biological function: Studying solvated biomolecules using terahertz absorption spectroscopy in conjunction with molecular dynamics simulations J. Am. Chem. Soc. 136(37), 12800-12807 (2014)

BP 56.2   Thu 10:00   H37
The Effect of Zwitterionic Ectoine on Local Water Dynamics — •Johannes Zeman and Jens Smiatek — Institute for Computational Physics, University of Stuttgart, Germany

Ectoine is known to have a stabilizing effect on proteins in aqueous solution. In order to investigate the plausibility of a suggested indirect mechanism [1], its effect on the local water dynamics at low molar concentrations has been examined by means of Molecular Dynamics simulations. The simulation data has been analyzed in terms of diffusion coefficients, hydrogen bond life times and angular distributions, power spectra, as well as dielectric spectra.

The observed influence of zwitterionic ectoine on water dynamics indicate a pronounced structural strengthening and therefore support the hypothesis of an indirect stabilization mechanism.

For comparison, similar simulations and analyses have been carried out with urea in aqueous solution, as urea is known to have a denaturing effect on proteins. As expected [2], the influence of urea on the local water dynamics is comparatively small.

[1] M. B. Hahn et al., The Influence of the Compatible Solute Ectoine on the Local Water Structure: Implications for the Binding of the Protein G5P to DNA, J. Phys. Chem. B (Nov 10, 2015) [Epub ahead of print]

[2] D. Bandyopadhyay et al., Molecular Dynamics Simulation of Aqueous Urea Solution: Is Urea a Structure Breaker?, J. Phys. Chem. B, 118 (40), pp 11757–11768 (2014)

Invited Talk   BP 56.3   Thu 10:15   H37
Dielectric and diffusional aspects of hydration water — •Roland Netz and Matej Kanduc — Physics Department, FU Berlin, Germany

The molecular layer of water molecules on surfaces is important for the properties of neutral and charged solutes and surfaces. We study how hydration and dielectric properties of interfacial water layers can be used to explain diverse phenomena such as the hydration repulsion between polar surfaces, dielectric spectra of salt solutions, and conformational transitions of polymers.

BP 56.4   Thu 10:45   H37
Salt Induced Hydrophobic Polymer Collapse Theoretical Model vs. Simulation — •Jan Heyda[1] and Joachim Dzubiella[2,3] — [1]Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic — [2]Soft Matter and Functional Materials, Helmholtz- Zentrum Berlin, Hahn-Meitner Platz 1, 14109 Berlin, Germany — [3]Department of Physics, Humboldt-University Berlin, Newtonstr. 15, 12489 Berlin, Germany

Smart materials are perspective due to their versatility. An soft-matter example are thermoresponsive polymers, which undergo volume transition, when crossing the lower critical solution temperature (LCST). Near the LCST, they become sensitive to other stimuli, such as salt type and concentration (dx.doi.org/10.1021/ja0546424).

In this contribution, we employed a hydrophobic polymer model (dx.doi.org/10.1073/pnas.0605139104), which possesses 2-state behavior, to study ion-specific effects. We performed replica-exchange molecular dynamics simulations and analyzed the data thermodynamically as well as in terms of Kirkwood-Buff theory, i.e., the preferential binding of salt over water to the polymer was determined.

We have found that the effect on LCST change of salts excluded from hydrophobic interfaces, such as KF and NaCl is strikingly different from attracted salts, such as NaI or GndCl. The surface area based model performs well for the first, but fail for the second group of salts.

To interpret the effect of 'binding' salts, we have employed recently proposed bridging mechanism (dx.doi.org/10.1021/ma302320y) and chain configuration entropy approach (dx.doi.org/10.1039/c4cp05314a).

15 min. break

Invited Talk   BP 56.5   Thu 11:15   H37
Neutron scattering clarifies the behaviour of water in cells —
●Giuseppe Zaccai — Institut Laue Langevin, Grenoble, France

Its essential role in biological structure and function is so well established that the search of extra-terrestrial Life is guided by a search of liquid water. Yet the H-bonding properties of water and their interactions with biological molecules are still not fully understood. Because of the strong H/D isotope effect in neutron scattering, neutron diffraction and neutron spectroscopy are particularly powerful experimental methods for the study of water in biology. Neutrons contributed important data to clarify the state of water in cells, following controversial reports on its dynamic state, which, by sustaining that in cell conditions are significantly different, put in question the relevance of in vitro studies. The atomic scale dynamics of intracellular water has been measured in vivo in mesophile and extreme halophile organisms. The results clearly show that intracellular water, other than in hydration interactions with macromolecules and membranes, flows as freely as bulk water, with similar effects on functional molecular dynamics as observed in vitro. Neutrons also characterised the state of water in the intracellular solvent of halotolerant bacteria, which contains molar concentrations of the compatible solute ectoine. All these observations underline the biological requirement of maintaining, within the physiological environment, the remarkable H-bonding properties of liquid water.

BP 56.6   Thu 11:45   H37
Explicitly implicit solutions: Cavity optimization on the cheap — ●David Egger, Christoph Scheurer, Karsten Reuter, and Harald Oberhofer — Technische Universität München, Garching, Germany

In recent years the importance of the solvent response in catalytic, bio- and photochemical processes has become more and more apparent. Yet, in ab-initio computer simulations treating the solvent effect in an efficient but accurate manner is still a major challenge. Unfortunately, an explicit inclusion of solvent molecules significantly increases the associated computational costs. Therefore, continuum solvation models which treat the solute-solvent interaction implicitly through their dielectric permittivities, are often the method of choice. The transitions between these permittivities define a dielectric 'cavity' that is generally defined over free parameters.

In our contribution, we study the validity of such an approach by comparing the implicit potential response to that of explicit classical MD simulations. We reverse engineer an optimal cavity by minimizing the differences between explicit and implicit spatially resolved electrostatic reaction potential of the solvent. To this end we also investigate a number of different models of the permittivity transition function and cavity. Finally, we present optimization results for ions and small molecules in water.

Invited Talk   BP 56.7   Thu 12:00   H37

Controlling Water Evaporation: self-assembly at air/liquid interfaces — ●Emma Sparr[1] and Kevin Roger[2] — [1]Physical chemistry, Lund University, Sweden — [2]Université de Toulouse, France

Land-living organisms face the challenge that the ambient air is much drier than what is found in a living cell. One strategy to counter this drying-out threat is through lipid-protein barrier membranes, like the human skin. One important property of the skin is that the evaporation rate across skin is nearly independent of the air humidity, which implies that skin is a responding membrane and its permeability depends on its boundary conditions.

Using aqueous solutions of amphiphilic molecules, we show that the response can be explained by changes in self-assembly structures in the water gradient across the interfacial layer. We have designed an experimental device coupled to a variety of characterization techniques (X-ray scattering, polarized & IR microscopy) to study the non-equilibrium time evolution at an air- liquid interface. Using this device we demonstrate for two model systems how multilayer interfacial structures are formed, and how these structures influence the water transport. We show that a dry phase with low water permeability forms at the air/liquid interface and adapts its thickness to counter changes in the air humidity. This responsive shield is a universal feature of systems for which the structure/permeability changes with the water content. Our findings can unveil mechanism of responding membrane in biological systems, for example, the skin, and it can lead to new possibilities to design robust and homogeneous coatings of amphiphilic molecules.

BP 56.8   Thu 12:30   H37
Anomalous and anisotropic diffusion of hydration water in fluid lipid membranes — ●Felix Roosen-Runge[1], Laura Toppozini[2], and Maikel Rheinstädter[2] — [1]Institut Laue-Langevin, Grenoble, France — [2]McMaster University, Hamilton, Ontario, Canada

Water diffusion in heterogeneous environments is a relevant and frequently studied phenomenon in experiment, simulation and theory. We report on water diffusion between phospholipid membranes using incoherent quasi-elastic neutron scattering (QENS) and computer simulations [1]. The combination of a well-aligned stack of DMPC membranes with the large, 2-dimensional detectors available at the neutron spectrometer Let (ISIS, UK) allows for simultaneous access to water motions lateral and perpendicular to the membranes. The resulting 2-dimensional maps of relaxation time, τ, and stretching exponent, β, evidence anomalous (sub-diffusive) and anisotropic diffusion of membrane hydration water varying on nanometer distances. By combining molecular dynamics and coarse-grained Brownian dynamics simulations, the overall behavior is reproduced, and the apparent features can be linked back to an intrinsic sub-diffusivity of water at picosecond time scales, and the anisotropy of confinement and local dynamical environments.

[1] Toppozini et al. Soft Matter 11 (2015) 8354

BP 57: Membranes and Vesicles I

Time: Thursday 9:30–12:45   Location: H43

Invited Talk   BP 57.1   Thu 9:30   H43
Monolayer curvature induced nanoscale structures in lipid membranes — ●Friederike Schmid — Institut fuer Physik, Johannes Gutenberg-Universitaet Mainz, Germany

Biological lipid membranes are believed to be laterally heterogeneous and filled with nanoscale ordered "raft" domains. However, the mechanisms stabilizing such small rafts are still under debate. Here we report the observation of raft-like structures of sizes in the order of 10 nm in a coarse-grained molecular model for multicomponent lipid bilayers [1]. Furthermore, we discuss a mechanism that generates nanoscale rafts by a coupling between monolayer curvature and local ordering. The theory rationalizes in a unified manner the observation of a variety of nanoscale structures in lipid membranes: Rippled states in one-component membranes, lipid rafts in multicomponent membranes. Both are observed in our generic simulations, with properties that are compatible with experimental observations [1-3]. Finally, we will discuss the interplay of this mechanism with a similar mechanism based on a coupling between *bilayer* curvature and local ordering, which is well known from the literature and can generate ordered microdomain

structures on the scale of 100 nm or more, and show how microdomains can be used to organize nanodomains [4].

[1] S. Meinhardt, R.L.C. Vink, F. Schmid, PNAS 119, 4476 (2013).
[2] O. Lenz, F. Schmid, Phys. Rev. Lett. 98, 058104 (2007).
[3] L. Toppozini et al, Phys. Rev. Lett. 113, 228101 (2014).
[4] L. Brodbek, F. Schmid, AEAM, to appear (2015).

BP 57.2   Thu 10:00   H43
Incorporation of Aescin in DMPC vesicles — ●Ramsia Sreij, Carina Dargel, and Thomas Hellweg — Physical and Biophysical Chemistry, Universitätsstraße 25, 33615 Bielefeld

The function of membrane proteins depends on the lipid bilayer thickness (d_z) and its properties. d_z is studied in model membrane systems in form of unilamellar vesicles (ULVs) consisting of 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC). DMPC vesicles undergo a phase transition from gel to fluid phase at a temperature $T_M = 23.6°C$. Saponins are a diverse class of natural, plant derived amphiphilic molecules with a peculiar molecular structure made of a hydrophobic scaffold and hydrophilic oligosaccharide chains. They have strong

surface activity and are used as natural emulsifiers and foaming agents in food, pharmaceutical and other industries. Their incorporation into the membrane of living cells reduces the cholesterol bioaccessibility by displacement of cholesterol molecules from the bile salt micelles. We studied the saponin Aescin to demonstrate the effect of its incorporation on the lipid bilayer thickness and T_M of small unilamellar DMPC vesicles produced by extrusion. We use small and wide angle X-ray scattering (SWAXS) to measure the effects on d_z in dependence of a varying amount of incorporated Aescin. By differential scanning calorimetry (DSC) and dynamic light scattering (DLS) experiments we show the influence of the saponin incorporation on T_M.

[1] B.A. Brüning, S. Prevost, R. Stehle, R. Steitz, P. Falus, B. Farago, and T. Hellweg, *Biochim. Biophys. Acta*, 1838, 2412-2419.

BP 57.3   Thu 10:15   H43

Squeezing vesicles on a supported lipid bilayer using osmolyte polymer chains: a neutron reflectivity study — •ALEXANDROS KOUTSIOUMPAS[1] and DIDIER LAIREZ[2] — [1]Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich GmbH, Outstation at MLZ, Lichtenbergstrasse 1, 85747 Garching, Germany — [2]Laboratoire Léon Brillouin, CEA/CNRS UMR 12, CEA-Saclay, 91191 Gif-sur-Yvette, France

The approach of two lipid bilayer segments in close proximity is an event of special interest in biophysics, due to its relation with several biological functions such as membrane fusion. Using the neutron reflectometry technique we attempt to gather structural information related to the interaction of a planar supported DPPC bilayer with DPPC vesicles that are "forced" at the interface by the addition of high concentrations of polyethylene glycol chains in bulk solution. At the adopted experimental conditions the major effect that is observed is related to the initial approach of vesicles close to the supported bilayer at temperatures below the liquid/gel transition, followed by their "spreading" and flattening at temperatures above the transition that is attributed to the radical decrease of their bending modulus. The experimental observation is backed up by semi-analytic calculations based on the Helfrich Hamiltonian that describes membrane mechanics. In all cases, no indication of any pre-fusion structure is found. These observations are also discussed in the context of alternative potential approaches for the formation of floating bilayers on a planar surface.

BP 57.4   Thu 10:30   H43

Acto-myosin dynamics drive local membrane component organization in an in vitro active composite layer — •DARIUS V. KÖSTER[1], KABIR HUSAIN[1], ELDA ILJAZI[1], PETER BIELING[2], DYCHE MULLINS[2], MADAN RAO[1,3], and SATYAJIT MAYOR[1] — [1]National Centre for Biological Sciences, Bangalore, India — [2]University of California, San Francisco, USA — [3]Raman Research Institute, Bangalore, India

Studies on the organisation of the cell surface have revealed a role for dynamic acto-myosin in membrane protein and lipid organization, suggesting that the cell surface behaves as an active composite. We reconstitute an analogous system in vitro that consists of a fluid lipid bilayer coupled via membrane-associated actin binding proteins to dynamic actin filaments and myosin motors. Varying actin concentration, filament length, and actin/myosin ratio in this minimal system revealed after consumption of a limited ATP pool a phase, characterized by a lattice of polar asters. During the self-organizing aster formation, advection drives transient clustering of membrane components. Increasing levels of ATP produces a constitutively remodelling state of the actin filaments which in turn drive active fluctuations of coupled membrane components, resembling those observed at the cell surface. In a multicomponent membrane bilayer, this remodelling acto-myosin layer contributes to distinct changes in the extent and dynamics of phase segregating domains. These results show how local membrane composition can be driven by active processes arising from acto-myosin which could have implications for the membrane organization in cells.

BP 57.5   Thu 10:45   H43

Structure and dynamics of phospholipid vesicles around the main phase transition — •BEATE BRÜNING[1], RAMSIA SREIJ[1], BELA FARAGO[2], and THOMAS HELLWEG[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Institut Laue-Langevin, Grenoble, France

We use complementary scattering probes to study the molecular and structural reorganization of unilamellar 1,2-dimyristoyl-sn-glycero-3-phosphatidylcholine (DMPC) vesicles undergoing the phospholipids main phase transition. Effects on vesicle morphology and collective shape fluctuations are hierarchically interlinked. We cover length scales from molecule distances to an ensemble of vesicles in solution, and time scales ranging from ns to ms. We find temperature-induced changes in the lipid chain order and bilayer thickness are reflected most strongly in curvature changes and shape fluctuations, rather than in inter-vesicle lipid exchange processes. We comment on the implications for vesicle-membrane budding processes.

[1] Structure and dynamics of phospholipid vesicles around the main phase transition (submitted).

30 min break

BP 57.6   Thu 11:30   H43

Fast tracking of single molecules in live cell membranes at ultra-high resolution with interferometric scattering microscopy (iSCAT) — •RICHARD TAYLOR and VAHID SANDOGHDAR — Max Planck Institute for the Science of Light, Erlangen, Germany

Conventional approaches to track diffusion of lipids and proteins in membranes use fluorescence microscopy, but a low fluorescence rate and inevitable photobleaching severely limit the localisation precision on both the short and long timescales. Furthermore, fluorescence microscopy traditionally also suffers from limited axial resolution. We report on the use of interferometric scattering microscopy (iSCAT) for monitoring of a gold nanoparticle-labelled protein within the live HeLa cell membrane. iSCAT particle tracking has previously demonstrated accurate tracking of labeled single lipids within synthetic membranes to nanometric precision at fast millisecond framerates [1]. Here, we demonstrate use of iSCAT microscopy to track the diffusion of gold labeled transmembrane proteins within the live HeLa cell membrane. We show that one may track the probe diffusion both in- and out-of-plane, with nanometer-level accuracy and microsecond framerates.

[1] C.-L. Hsieh, S. Spindler, J. Ehrig, V. Sandoghdar, J. Phys. Chem. B. 118, 1545-1554, (2014).

BP 57.7   Thu 11:45   H43

Passive Translocation of Hydrophobic Nanoparticles through a Phospholipid Bilayer — YACHONG GUO[1], EMMANUEL TERAZZI[2], RALF SEEMANN[3,4], •JEAN-BAPTISTE FLEURY[3], and VLADIMIR BAULIN[1] — [1]Departament d'Enginyeria Quimica, Universitat Rovira i Virgili, 26 Av. dels Paisos Catalans, 43007 Tarragona, Spain — [2]Department of Inorganic and Analytical Chemistry, University of Geneva, 30 quai E. Ansermet, CH-1211 Geneva 4, Switzerland — [3]Universitat des Saarlandes, Experimental Physics, 66123 Saarbruecken, Germany — [4]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Hydrophobic nanoparticles introduced into living systems may lead to increased toxicity, can activate immune cells or can be used as nanocarriers for drug and gene delivery. The interaction of nanoparticles with bilayers is essential of an in depth understanding of these processes. It is known that small hydrophobic nanoparticles can insert into a lipid bilayer and accumulate in the bilayer core, representing a potential well. Therefore it is generally accepted that escaping the bilayer is unlikely for these nanoparticles. In contrast to this assumption, we demonstrate theoretically how large hydrophobic nanoparticles can cross lipid bilayers with almost no energy barrier, while small hydrophobic nanoparticles stay trapped in the core of the bilayer. This size-dependent translocation was confirmed experimentally using a microfluidic device. Moreover, the kinetic pathway of a single passive translocation event was directly measured and analyzed. (Submitted)

BP 57.8   Thu 12:00   H43

Shaping the Endoplasmic Reticulum network in vitro — •GERNOT GUIGAS, CSILLA FERENCZ, and MATTHIAS WEISS — Experimental Physics I, University of Bayreuth

Many organelles in eucaryotic cells have complex shapes that deviate significantly from simple spheres. A prime example is the Endoplasmic Reticulum (ER) which forms an extensive network of membrane tubules throughout the cytoplasm of mammalian cells. In order to explore the self-assembly capacity of ER networks we have used an in-vitro reconstitution system and spinning disk confocal microscopy. In particular, we monitored how purified ER microsomes from Xenopus laevis eggs fuse in the presence of purified cytosol, ATP, and GTP. As a result, we observed that a complex network with an ER-like topology and a typical mesh size of some 10 micrometers grew almost instantly on the surface of the incubation chamber. In a subsequent

relaxation process, single tubules of the network moved and rearranged until the network had reached a stable configuration. Tubular networks only grew on charged surfaces and they were most stable on surfaces with a medium elasticity. When vesicles were mixed with small silicon oil droplets, tubular networks with a significantly reduced mesh size formed on these droplets, i.e. the ER network structure resembled more closely the native form found in mammalian cells. We conclude from our experiments that ER microsomes have an inherent capacity to self-assemble into a network structure with a mesh size that is influenced by the surface on which the structure grows.

BP 57.9   Thu 12:15   H43
Developing of biomimetic model-membranes to investigate transport processes via X-ray and neutron reflectometry — ●Irena Kiesel, Yuri Gerelli, and Giovanna Fragneto — Institut Laue Langevin, Grenoble, France

Transport processes through membranes are fundamental for the biological function of cells in living organisms. To investigate these processes, e.g. transport of drugs into cells, it is necessary to build a reproducible and stable model membrane system, accessible for analytical methods. Typically, model membranes are created as solid-supported lipid bilayers, as they are feasible for surface-sensitive techniques as X-ray- or neutron reflectivity (XRR, NR). In order to allow the penetration of guest molecules through membranes, it is necessary to use a highly hydrated spacer (e.g. polymer brushes). Furthermore, natural membranes are composed by several different saturated and unsaturated lipid species, which is in contrast to normally used model systems, using one or few comercially availible lipid species. Extracted lipids from *Pichia pastoris* yeast are used here in order to model a more natural mimicking membrane. The availability of natural extracts in both hydrogenated and deuterated forms allow the use of the so-called contrast variation method with neutrons. The aim of this project is to create reproducible, stable and tethered model membranes with natural extracted lipids to mimic real membranes and to allow the investigation of transport processes through this membrane. First reults from XRR, NR and other methods (AFM, fluorescence microscopy, QCM) will be presented.

BP 57.10   Thu 12:30   H43
Standing-Wave X-Ray Fluorescence Enables Near-Angstrom Precision Localization of Biologically Important Chemical Elements in Molecular Layers — ●Emanuel Schneck[1], Ernesto Scoppola[2,3], Jakub Drnec[4], Cristian Mocuta[5], Roberto Felici[4], Dmitri Novikov[6], Giovanna Fragneto[2], and Jean Daillant[5] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Institut de Chimie Séparative de Marcoule, France — [4]European Synchrotron Radiation Facility, Grenoble, France — [5]Synchrotron Soleil, Gif-sur-Yvette, France — [6]Deutsches Elektronen-Synchrotron, Hamburg, Germany

In nature, biomolecules are often organized as functional thin layers in interfacial geometries. The most prominent examples are the biological membranes. But biomolecular layers also play important roles in context with biotechnological surfaces, for instance when they are the result of adsorption processes. For the understanding of many biological or biotechnologically relevant processes, detailed structural insight into the involved biomolecular layers is required. Here, we use standing-wave x-ray fluorescence to determine element-specific density profiles in solid-supported lipid and protein monolayers with near-Angstrom resolution. The technique complements traditional reflectometry experiments which merely yield the layers' "global" density profiles. While earlier work mostly focused on relatively heavy elements, typically ions, we also localize the comparatively light elements S and P, which are found in many biomolecules and therefore particularly interesting.

BP 58: Cytoskeletal Filaments

Time: Thursday 9:30–13:00   Location: H44

Invited Talk   BP 58.1   Thu 9:30   H44
Cytoskeletal coordination — ●Gijsje Koenderink — FOM Institute AMOLF, Amsterdam, Netherlands

Cell shape and mechanics are determined by the interplay of the plasma membrane with three distinct cytoskeletal networks, made of actin filaments, microtubules, and intermediate filaments. These cytoskeletal polymers markedly differ in their structure and physical properties, and have traditionally been thought to have distinct cellular functions. However, there is growing evidence that they also exhibit strongly coupled functions necessary for cell migration, cell division, and mechanoresponse [1]. Our goal is to resolve physical mechanisms that contribute to cytoskeletal coordination. For this purpose, we study cell-free model systems reconstituted from purified cellular components. I will illustrate this approach by discussing two examples. First, I will demonstrate a model system where we introduced interactions between the actin and microtubule (MT) cytoskeletons via MT end-tracking proteins (+TIPs) that also bind F-actin [2]. We showed that the interaction between growing MT ends and actin is sufficient to capture and re-direct MT growth along actin bundles. Second, I will show how a fourth cytoskeletal filament, septins, interact with actin as well as the plasma membrane.

BP 58.2   Thu 10:00   H44
Overlap microtubules link sister k-fibers and balance the forces on bioriented kinetochores — ●Maja Novak[1], Janko Kajtez[2], Anastasia Solomatina[2], Iva M. Tolic[3,2], and Pavin Nenad[1] — [1]Department of Physics, Faculty of Science, University of Zagreb, Bijenicka cesta 32, 10000 Zagreb, Croatia — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany — [3]Division of Molecular Biology, Rudjer Boskovic Institute, Bijenicka cesta 54, 10000 Zagreb, Croatia

During metaphase, forces on kinetochores are exerted by k-fibers, bundles of microtubules that end at the kinetochore. Interestingly, non-kinetochore microtubules have been observed between sister kinetochores, but their function is unknown. Here we show by laser-cutting of a k-fiber in HeLa and PtK1 cells that a bundle of non-kinetochore microtubules, which we term 'bridging fiber', bridges sister k-fibers and balances the inter-kinetochore tension [1]. We found PRC1 and EB3 in the bridging fiber, suggesting that it consists of anti-parallel dynamic microtubules. By using a theoretical model that includes a bridging fiber, we show that the forces at the pole and at the kinetochore depend on the bridging fiber thickness. Moreover, our theory and experiments show larger relaxation of the inter-kinetochore distance for cuts closer to kinetochores. We conclude that the bridging fiber, by linking sister k-fibers, withstands the tension between sister kinetochores and enables the spindle to obtain a curved shape.

[1] Kajtez, Solomatina, Novak et al., Nature Communnications (Accepted)

BP 58.3   Thu 10:15   H44
Why microtubules run in circles — ●Falko Ziebert[1], Herve Mohrbach[2], and Igor Kulic[3] — [1]Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Groupe BioPhysStat, LCP-A2MC, Université de Lorraine, 57078 Metz, France — [3]Institut Charles Sadron UPR22-CNRS, 67034 Strasbourg, France

The fate of every eukaryotic cell subtly relies on the exceptional mechanical properties of microtubules. Despite significant efforts, understanding their unusual mechanics remains elusive. One persistent, unresolved mystery is the formation of long-lived arcs and rings, e.g., in kinesin-driven gliding assays. To elucidate their physical origin we develop a model of the inner workings of the microtubule lattice, based on recent experimental evidence for a conformational switch of the tubulin dimer. We show that the microtubule lattice itself coexists in discrete polymorphic states. Metastable curved states can be induced via a mechanical hysteresis involving torques and forces typical of few molecular motors acting in unison, in agreement with the observations.

BP 58.4   Thu 10:30   H44
Microtubule bundle formation is driven by angular diffusion of microtubules and forces exerted by cross-linkers — ●Marcel Prelogović[1], Lora Winters[2], Ana Milas[3], Iva Tolić[3], and Nenad Pavin[1] — [1]Department of Physics, Faculty of Science, University of Zagreb, Bijenička cesta 32, 10000 Zagreb, Croatia —

[2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstr. 108, 01307 Dresden, Germany — [3]Division of Molecular Biology, Ruder Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

During mitosis, microtubules (MTs) form a spindle, which is responsible for proper segregation of the genetic material. Most of the spindle MTs are organized into bundles by cross-linking proteins. A key question is what are the physical principles underlying the formation and stability of MT bundles. Here we show (Prelogović et.al., submitted), by introducing a model and experimentally testing its predictions, that random angular movement of MTs around the spindle pole and forces exerted by passive cross-linking proteins are sufficient for the formation of stable MT bundles. Our model predicts that the time needed for bundle formation depends mainly on the concentration of cross-linking proteins and the angular diffusion of the MT, but weakly on MT length. We confirmed these predictions by experiments in wild-type and ase1Δ fission yeast cells. In conclusion, the angular motion drives the alignment of MTs, which in turn allows the cross-linking proteins to connect the MTs into a stable bundle.

BP 58.5 Thu 10:45 H44
Axonal microtubule bundle polarity is maintained by mechanically mediated depolymerization of ill-oriented microtubules — •Maximilian Jakobs and Kristian Franze — University of Cambridge, UK

The microtubule (MT) bundles found in neuronal axons are highly polar with around 90% of all MTs pointing with their +end away from the cell body. Disruption of this polarity is thought to be involved in a variety of neurodegenerative diseases. Although the MT array polarity has been discovered more than 30 years ago, its origin is still poorly understood. We here tracked growing MT +ends in dissociated primary neurons to look for correlations between bundle polarity, MT growth and transport velocities, and MT growth lifetimes. Even though the +ends moved in the anterograde (away from the cell body) and retrograde (towards the cell body) direction with similar velocities, the fraction of velocities above 15μm/min was larger in the retrograde direction, implying that active transport drives -end out MTs back into the cell body. Additionally, MTs stopped growing more frequently when pointing with their +end towards the cell body than vice versa. This behaviour might be explained by an increased drag force acting on retrogradely growing MTs, which originates from an anterogradely directed viscous flow within the axon. This flow acts as a mechanical barrier for retrogradely growing MTs, facilitating their depolymerization and thus keeping the MT array polar. Understanding the mechanism that polarises the axonal MT array might yield new approaches towards preventing neuronal degeneration during disease.

BP 58.6 Thu 11:00 H44
Small-Angle X-ray Scattering Investigation of Structural and Organizational Changes Induced by Ions on Keratin Filaments — •Clément Hémonnot[1], Daniel Schmitz[1], Manuela Denz[1], Monika Mauermann[2], Harald Herrmann[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, Uni. Göttingen, Germany — [2]DKFZ, Heidelberg, Germany

Keratin intermediate filaments (IF) proteins play an important role for cell mechanics as they form extended filaments (5 nm radius) and complex, highly ordered intracellular networks, which provide integrity and stability to epithelial cells. We present a study of the assembly of keratin in presence of monovalent and divalent ions by small-angle X-ray scattering (SAXS). As SAXS can reveal structures on the nanometer length scale, we investigate the impact of K+ and Mg2+ ions on the internal structure and organization of keratin filaments and assemblies. We show that the radius of the filaments follows a linear trend with increasing ion concentration. Moreover, we are able to determine where in the filaments the ions accumulate by using a model consisting of a core filament and Gaussian chains representing the N- and C- terminals. Because of Coulomb screening, at low concentrations both ion species accumulate in the side chains; at intermediate concentrations, the ions start to bind to the core of the filament; at high concentration, ions eventually lead to bundling events. Such bundling was not observed in the case of monovalent ions for other IFs such as vimentin. These results help to understand the differences in structure formation in different IFs, leading to different mechanical roles in the cell.

BP 58.7 Thu 11:15 H44
Mechanical Properties of Single Vimentin Intermediate Filaments — •Johanna Block[1], Andrea Candelli[2], Jordi Ca-

banas Danes[3], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]LUMICKS, Amsterdam, The Netherlands — [3]Physics of Living Systems, VU Amsterdam, The Netherlands

The cytoskeleton plays a fundamental role for the mechanical integrity of biological cells. The cytoskeleton of eukaryotic cells is composed of three types of filaments: microfilaments (MFs) built up from actin monomers, microtubules (MTs) and intermediate filaments (IFs). While MFs and MTs have been of interest for biophysicists since decades, IFs moved to the center of attention only some years ago. The aim of our work is to characterize the mechanical properties of fluorescently labeled single vimentin filaments in solution. Using combined optical tweezers and fluorescent microscopy we test the mechanical properties of the filaments in a very controlled way and image them simultaneously. By analyzing the filament behavior under different stretching conditions and comparing glutaraldehyde-fixed and unfixed filaments, we gain knowledge about the stretchability, the elastic behavior and the involved molecular mechanisms such as subunit gliding or α-helix to β-sheet transition. From our data we hypothesize that many of the specific mechanical properties of IFs are encoded in their molecular architecture, which differs considerably from that of MTs and MFs. By probing single vimentin IFs we further the understanding of these important determinants for cell mechanics.

15 min break

Invited Talk BP 58.8 Thu 11:45 H44
Single molecule studies on myosin motors — •Claudia Veigel — Lehrstuhl Cellular Physiology and Center for Nanosciences (CENS), LMU München

Many types of cellular motility are based on the myosin family of motor proteins. There are now known to be at least 35 different classes of myosins, involved in intracellular transport processes, cytokinesis, muscle contraction, exo- and endocytosis or even signal transduction in vision or hearing. The ability to coordinate the timing of motor protein activation lies at the very centre of this wide range of cellular motile processes. Using a combined approach of recombinant protein expression and single molecule techniques including optical tweezers we study the basic mechanisms of activation, force production and movement of these molecular machines at the single molecule level. In this talk we will report on our recent studies on myosins class XXI and VI, which interact with lipids and transport cargo, such as cytoplasmic vesicles, over micrometer distances along the actin cytoskeleton in the cell.

BP 58.9 Thu 12:15 H44
Stabilization of small myosin II ensembles by mechanical load and ATP concentration — •Thorsten Erdmann, Kathrin Bartelheimer, and Ulrich S. Schwarz — Institute for Theoretical Physics and BioQuant, Heidelberg University, Heidelberg, Germany

Biological systems use ensembles of non-processive myosin II motor molecules to generate contractile forces. In muscle, large myosin II ensembles remain continuously attached to actin filaments to ensure effective force generation. In the cytoskeleton or in reconstituted actomyosin gels and motility assays, by contrast, small myosin II ensembles detach from actin with probabilities depending on both internal and external parameters. We study the influence of mechanical load and ATP concentration on small myosin II ensembles using a five-state crossbridge model. Increasing mechanical load or decreasing ATP concentration both increase the number of bound motors and stabilize ensemble attachment. While ensemble velocity is always reduced by increased mechanical load, lowering ATP concentration can increase ensemble velocity and stall force due to load-sharing between increased numbers of bound motors. To facilitate the use of our model in higher level modelling, we first reduce it to a three-state cross bridge model with conserved mean-first passage times in the motor cycle. Next, we exploit a separation of time-scales in the motor cycle to project the stochastic reaction network to a one-step master equation. We test the validity of each reduction step by comparison to the full model.

BP 58.10 Thu 12:30 H44
Structure and formation dynamics of stress fibers in adult stem cells — •Carina Wollnik[1], Benjamin Eltzner[2], Stephan Huckemann[2], and Florian Rehfeldt[1] — [1]Third Institute of Physics - Biophysics, Georg-August-University, Göttingen, Germany — [2]Institute for Mathematical Stochastics, Georg-August-University,

Göttingen, Germany

During differentiation, pluripotent adult human mesenchymal stem cells (hMSCs) become various cell types like nerve, bone or muscle precursor cells. Here, substrate stiffness is sufficient to guide hMSCs towards different lineages in the absence of additional biochemical stimuli [1]. Key players are stress fibres that generate and transmit contractile forces throughout the cell [3] and mediate cell-matrix mechanics. Characteristic reorganisation of stress fibres is detected within 24 hours and can be used as early morphological marker [2]. Using massive parallel life-cell imaging of RFP-Lifeact transfected hMSCs on substrates of different stiffness during early stem cell differentiation, we detect distinct pattern formation strategies of stress fibres, traced with novel 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 (2015) - to appear;

BP 58.11   Thu 12:45   H44

Force distributions in disordered fiber networks — •Knut M. Heidemann[1], Abhinav Sharma[2], Florian Rehfeldt[2], Christoph F. Schmidt[2], and Max Wardetzky[1] — [1]Institut für Numerische und Angewandte Mathematik, Georg-August-Universität, Göttingen, Germany — [2]Drittes Physikalisches Institut, Georg-August-Universität, Göttingen, Germany

Disordered fiber networks determine the mechanical response of many materials in nature. Due to the filamentous character of these networks, the strain field, and hence the force distributions, can be highly inhomogeneous. Large local stresses can result in an increased susceptibility for local rearrangements due to rupture or unbinding events.

In our study, we introduce a quantitative measure to characterize the emergence of highly stressed one-dimensional paths, so-called force chains, in three-dimensional nonlinear fiber networks. Furthermore, we provide an analytical approach, based on graph theory, that quantitatively describes the force distributions in one-dimensional periodic spring networks. Our analytical results are in excellent agreement with our numerical simulations.

BP 59: DNA, RNA and Related Enzymes

Time: Thursday 9:30–11:00   Location: H45

Invited Talk   BP 59.1   Thu 9:30   H45
RNA-based gene circuits in vitro and in vivo — •Friedrich Simmel — TU München, Garching, Germany

The sequence-progammability of nucleic acids not only allows the design of complex supramolecular structures, but also the realization of dynamically switchable molecular devices. In particular RNA-based switches can be utilized as "rationally designed" genetic regulators, and can thus be used for the realization of artificial gene regulatory circuits. In this talk, a variety of examples of dynamical systems will be described, which can be implemented with such components - either using in vitro gene transcription, cell-free gene expression, or even in vivo.

BP 59.2   Thu 10:00   H45
Knots in DNA and nanopore sequencing — •Stefanie Stalter, Florian Rieger, and Peter Virnau — Institut für Physik, JGU Mainz, Staudingerweg 9, 55128 Mainz

We determine knotting probabilities as a function of salt concentration for DNA strands of up to 150000 base pairs with coarse-grained Monte Carlo simulations. At this size DNA is highly knotted, which has severe implications for the future of nanopore sequencing devices. We also provide evidence for an entropic attraction of knots on the strand and demonstrate how two knots can pass through each other.

BP 59.3   Thu 10:15   H45
Accumulation and Replication in shallow thermal gradients: towards volcanic settings — •Michael Hartmann, Lorenz Keil, and Dieter Braun — Biophysics Department, Ludwig-Maximilians-Universität München, Amalienstraße 54, 80799 München, Germany

The most likely low concentration of molecules in a prebiotic ocean is a central problem for the origin of life. We have argued in the past that focused temperature gradients in hydrothermal, porous systems can thermophoretically accumulate, thermally cycle, and continuously feed the first prebiotic molecules for evolution [Mast, PRL 2010; Mast et al., PNAS 2013; Kreysing et al., Nature Chemistry 2015]. But the applied gradients of $10 - 100K/mm$ limit the scope of the approach to hydrothermal orifices.

We simulate in silico that a strong molecular accumulation (of nucleotides in particular) more than 10^{20}-fold still takes place in thermal gradients of $0.1K/mm$ ($100K/m$), about $100 - 1000$ fold more shallow than considered before. Accumulations remain stable under various pore widths and tilt angles. We investigate the stochastic thermal cycling of single molecules by two-dimensional random walk in the convection.

With the findings, more shallow gradients in steam heated, porous volcanic rock can be considered. This is important since wet-dry cycles under UV illumination seem important for the generation of nucleotides [Powner et al., Nature 2009]. To conclude, the study expands the thermal gradient scenario for the onset of molecular evolution towards shallow thermal gradients.

BP 59.4   Thu 10:30   H45
RNAi revised - target mRNA-dependent enhancement of gene silencing — •Simon Dornseifer[1], Sarah Willkomm[1], Rosel Kretschmer-Kazemi Far[1], Janine Libschwager[1], Foteini Beltsiou[1], Kirsten Frank[1], Sandra D. Laufer[1], Thomas Martinetz[2], Georg Sczakiel[1], Jens Christian Claussen[3,2], and Tobias Restle[1] — [1]Inst. Molecular Medicine, Univ. Lübeck — [2]INB, Univ. Lübeck — [3]Comp. Systems Biol., Jacobs Univ. Bremen

The discovery of RNA interference (RNAi) gave rise to the development of new nucleic acid-based technologies as powerful investigational tools and potential therapeutics. Mechanistic key details of RNAi in humans need to be deciphered yet, before such approaches take root in biomedicine and molecular therapy.

We developed and validated an in silico-based model [1] of siRNA-mediated RNAi in human cells in order to link in vitro-derived pre-steady state kinetic data with a quantitative and time-resolved understanding of RNAi on the cellular level. The observation that product release by Argonaute 2 is accelerated in the presence of an excess of target RNA in vitro inspired us to suggest an associative mechanism for the RNA slicer reaction where incoming target mRNAs actively promote dissociation of cleaved mRNA fragments. This novel associative model is compatible with high multiple turnover rates of RNAi-based gene silencing in living cells and accounts for target mRNA concentration-dependent enhancement of the RNAi machinery [1].

[1] S. Dornseifer et al, Nucleic Acids Research (Epub ahead of print 2015) http://dx.doi.org/10.1093/nar/gkv1200

BP 59.5   Thu 10:45   H45
The TASEP with reinitiation before the steady state — David W. Rogers, •Marvin A. Böttcher, Arne Traulsen, and Duncan Greig — Max Planck Institute for Evolutionary Biology, Plön, Germany

The *totally asymmetric simple exclusion process* (TASEP) was initially developed as a stochastic model for mRNA translation. It has subsequently attracted a lot of attention, since it can be applied to a variety of systems, including molecular transport, traffic, or spread of epidemics, and can be solved analytically in multiple cases. However, recent experimental evidence for the translation process shows a negative correlation between transcript length and observables such as ribosome density, protein abundance and codon adaption, which can not be explained with the original TASEP.

We examine the influence of ribosome reinitiation on translation, that is the finishing ribosome directly initiates again without leaving into the ribosome pool, by using an implementation of the TASEP with the Gillespie algorithm. In contrast to previous work we explicitly take the initial phase into account, before steady state is reached. Thereby we demonstrate that reinitation leads to a strong length dependency on both ribosome density on the transcript and protein yield consistent with current experimental evidence, allowing powerful prediction of translational regulation across eukaryotes.

BP 60: Pattern Formation (Joint Session with DY)

Time: Thursday 9:30–13:00   Location: H46

Invited Talk   BP 60.1   Thu 9:30   H46
Patterns formation through elastic instabilities, from thin sheets to twisted ribbons — •Pascal Damman — Université de Mons, Mons, Belgium

Hydrodynamics instabilities, such as Bénard-Marangoni convection, Rayleigh-Plateau, Rayleigh-Taylor and many others, are well known to produce beautiful patterns. Capillary, viscous and/or inertial forces conspire to generate very regular morphologies. In this seminar, we will see that elasticity can also produce complex structures, either regular or fully random, provided that slender objects are used. These objects are usually classified as rods, shells or sheets.

In the "classical picture", thin sheets constrained by external forces minimize the elastic energy through focalization of deformation in singularities. We will see that, due to geometric constraints, these origami structures cannot always be obtained. In the second part, the formation of very regular wrinkles in sheets "glued" on a soft foundation will be discussed. At the threshold, these wrinkles reflect the competition between various forces. For large deformations, however, the morphology is surprisingly determined by the nature of the foundation. Fold localization or period-doubling bifurcations are indeed observed for liquid or solid substrate, respectively. Finally, the effect of specific geometrical constraints produced by twisting thin ribbon of elastic materials will be discussed.

Finally, these various studies also highlight the effort of this growing interdisciplinary researcher community to the emergence of a global picture of elastic instability.

BP 60.2   Thu 10:00   H46
Shear driven instabilities in hard–core anisotropic colloids: Pressure tensor dynamics — •Henning Reinken, Rodrigo Lugo-Frias, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Systems of hard anisotropic particles display interesting flow induced behavior that modifies their internal structure and rheological properties [1, 2]. In soft matter theory, using the well known Doi–Hess approach, these systems have been studied in the bulk [3] and close to the boundaries [4].
Within this framework, we study how the pressure tensor is influenced by the average orientation of the particles coupled to the velocity field. To do so, we start from an isotropic or nematic equilibrium configuration and apply simple shear flow (Couette geometry) observing the emergence of instabilities (shear banding) in both scenarios. A novel finding is the appearance of coexisting stationary and oscillatory dynamics within the bands. We also discuss the resulting stress-strain relations.

[1] S. M. Fielding, Soft Matter, **3**, 1262-1279 (2007).
[2] J. K. G. Dhont, M. P. Lettinga, *et al.*, Faraday Discuss, **123**, 157-172 (2003).
[3] D. Strehober, H. Engel and S. H. L. Klapp, Phys. Rev. E **88**, 012505 (2013).
[4] S. Heidenreich, P. Ilg, and S. Hess, Phys. Rev. E **75**, 066302 (2007).

BP 60.3   Thu 10:15   H46
Towards a more thorough understanding of dislocation contributions in shape-memory alloys — •Heike Emmerich[1] and Julia Kundin[2] — [1]Universität Bayreuth, Lehrstuhl Material- und Prozesssimulation, Universitätsstraße 30, D-95447 Bayreuth — [2]Universität Bayreuth, Lehrstuhl Material- und Prozesssimulation, Universitätsstraße 30, D-95447 Bayreuth

The scientific interest in solid state cooling technologies has been renewed and increased since the discovery of of new materials with giant ferrocaloric effects - and with it the interest in understanding the hysteresis effects associated with the rise of crystal defect evolution as a result of plastic deformations at diverse time scales more thoroughly. In this contribution we show how phase-field modeling including elastic and plastic contributions tight to incoherent martensitic phase transitions can contribute to shade light into this scenario. Additionally we elucidate from a fundamental point of view how the associated enthalpic contributions can be reconciled and validated with atomistic concepts.

BP 60.4   Thu 10:30   H46
Pattern orientation in finite domains without boundaries — •Lisa Rapp, Fabian Bergmann, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate the orientation of nonlinear stripe patterns in finite domains. Motivated by recent experiments, we introduce a control parameter drop from supercritical inside a domain to subcritical outside without boundary conditions at the domain border. As a result, stripes align perpendicular to shallow control parameter drops. For steeper drops, non-adiabatic effects lead to a surprising orientational transition to parallel stripes with respect to the borders. We demonstrate this effect in terms of the Brusselator model and generic amplitude equations. Preprint available at arXiv:1512.05576 [cond-mat.soft]

BP 60.5   Thu 10:45   H46
Reflection and orientation of nonlinear traveling waves in finite domains without boundaries — •Fabian Bergmann, Lisa Rapp, and Walter Zimmermann — Theoretische Physik, Universitaet Bayreuth, Bayreuth, Germany

We investigate the reflection and orientation of nonlinear traveling waves in finite domains. In a finite domain (part of large system) the control parameter is assumed to be supercritical inside the domain and to drop to subcritical values outside. In 2d systems we find that a control parameter drop orients the propagation of traveling waves parallel to the domain boundaries. In quasi 1d systems steep control parameter variations at the ends of a finite domain cause reflections of traveling waves. Steep drops may also lead to complex spatio-temporal scenarios inside the finite domain. This study is motivated by recent experiments [1], where traveling waves in finite stripes have been investigated. Our analysis is compared with a recent work on stationary stripe patterns in finite domains without boundary conditions for the dynamical fields [2].
[1] J. Schweizer, M. Loose, M. Bonny, K. Kruse, I. Moench, P. Schwille, Proc. Natl. Acad. Sci. (USA)109, 15283 (2012)
[2] L. Rapp, F. Bergmann, W. Zimmermann, arXiv:1512.05576 (2015)

15 min. break

BP 60.6   Thu 11:15   H46
Self-assembly in colloidal systems with tunable particle interactions — •Hauke Carstensen, Vassilios Kapaklis, and Max Wolff — Dept of Physics & Astronomy, Box 516, SE-751 20 Uppsala, Sweden

We present a system that allows tunable magnetic self-assembly of microbeads. Two types of beads, magnetic and non-magnetic ones, are dispersed in a ferrofluid (FF), which alters their effective magnetic behaviour. By changing the FF concentration, the interactions between the beads can be tuned. The particles are confined in two dimensions. Depending on the interaction and the particle composition, lattices like square or hexagonal are assembled. Additionally, in less dense conditions metastable structures like branching chains are observed. The samples are analysed by transmission optical microscopy and images are taken in a scanning mode. Sets of images can be stitched together to create large scale maps of each sample. The particle positions are extracted by image analysis. Phases are detected via characteristic angles and lattice constants. A phase diagram is created by combining the observed phases with the particle interactions and the sample compositions. This can be applied to the fundamental understanding of colloidal crystal formation and chain formation in magnetorheological fluids.

BP 60.7   Thu 11:30   H46
Subcritical chaos and localized convection in the asymptotic suction boundary layer over a heated plate — •Stefan Zammert[1] and Bruno Eckhardt[1,2] — [1]Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]J.M. Burgerscentrum, Delft University of Technology, 2628 CD Delft, The Netherlands

The asymptotic suction boundary layer over a heated plate, a parallel and open flow, can be considered as a model for the properties of thermal boundary layers. A stability analysis of the base state

shows that the flow undergoes a subcritical instability with increasing Rayleigh number. This instability creates spatially periodic convection patterns. We will show how bifurcations of these secondary solutions create a chaotic attractor in the subcritical regime which is turned into a chaotic saddle by a crisis bifurcation. Long-wavelength instabilities of the secondary solutions create various stationary convection solutions which are localized in one or two directions parallel to the plate. These localized structures also exist in subcritical regime and can potentially be used to study plume dynamics in thermal boundary layers.

BP 60.8   Thu 11:45   H46

Spontaneous autocatalysis in a primordial broth — •Sabrina Scherer[1], Eva Wollrab[2], Varun Giri[1], and Albrecht Ott[1] — [1]Biologische Experimentalphysik, Universität des Saarlandes — [2]Laboratory of Microbial Morphogenesis and Growth, Institut Pasteur

Driven non-linearities lead to pattern formation. Here 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. Using real-time mass spectrometry, we observe the generation of a primordial broth composed of thousands of different molecules in a mass range from 50 to 1000 Dalton. The temporal development of the primordial broth reveals the spontaneous emergence and disappearance of oligomeric surfactants. Strong non-linearities are required for these aperiodic chemical oscillations. The phenomenon is robust against different gas compositions and concentrations, temperatures and many details of the experimental set-up. We analyze the chemical composition of the solution by different methods like (high-resolution) mass spectrometry, NMR and gas-chromatography to find high-reactive molecules and possible catalysts. We find that oxidation and doping with small amounts of an active broth can trigger the production of the oligomers. We suggest that surface active molecules lead to phase transfer catalysis in the oil/water mixture and self-organize to a spontaneously emerging autocatalytic network.

BP 60.9   Thu 12:00   H46

A Protein Flux-based Mechanism for Midcell Sensing in Bacteria — •Silke Bergeler[1], Dominik Schumacher[2], Lotte Søgaard-Andersen[2], and Erwin Frey[1] — [1]ASC for Theoretical Physics, Ludwig-Maximilians-Universität, München, Germany — [2]Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

Precise positioning of the cell division site is crucial for the correct separation of the genetic material into the two daughter cells. In myxobacteria a cluster of Pom proteins (PomX, PomY, PomZ) is formed on the chromosome that performs a biased random walk to midcell and positively regulates cell division. To investigate how the Pom cluster, consisting of PomX and PomY, moves to midcell, we introduce a mathematical model in which PomZ dimers can attach to, diffuse on the nucleoid and can hydrolyze ATP and subsequently detach from the nucleoid primarily at the cluster. 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, but it is not known how the force to move the cluster is generated. We model the PomZ dimers as springs, based on the observation that the bacterial chromosome and several proteins have elastic properties. As springs the PomZ dimers can exert a force on the PomXY cluster. Our model explains mid-plane localization of the Pom cluster. It predicts a decrease in the efficiency to find midcell for a large number of PomZ dimers in the cell and small ATP-hydrolysis rates of the ATPase PomZ, which is in agreement with our experimental findings. In summary, our study provides new mechanistic insights into intracellular positioning.

BP 60.10   Thu 12:15   H46

Cyclosis-mediated transfer of reactive oxygen species and its relation to the formation of pH bands in Chara alga cells — •Alexey Eremin[1], Ralf Stannarius[1], Anna Komarova[2], and Alexander Bulychev[2] — [1]Institute of Experimental Physics,

Otto von Guericke University Magdeburg — [2]Faculty of Biology, Lomonosov Moscow State University, 119992 Moscow, Russia

In internodal cells of characean algae, cyclosis participates in formation of light-dependent patterns of surface pH and photosynthetic activity. Hydrogen peroxide, being a signalling molecule and a stress factor, is known to accumulate under excessive irradiance. In our study, we explore the spatio-temporal dynamics of pH-band formation on the surfaces of internodal Chara corallina cells and study the kinetics of H2O2 production in chloroplasts and its release into the cytoplasm under local illumination. We demonstrate that in cells exhibiting active streaming, H2O2 first accumulates in the illuminated region and then enters into the streaming cytoplasm. The results suggest that H2O2 released from chloroplasts is transported along the cell with the cytoplasmic flow. It is proposed that the shift of cytoplasmic redox poise and light-induced elevation of cytoplasmic pH facilitate the opening of H+/OH-permeable channels in the plasma membrane.

BP 60.11   Thu 12:30   H46

Improvement of unpinning and termination of spiral waves by reducing excitability — •Jiraporn Luengviriya[1], Malee Sutthiopad[2], Metinee Phantu[2], Porramain Porjai[2], Jarin Kanchanawarin[2], Stefan C. Müller[3], and Chaiya Luengviriya[2] — [1]Department of Industrial Physics and Medical Instrumentation, King Mongkut's University of Technology North Bangkok, Thailand — [2]Department of Physics, Kasetsart University, 50 Phaholyothin Road, Jatujak, Bangkok 10900, Thailand — [3]Institute of Experimental Physics, Otto-von-Guericke University Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Spiral waves are common found in excitable systems. Such waves may drift and eventually annihilate at the boundary. However, they can be stabilized when pinned to obstacles. Spiral waves of electrical excitations in cardiac systems connect to some arrhythmias so that they should be eliminated. We present an investigation of the release of pinned spiral waves from unexcitable obstacles and the termination of free spiral waves at the boundary in a reaction-diffusion system. An advective field is applied as the external forcing. For a given obstacle size, the critical value of advection to release as well as that to terminate the spiral waves decrease when the excitability of the system is reduced. Therefore, this study shows that decreasing the excitability can facilitate elimination of spiral waves, either in the presence of obstacles or not.

BP 60.12   Thu 12:45   H46

Coexistence of stable branched patterns in anisotropic inhomogeneous systems — Badr Kaoui[1,2], Achim Guckenberger[1], Alexei Krekhov[1,3], Falko Ziebert[1,4], and •Walter Zimmermann[1] — [1]Theoretische Physik, Universitaet Bayreuth, Bayreuth, Germany — [2]Biomechanics and Bioengineering, Universite de Technlogie de Compiegne, Compiegne, France — [3]Max-Planck-Institute for Dynamics and Self-Organization, Goettingen, Germany — [4]Physikalisches Institut, Albert-Ludwigs-Universitaet Freiburg, Freiburg, Germany

A new class of pattern forming systems is identified and investigated: anisotropic systems that are spatially inhomogeneous along the direction perpendicular to the preferred one. By studying the generic amplitude equation and a model equation, we show that branched stripe patterns emerge, which for a given parameter set are stable within a band of different wavenumbers and different numbers of branching points (defects). Moreover, the branched patterns and unbranched ones (defect-free stripes) coexist over a finite parameter range. We propose two systems where this generic scenario can be found experimentally, surface wrinkling on elastic substrates and electroconvection in nematic liquid crystals, and relate them to the findings from the amplitude equation.

B. Kaoui, A. Guckenberger, A. Krekhov, F. Ziebert, W. Zimmermann, New J. Phys. 17, 103015 (2015); B. A. Glatz, M. Tebbe, B. Kaoui, R. Aichele, C. Kuttner, A. E. Schedl, H.-W. Schmidt, W. Zimmermann, A. Fery, Soft Matter 11, 3332 (2015)

BP 61: Anomalous Diffusion in Complex Environments (Focus Session)

Joint session with DY, organized by Reza Shaebani and Ludger Santen, Saarland University, for BP.

Time: Thursday 11:30–13:00   Location: H45

BP 61.1   Thu 11:30   H45

Apparent Super-Diffusion Induced by Trail-Mediated Self-Interaction of Microorganisms — •Till Kranz, Anatolij Gelimson, and Ramin Golestanian — Rudolf-Peierls Centre for Theoretical Physics, University of Oxford

Many microorganisms, namely surface bound bacteria [1] and amoeboid slime moulds [2], leave trails of sticky substances. We will present a simple model of a self-propelled microorganism whose propulsion force depends on the concentration of trail material [3]. The trail-mediated self-interactions of a single microorganism and its own trail profoundly alter the dynamics. Above a critical interaction strength with the trail a discontinuous localisation transition emerges. Close to the transition, the orientational dynamics becomes super-diffusive and, in fact, super-ballistic, on a diverging timescale. Interestingly, no such super-diffusive regime appears for the translational dynamics. We will discuss the implications for real biological systems and the interplay of their finite timescales with the emergent diverging timescale.
[1] K. Zhao *et al.*, Nature **497**, 388 (2013)
[2] B. Rodiek and M. J. B. Hauser, EPJ ST **224**, 1199 (2015)
[3] W. T. Kranz, A. Gelimson, and R. Golestanian, arXiv:1504.06814

BP 61.2   Thu 11:45   H45

Transport of active Brownian particles in complex environments — •Maria Zeitz and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

From the perspective of physics, biological microswimmers such as bacteria can be viewed as active particles. Since bacteria often inhabit porous or crowded environments, we examine the dynamics and transport of active particles in a complex environment. We focus on active Brownian particles (APB), which provide a simple model for microswimmers. ABPs have an intrinsic speed and perform rotational as well as translational diffusion.

We study the transport of ABPs moving in a two-dimensional environment of randomly placed and fixed obstacles of a given area fraction ϕ_o. For increasing ϕ_o we observe a transition from diffusive transport to trapping on long time scales, which happens close to the percolation threshold of the void space $1 - \phi_0 \approx 0.67$. The behavior on long time scales is universal and depends only on the obstacle density and not on the intrinsic dynamics of the particle. However, on time scales much shorter than the rotational diffusion time, we find ballistic transport and on intermediate timescales we find subdiffusive transport. The crossover times between the three regimes depend not only on ϕ_o but also on the details of particle propulsion, e.g. Peclét number.

In a second step we study how obstacles can serve as nucleation seeds for clustering in collective motion of ABPs and therefore promote clogging.

BP 61.3   Thu 12:00   H45

Impact of detachment frequency on transport dynamics of cytoskeletal motor proteins — •Anne E Hafner, M Reza Shaebani, Ludger Santen, and Heiko Rieger — Department of Theoretical Physics, Saarland University, Saarbrücken, Germany

Cytoskeletal motor proteins are involved in key intracellular transport processes which are vital for maintaining appropriate cellular function. The motors exhibit distinct states of motility: active motion along filaments, and inactive state in which the motor detaches from the filament and remains effectively stationary by performing passive diffusion in the vicinity of the detachment point due to cytoplasmic crowding until it attaches again to the cytoskeleton. The rates of transitions between motion and pause states are considerably affected by changes in environmental conditions which influences the efficiency of cargo delivery to specific targets. By considering the motion of molecular motor on a single filament as well as a dynamic filamentous network, we present an analytical model for the dynamics of self-propelled particles which undergo frequent pause phases, and validate the theoretical predictions by performing extensive Monte Carlo simulations. The transition rates between the two states drastically change the dynamics: multiple transitions between different types of anomalous diffusive dynamics may occur and the crossover time to the asymptotic diffusive or ballistic motion varies by several orders of magnitude. We map out the phase

diagrams in the space of transition rates, and address the role of initial conditions of motion on the resulting dynamics.

BP 61.4   Thu 12:15   H45

The Power Spectrum of Ionic Nanopore Currents: The Role of Ion Correlations — •mira zorkot, Ramin Golestanian, and Douwe Jan Bonthuis — Rudolf Peierls Centre for Theoretical Physics, Oxford University, Oxford, OX13NP, United Kingdom

Measuring the ionic current passing through a nanometer-scale membrane pore has emerged over the past decades as a versatile technique to study molecular transport. These measurements su*er from high noise levels that typically exhibit a power law dependence on the frequency. A thorough theoretical understanding of the power spectrum is essential for the optimisation of experimental setups and for the use of measurement noise as a novel probe of the nanopores microscopic properties.

We calculate the power spectrum of electric-*field-driven ion transport through nanopores using both linearized mean-fi*eld theory and Langevin dynamics simulations. With only one *tting parameter, the linearized mean-*field theory accurately captures the dependence of the simulated power spectrum on the pore radius and the applied electric *field. Remarkably, the linearized mean-*field theory predicts a plateau in the power spectrum at low frequency f, which is con*rmed by the simulations at low ion concentration. At high ion concentration, however, the power spectrum follows a power law that is reminiscent of the $1/f$ dependence found experimentally at low frequency. Based on simulations with and without ion-ion interactions, we attribute the low-frequency power law dependdence to ion-ion correlations.

BP 61.5   Thu 12:30   H45

Fluctuation relations for anomalous dynamics generated by time fractional Fokker-Planck equations — Peter Dieterich[1], •Rainer Klages[2,3], and Aleksei V. Chechkin[2,4,5] — [1]Institut fuer Physiologie, Technische Universitaet Dresden — [2]Max Planck Institute for the Physics of Complex Systems, Dresden — [3]Queen Mary University of London, School of Mathematical Sciences — [4]Institute for Theoretical Physics NSC KIPT, Kharkov, Ukraine — [5]Institute of Physics and Astronomy, University of Potsdam

Anomalous dynamics characterized by non-Gaussian probability distributions (PDFs) and/or temporal long-range correlations can cause subtle modifications of conventional fluctuation relations (FRs). As prototypes we study three variants of a generic time-fractional Fokker-Planck equation with constant force. Type A generates superdiffusion, type B subdiffusion and type C both super- and subdiffusion depending on parameter variation. Furthermore type C obeys a fluctuation-dissipation relation whereas A and B do not.We calculate analytically the position PDFs for all three cases and explore numerically their strongly non-Gaussian shapes. While for type C we obtain the conventional transient work FR, type A and type B both yield deviations by featuring a coefficient that depends on time and by a nonlinear dependence on the work.We discuss possible applications of these types of dynamics and FRs to experiments.
P. Dieterich et al., New J. Phys. **17**, 075004 (2015)

BP 61.6   Thu 12:45   H45

Induced anomalous diffusion nearby cell membranes — •Abdallah Daddi-Moussa-Ider, Achim Guckenberger, and Stephan Gekle — Biofluid Simulation and Modeling, University of Bayreuth, 95440 Bayreuth, Germany

The approach of a small particle to the cell membrane represents the crucial step before active internalization and is governed by thermal diffusion. Using a fully analytical theory, we show that the membrane induces a long-lived subdiffusive behavior on the nearby particle, during which the residence time is increased by up to 50 % for a typical scenario. The corresponding scaling exponent is found to be as low as 0.87 in the perpendicular direction, and as low as 0.92 in the parallel direction. Such behavior is qualitatively different from the normal diffusion near a hard wall or in a bulk fluid. A good agreement is found for the frequency dependent mobility between the analytical predictions and the numerical simulations that we performed using a boundary integral method.

BP 62: Biomaterials and Biopolymers II (Joint Session MM/CPP/BP)

Time: Thursday 11:45–13:00   Location: H52

BP 62.1   Thu 11:45   H52

Stimuli responsiveness of electron irradiated gelatin — •STEFANIE RIEDEL[1,2], EMILIA I. WISOTZKI[1,2], KATHARINA APEL[1], WOLFGANG KNOLLE[1], and STEFAN G. MAYR[1,2] — [1]Leibniz-Institut für Oberflächenmodifizierung, Leipzig — [2]Fakultät für Physik und Geowissenschaften, Universität Leipzig

Stimuli responsive materials have attracted considerable interest during the past years due to their potential use in sensor and actuator applications. They are designed to transform small external stimuli e.g. temperature and humidity changes into a significant response.

While a large number of alloys or synthetic polymers are well-established at this point, we explore the potential of the biomaterial gelatin to respond to humidity changes. We demonstrate how irradiation with high-energetic electrons allows fine-tuning of the response. In addition, this treatment enhances thermal stability providing high attractiveness for biomedical applications.

BP 62.2   Thu 12:00   H52

Langzeitverhalten von Seide und "Selbstheilung" — •JAN ROSIGKEIT[1], IGOR KRASNOV[1] und MARTIN MÜLLER[1,2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel — [2]Institut für Werkstoffforschung, Helmholtz-Zentrum Geesthacht

Durch Streckexperimente haben wir mechanische Eigenschaften des biologischen Nanokomposits Seide unter Verwendung eines Modells aus der linearen viskoelastischen Theorie [1] über lange Zeiten bestimmt. Wir stellen fest, dass sich die mechanischen Eigenschaften der Seide auf langen Zeiten "fraktional" viskoelastisch ("Memory"-Effekt) beschreiben lassen.

Seidenfasern können sich in zwei Zuständen befinden. Einer dieser Zustände ist ein stabiler Zustand der nicht vorgestreckten Faser. Der andere Zustand wird durch äußere Krafteinwirkung hervorgerufen, wodurch eine vorgestreckte Faser entsteht. Wir haben experimentell gezeigt, dass der Übergang vom vorgestreckten zum Anfangszustand in einer nassen Umgebung innerhalb von 24 Stunden stattfindet. Der vorgestreckte Zustand ist daher ein metastabiler Zustand. [2]

[1] W. Glöckle und T. Nonnenmacher, Macromol., **24:**6426-6434 (1991).
[2] J. Rosigkeit, Bachelorarbeit, Christian-Albrechts-Universität Kiel (2014).

BP 62.3   Thu 12:15   H52

Fractional dynamics in silk — •IGOR KRASNOV[1], TILO SEYDEL[3], and MARTIN MÜLLER[2] — [1]IEAP, Universität Kiel, Germany — [2]Institute of Materials Research, HZG, Germany — [3]ILL, Grenoble, France

Structural relaxations in humid silk fibers exposed to tensile stress have been observed to take place on a very wide range of time scales from a few milliseconds to several hours. The time-dependence of the measured tensile force following a quasi-instantaneously applied external strain on the fibers can be understood in terms of a fractional viscoelastic relaxation function introducing memory effects by which the mechanical state of a fiber depends on its tensile history. [1] An analog fractional relaxation also gives rise to the subdiffusion observed on picosecond time scales, which governs the mobility of the amorphous polymer chains and adsorbed water on the molecular level. The reduction of the subdiffusive memory effect in stretched fibers compared to native fibers is consistent with the higher order of the polymers in the stretched state.

[1] I. Krasnov, T. Seydel, and M. Müller, Phys. Rev. E 91, 042716 (2015)

BP 62.4   Thu 12:30   H52

Mechanical properties of branched actin filaments — •MOHAMMADHOSEIN RAZBIN[1], MARTIN FALCKE[3,4], PANAYOTIS BENETATOS[5], and ANNETTE ZIPPELIUS[1,2] — [1]Georg August University — [2]Max Planck Institute for Dynamics and Selforganization — [3]Humboldt University — [4]Max Delbrueck Center for Molecular Medicine — [5]Kyungpook National University

Motile cells on a 2dimensional substrate generate motion by flat membrane protrusion called lamellipodia. Within lamellipodia, actin filaments are generated by branching off existing ones, giving rise to branched network structures. We investigate the force-extension relation of branched actin filaments, grafted on an elastic substrate at one end and pushing with the free ends against a flat and stiff wall. We compute the thermal fluctuation of the endpoints and the resulting entropic forces on a membrane, restricting the fluctuations of the endpoints. The entropic forces are shown to depend sensitively not only on the persistence length but also on the geometry of the structure. It depends on branch point position and filament orientation, being most pronounced for intermediate tilt angles and intermediate branch point positions. We describe filament networks without cross-linkers to focus on the effect of branching. We compare properties of branched and unbranched networks. The ratio of the network average of the force per branched filament to the average force per unbranched filament exhibits compression dependence and may go up to about 4.5 in networks with a narrow orientation distribution. With orientation distributions measured in lamellipodia, it is about 2.

BP 62.5   Thu 12:45   H52

Tension, Balance and Flex: Auxetic periodic tensegrities — •MYFANWY EVANS — TU Berlin, Berlin, Germany

We present here a class of triply-periodic tensegrity structures that have a negative Poisson's ratio: they are auxetic. These theoretical materials are derived from periodic rod packings or more general periodic filament packings with a dilatant property. We show that these chiral tensegrity structures are periodically rigid but affinely flexible. The affine flex leads to isotropic expansion or contraction. A parallel can be drawn between these tensegrity structures and woven materials with elastic filaments, which also display an auxetic behaviour. Such materials are an exciting target for functional materials and biomaterials, from metal-organic frameworks to woven polymeric or filamentous structures.

BP 63: Plenary Talk of Ben Schuler

Time: Thursday 14:00–14:45   Location: H15

Plenary Talk   BP 63.1   Thu 14:00   H15
Single-Molecule Spectroscopy of Biomolecular Dynamics at the Nanoscale — •BEN SCHULER — University of Zurich, Switzerland

Proteins are the most versatile constituents of the molecular machinery of life. Understanding their remarkable mechanisms of self-organization and their functional properties requires detailed knowledge of their structure and dynamics. Single-molecule spectroscopy provides an opportunity for investigating these properties on nanometer lengthscales and down to nanosecond timescales. By probing individual molecules, both structural and dynamic heterogeneity, which would be hidden in the ensemble average, can often be identified. Förster resonance energy transfer (FRET) combined with correlation spectroscopy, microfluidics, and the quantitative analysis of photon statistics enables us to probe distances, distance distributions, and both the equilibrium and non-equilibrium dynamics of biomolecules, even in complex environments, including live cells. A thorough understanding of the physics underlying biomolecular behavior is becoming accessible via the growing synergy of experiment with analytical theory and molecular simulations. I will present the basic conceptual and experimental ideas, and illustrate them with recent investigations of the dynamics, folding, assembly, and interactions of proteins in the context of their roles in living systems.

BP 64: Symposium - Anomalous Diffusion in Complex Environments (SYAD)

Time: Thursday 15:00–17:45   Location: H15

Invited Talk   BP 64.1   Thu 15:00   H15
Phenomenology of Collective Chemotaxis in Artificial and Living Active Matter — •Ramin Golestanian — University of Oxford

The non-equilibrium dynamics of active particles that send and receive chemical signals could lead to enhanced and/or anomalous diffusion, as well as spontaneous formation of interesting structures and patterns due to the long-range nature of the interactions. We examine theoretically the consequences of this interaction, and present some results that exemplify the type of emergent properties that could result from them, including: spontaneous formation of small stable clusters or "molecules" that can exhibit functionality that depends on geometry, collective chemotaxis in a solution of catalytically active colloids that could lead to cluster formation, aster condensation, and spontaneous oscillations, swarming - in the form of a comet - of light-induced thermally active colloids with negative Soret coefficient due to a shadowing interaction, and collective behaviour of a colony of cells that divide and interact chemotactically.

Invited Talk   BP 64.2   Thu 15:30   H15
First-passage times of Markovian and non Markovian random walks in confinement — •Raphael Voituriez — CNRS/ Université Pierre et Marie Curie, Paris, France

The first-passage time is a key quantity for evaluating the kinetics of various processes, and in particular chemical reactions involving "small" numbers of particles. A striking example is given by gene transcription, where specific proteins search for target sequences on DNA. I will present asymptotic results which enable the evaluation of the distribution of the first-passage time to a target site for a wide range of random processes in confined domains, and show how these results can be extended to non Markovian processes.

Invited Talk   BP 64.3   Thu 16:00   H15
Cytoskeleton organization as an optimized, spatially inhomogeneous intermittent search strategy — •Heiko Rieger, Yannick Schröder, and Karsten Schwarz — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

The efficiency of intracellular transport of cargo from specific source to target locations is strongly dependent upon molecular motor assisted motion along cytoskeleton filaments, microtubules and actin. Radial transport along microtubules and lateral transport along the filaments of the actin cortex underneath the cell membrane are characteristic for cells with a centrosome. Here we show that this specific filament organization for ballistic transport in conjunction with intermittent diffusion realizes a spatially inhomogeneous intermittent search strategy that is in general optimal for small thicknesses oft he actin cortex. We prove optimality in terms of mean first passage times for three different, frequently encountered intracellular transport tasks: 1) the narrow escape problem (e.g. transport of cargo to a synapse or other specific region of the cell membrane), 2) reaction kinetics enhancement (e.g. binding of two mobile reaction partners within the cell), 3) the reaction-escape problem (e.g. release of cargo at a synapse after in-

tracellular vesicle pairing). Since homogeneous search strategies could only be realized by completely filling the search volume with randomly oriented cytoskeleton filaments, our results indicate that living cells realize optimal search strategies for various intracellular transport problems *economically* through a spatial cytoskeleton organization that involves only small amounts of randomly oriented actin filaments.

15 min break

Invited Talk   BP 64.4   Thu 16:45   H15
Ergodicity violation and ageing in living biological cells — •Ralf Metzler — Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

In 1905 Einstein formulated the laws of diffusion, and in 1908 Perrin published his Nobel-prize winning studies determining Avogadro's number from diffusion measurements. With similar, more refined techniques the diffusion behaviour in complex systems such as the motion of tracer particles in living biological cells is nowadays measured with high precision. Often the diffusion turns out to deviate from Einstein's laws.

This talk will discuss the basic mechanisms leading to anomalous diffusion as well as point out the physical and biological consequences, for instance, in gene regulation or cargo transport in cells. In particular the unconventional behaviour of non-ergodic, ageing systems will be discussed. Concrete examples include the motion of submicron and nanoprobes in biological cells, uncrowded and crowded lipid membranes, as well as interacting many particle systems.

Invited Talk   BP 64.5   Thu 17:15   H15
Anomalous diffusion within cells — Sarah Klein[1,2], •Cecile Appert-Rolland[1], and Ludger Santen[2] — [1]Laboratory of Theoretical Physics, CNRS, Univ. Paris-Sud, Bat 210, 91405 Orsay, France — [2]Fachrichtung Theoretische Physik, Univ. des Saarlandes D-66123 Saarbrücken, Germany

Within cells, various objects (vesicles, organelles,...) need to be transported. Some processive molecular motors get attached to these objects (or cargos) to form a complex that will have a stochastic motion along a network of microtubules. Intriguingly, there is some evidence that this motion results from a tug-of-war between teams of motors that pull in opposite directions.

A stochastic model for cargo-motors complex allows us to study the properties of the resulting motion along a single microtubule. We find some anomalous diffusion, both subdiffusive or superdiffusive depending on the timescale. Interestingly, such anomalous diffusion has indeed been observed experimentally. I will discuss the importance of fluctuations in the dynamics, and present some hypotheses why nature chose such a transport process to carry cargos through the crowded interior of cells.

[Klein, Appert-Rolland, Santen, EPL 107 (2014) 18004,
Eur. Phys. J. Special Topics 223 (2014) 3215,
EPL 111 (2015) 68005]

BP 65: Membranes and Vesicles II

Time: Thursday 15:00–16:15   Location: H43

Invited Talk   BP 65.1   Thu 15:00   H43
Design features of a membrane-assisted protein oscillator — •Petra Schwille — Max Planck Institute of Biochemistry, Martinsried

The MinCDE protein machinery, which orchestrates the positioning of the division ring in E.coli bacteria, shows a distinct oscillation of protein concentrations between the two cell poles, which are based on self-organization through reaction-diffusion. We have been able to reconstitute these self-organized oscillations of purified proteins in artificial cell-shaped compartments, as well as the faithful downstream positioning of protofilaments of the Z division ring. This could be the first step towards autonomous division of an artificial cell system which we aim to establish in a bottom-up synthetic biology approach. In my

talk, I will discuss the design features of this very simple and archetypical kind of a biological oscillator and particularly highlight the role of the membrane, acting as a heterogenous catalyst and providing spatial cues in two and three dimensions.

BP 65.2   Thu 15:30   H43
Electrostatically driven formation of double lipid membranes studied by evanescent light scattering microscopy — Björn Agnarsson[1], Hannah Wayment-Steele[2], Sofia Svedhme[1], Fredrik Höök[1], and •Angelika Kunze[3] — [1]Dept. of Applied Physics, Chalmers Univ. of Technology, Göteborg, Sweden — [2]Dept. of Chemistry, Pomona College, CA, USA — [3]Inst. of Physical Chemistry, Univ. of Göttingen, Göttingen, Germany

Since their introduction, solid-supported lipid membranes (SLMs) have been widely and successfully applied as platforms to study membrane-related processes and interactions. Remaining challenges when it comes to model studies involving SLMs are to ensure the formation of defect-free membranes and to minimize side effects of the underlying substrate. As a consequence, great efforts have been devoted to the development of surface sensitive techniques allowing for the characterization of SLM formation as well as to the development of highly mobile membranes or multiple membranes. Here, the formation of a highly fluid SLM and a double lipid membrane is demonstrated and monitored using label-free evanescence light scattering microscopy (EvSM) in combination with acoustic sensing and fluorescence microscopy. The dominating driving force for the formation of both lipid structures is electrostatic interaction. We propose this demonstrated approach to be a promising tool for the preparation of highly fluid lipid membranes and double membranes for the study of membrane processes. Furthermore, is EvSM shown to be and an excellent tool for probing membrane related interactions with a single vesicle resolution.

BP 65.3   Thu 15:45   H43
A new free energy-based lattice model of lipid membranes — ●Andreas Heuer and Davit Hakobyan — Institute f. Phys. Chemistry, WWU Münster

The thermodynamic properties of lipid mixtures in membranes are, on the one hand, strongly influenced by the specific enthalpic interactions among lipids and, on the other hand, by the entropic degrees of freedom of the hydrocarbon chains [1]. We suggest the formulation of a lattice model, each site corresponding to one lipid, where the enthalpic and the entropic effects are taken into account in a quantitative way. The chain entropy is reflected by an appropriately chosen order parameter distribution. All properties of the lattice model are extracted from atomistic molecular dynamics simulations of saturated and unsaturated lipids, respectively.

We can show via kinetic Monte Carlo simulations that the lattice model displays on a quantitative level the same temperature effects as the atomistic system. Specifically, we discuss gel formation for the pure saturated lipid and phase separation for a mixed system upon cooling. This agreement reflects the fact that the different free energy contributions of the atomistic system are contained in the lattice model.

[1] D.Hakobyan, A. Heuer, PLoS ONE 9/2, e87369 (2014).

BP 65.4   Thu 16:00   H43
An entropic attraction mediates vesicle tethering in early endosomes — ●Marcus Jahnel[1,2], David Murray[1], Marino Zerial[1], and Stephan Grill[1,2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Biotechnology Center, TU Dresden, Dresden, Germany

Vesicle tethering is mediated by long, rather rigid coiled-coil membrane proteins that can bind Rab GTPases at their free end. Yet it is still unclear how these large fibrous proteins help to decrease the initial separation between two membranes for downstream docking and fusion. Which mechanism brings the two ends together?

Here, we address this question with a minimal tethering system consisting of the small GTPase Rab5 and the coiled-coil tethering protein early endosome antigen 1 (EEA1). Importantly, we show through a combination of high-resolution optical tweezer and EM experiments that EEA1 undergoes a global conformational change upon binding to Rab5 in the presence of GTP.

In the unbound (free) state EEA1 is rather rigid with a persistence length larger than its contour length of around 220 nm. However, in the bound state, the EEA1 dimer adopts a more flexible configuration with a persistence length of < 30 nm. This sudden, over 10-fold reduction in persistence length upon binding gives rise to an elegant physical mechanism for vesicle capture and tethering: an entropic collapse force — the result of an extended rigid structure suddenly becoming more flexible — pulls the membranes together to potentially initiate docking and fusion.

BP 66: Biomaterials and Biopolymers III (Joint Session BP/CPP/MM)

Joint session with CPP and MM organized by BP.

Time: Thursday 15:00–16:15   Location: H45

BP 66.1   Thu 15:00   H45
Contribution of Biofilm Matrix Components to Physical Material Properties of Bacterial Biofilms — ●Sara Kesel, Stefan Grumbein, Ina Gümperlein, Anna-Kristina Marel, Marwa Tallawi, Oliver Lieleg, and Madeleine Opitz — Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany

Bacteria can be protected from antibiotics, chemicals and mechanical stresses by a self-produced matrix, the so called biofilm. As biofilms can grow on various surfaces such as medical implants, this poses a big problem in health care and industry. Biofilm matrices can thereby consist of different extracellular substances (EPS) such as polysaccharides, proteins, lipids and nucleic acid. Understanding of the individual contributions to the above described resistances by the different biofilm matrix components is therefore necessary, in order to prevent and fight biofilm growth. In particular, it is important to understand at what stage of biofilm formation the observed resistances are developed. In this study, different stages of biofilm growth (attachment of single cells, microcolony growth, as well as mature biofilms) were investigated using several techniques such as e.g. cantilever arrays, time-lapse microscopy and atomic force microscopy. The attachment of single bacteria onto solid surfaces and further physical material properties of two B. subtilis wild-type strains that differ in their biofilm matrix composition were analyzed. Furthermore, using several mutant strains the impact of specific biofilm matrix elements on the observed biofilm properties was quantitatively analyzed.

BP 66.2   Thu 15:15   H45
Multiple bio-functionalization in 3D-scaffolds for cell manipulation realized by orthogonal (photo)chemistry — ●Vincent Hahn[1], Benjamin Richter[2], Tanja Claus[3,4], Guillaume Delaittre[3,5], Christopher Barner-Kowollik[3,4], Martin Wegener[1,6], and Martin Bastmeyer[2] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT) — [2]Zoological In-

stitute and Institute for Functional Interfaces, KIT — [3]Institute for Chemical Technology and Polymer Chemistry, KIT — [4]Institute for Biological Interfaces, KIT — [5]Institute for Toxicology and Genetics, KIT — [6]Institute of Nanotechnology, KIT

In recent years, we have applied Direct Laser Writing to fabricate 3D-microscaffolds for culturing cells in a well-defined environment and investigated cellular responses, e.g., contractility, adhesion and shape.

By sequential writing of different photoresists, patterned scaffolds are realized. They consist of protein-binding polymers next to regions containing light-activatable monomers in a non-protein binding background. Upon light-activation we were able to biotinylate specific regions in the passivating backbone. When incubated with a protein solution, proteins adsorb only onto protein-binding polymer areas. The biotin-linker is subsequently addressed by using avidin and any other biotinylated protein of choice. This technique has been successfully applied to fabricate scaffolds functionalized with two different adhesion proteins that selectively direct cell adhesion.

Such scaffolds might prove useful for applications in tissue engineering and stem cell differentiation.

BP 66.3   Thu 15:30   H45
Different protein adsorption rates on different grain orientations in hydroxyapatite — ●Thomas Faidt, Jörg Schmauch, Michael Deckarm, Samuel Grandthyll, Frank Müller, and Karin Jacobs — Saarland University, Dept. of Experimental Physics, 66041 Saarbruecken

As a model system for tooth enamel, hydroxyapatite (HAP) pellets with a density of $> 97\%$ of the theoretical crystallographic density of HAP have been produced by compacting and sintering commercially available HAP powder. Atomic force microscopy (AFM) combined with electron backscatter diffraction (EBSD) measurements reveal the smoothness and the crystal orientation of the HAP grains on the surface of the pellets. On these surfaces, single molecule BSA adsorption experiments are performed in a microfluidic setup and reveal that

different grain orientations provoke different adsorption rates. These findings open a pathway to control protein adsorption.

BP 66.4 Thu 15:45 H45
Studying Biomineralization with ultrathin silica sheets grown at the air-water interface. — •Helmut Lutz[1], Vance Jaeger[2], Rüdiger Berger[1], Mischa Bonn[1], Jim Pfaendtner[2], and Tobias Weidner[1] — [1]Max Planck Institute for Polymer Research Ackermannweg 10, Mainz 55128, Germany — [2]Chemical Engineering University of Washington 105 Benson Hall, Seattle, WA 98195-1750, USA

Inspired by diatom silification we used amphiphilic peptides consisting of leucine and lysine (LK peptides) to investigate biomineralization at surfaces. Depending on hydrophobic periodicity, these peptides adopt alpha helical or beta sheet structures at the air-water interface. Upon addition of a silica precursor we obtained surface-tailored peptide-silica hybrid films with a thickness of ~4 nm. We probed film composition and interactions between peptides and silica at early stages of biomineralization by means of surface sensitive techniques, such as sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS). Electron and atomic force microscopy show similarities of the film fine structure and the surface of in-solution silica precipitates. Experimental findings were complemented with molecular dynamics simulations. We believe that our results provide insights into the biomineralization of structured films, which might prove useful in materials design and surface engineering.

H. Lutz, V. Jaeger, R. Berger, M. Bonn, J. Pfaendtner, T. Weidner, Advanced Materials Interfaces 2015, 2, n/a. J. E. Baio, A. Zane, V. Jaeger, A. M. Roehrich, H. Lutz, J. Pfaendtner, G. P. Drobny, T.

Weidner, Journal of the American Chemical Society 2014, 136, 15134.

BP 66.5 Thu 16:00 H45
AFM force spectroscopy with S. aureus and Strep. mutans to reveal biopolymer binding properties — •Friederike Nolle[1], Nicolas Thewes[1], Christian Spengler[1], Kordula Schellnhuber[1], Peter Loskill[1], Alexander Thewes[2], Ludger Santen[2], and Karin Jacobs[1] — [1]Saarland University, Dept. of Experimental Physics, 66041 Saarbruecken — [2]Saarland University, Dept. of Theoretical Physics, 66041 Saarbruecken

The adhesion of pathogenic bacteria is a crucial step in the development of implant-related infections. The adhesion of bacteria is mediated by biopolymers, the properties of which we are able to characterize by AFM force spectroscopy, where the probe is a single bacterium. To deepen the understanding, we combine the AFM studies with computer simulations [1]. For bacteria (Staphylococcus aureus) in contact with hydrophobic surfaces, thermally fluctuating cell wall proteins of different stiffness attach to the surface via short range forces and subsequently * due to entropic forces * pull the bacterial cell into close contact. That way, S. aureus is able to substantially increase its interaction range for contact initiation. Bacteria like Streptococcus mutans also attach to hydrophilic surfaces (e.g. titanium or hydroxyapatite) in the presence or absence of other biomolecules (proteins, enzymes). Our study reveals the importance of specific parameters (e.g. roughness) and proposes that fluctuations in protein density and structure are much more relevant than the exact form of the binding potential.

[1] N. Thewes, P. Loskill, P. Jung, H. Peisker, M. Bischoff, M. Herrmann, K. Jacobs, Soft Matter 2015, 11, 8913-8919

BP 67: Networks: From Topology to Dynamics III (Joint Session DY/SOE/BP)

Time: Thursday 15:30–17:00 Location: H47

BP 67.1 Thu 15:30 H47
Complex Quantum Networks: From Universal Breakdown to Optimal Transport — •Oliver Mülken — Physikalisches Institut, Universität Freiburg, Freiburg, Deutschland

We study the transport efficiency of excitations on complex quantum networks with and without loops. For this we consider sequentially growing networks with different topologies of the sequential subgraphs. This can lead to a universal complete breakdown of transport for tree-like [1] or complete-graph-like [2] sequential subgraphs, while it leads to optimal transport for linear [1] or ring-like [2] sequential subgraphs. The transition to optimal transport for networks with loops can be triggered by systematically reducing the number of loops of complete-graph-like sequential subgraphs in a small-world procedure. These effects are explained on the basis of the spectral properties of the network's Hamiltonian. Our theoretical considerations are supported by numerical Monte-Carlo simulations for complex quantum networks with a scale-free size distribution of sequential subgraphs and a small-world-type transition to optimal transport in the case of loops.

[1] Phys. Rev. Lett. 115, 120602 (2015)
[2] arXiv:1511.00910

BP 67.2 Thu 15:45 H47
Resilience of complex networks — •Baruch Barzel — Bar-Ilan University, Ramat-Gan, Israel

Resilience, a system's ability to adjust its activity to retain its basic functionality under errors, failures and environmental changes, is a defining property of many complex systems. Despite widespread consequences on human health, economy and the environment, events leading to loss of resilience, from economic collapse to mass extinctions in ecological networks, are rarely predictable and often irreversible. These limitations are rooted in a theoretical gap: the current analytical framework of resilience is designed to treat low dimensional models of a few interacting components, and hence it is unsuitable for characterizing multidimensional systems consisting of a large number of components that interact through a complex network.In this talk we will bridge this theoretical gap by introducing a set of analytical tools to identify the natural control and state parameters of a multidimensional complex system. This analytical framework allows us to systematically separate the role of the system's dynamics and topology, collapsing the behavior of different networks onto a single universal resilience pattern. Our results unveil the network characteristics that can

enhance or diminish resilience, offering avenues to prevent the collapse of environmental, infrastructural or socio-economic systems.

BP 67.3 Thu 16:00 H47
The totally asymmetric inclusion process (TASIP): how network topology determines condensation and transport properties — •Johannes Knebel, Markus F. Weber, Philipp Geiger, and Erwin Frey — Ludwigs-Maximilians-Universität, München, Deutschland

Transport phenomena are often modeled by the hopping of particles on regular lattices or networks. Such models describe, for example, the exclusive movement of molecular motors along microtubules: no two motors may occupy the same site. In our work, we study *inclusion processes* that are the bosonic analogues of the fermionic exclusion processes. In inclusion processes, many particles may occupy a single site and hopping rates depend linearly on the occupation of departure and arrival sites. Particles thus attract other particles to their own site. Condensation occurs when particles collectively cluster in one or in multiple sites, whereas the other sites become depleted.

We showed that inclusion processes on a network describe both the selection of strategies in evolutionary zero-sum games and the condensation of non-interacting bosons into multiple quantum states in driven-dissipative systems. The condensation is captured by the antisymmetric Lotka-Volterra equation (ALVE), which constitutes a nonlinearly coupled dynamical system. We derived an algebraic method to analyze the ALVE and to determine the condensates. Our approach allows for the design of networks that result in condensates with oscillating occupations, and yields insight into the interplay between network topology and transport properties.

BP 67.4 Thu 16:15 H47
Growing Boolean networks together with their attractors — Andrey Sakryukin and •Konstantin Klemm — School of Science and Technology, Nazarbayev University, Astana, Kazakhstan

We present a computational method for finding attractors of Boolean dynamics under asynchronous update. Starting from a single node or small network, it builds up the queried network by iterative node addition. The core idea is the mechanism for restricting Boolean dynamics to a subnetwork. Here a natural restriction rule is defined so that node addition never leads to shrinking of an attractor's state set. This facilitates tracking growth, merging and annihilation of attractors as the network itself is being built up.

Applications to Boolean models of biological regulation as well as metastable states of discrete energy landscapes, e.g. NK model, are discussed. At `http://goo.gl/eRzFoo` the implementation of the method and further material are available for download.

BP 67.5   Thu 16:30   H47

Synchronization of heterogeneous chemical relaxation oscillators — •Jan Frederik Totz[1], Julian Rode[1], Kenneth Showalter[2], and Harald Engel[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]West Virginia University, Morgantown, USA

Recently discovered synchronization patterns, such as chimera states and intertwined cluster synchronization in networks of identical nonlinear oscillators lead to the emergence of new theoretical concepts, most notably an extended master stability function for networks with permutation symmetries [1].

Optically coupled catalytic beads provide a versatile experimental tool to study the emergence of collective synchronization patterns with real oscillators under well-controlled laboratory conditions [2].

One important aspect is the impact of a broad oscillator frequency distribution. Instead of in-phase or cluster synchronization, experiments reveal phase wave synchronization through neighboring permutation symmetry clusters [3].

[1] Kuramoto, Battogtokh. Complex Syst. 4, 380 (2002); Pecora et al. Nat. Commun. 5, 4079 (2014) [2] Tinsley. Nat. Phys. 8, 662 (2012); Taylor et al. PCCP (2015) [3] Totz et al. PRE 92, 022819 (2015)

BP 67.6   Thu 16:45   H47

Biologically implementable attractors in Boolean network models of gene regulation — •David F. Klosik and Stefan Bornholdt — Institut für Theoretische Physik, Universität Bremen

Boolean networks have successfully been used as a modeling approach for gene regulatory networks. It is a well-known fact that in general the attractor landscape can change dramatically when moving from the original parallel deterministic update scheme applied in the first studies to asynchronous or otherwise noisy schemes believed to more plausibly represent the actual processes in the cell. However, the main dynamical features of many biological regulatory networks (e.g., the cell cycle network in yeast) can be captured in a parallel Boolean model, as well, in addition to its own stochastic biochemical implementation within the cell. This leads to the question of when Boolean networks are in fact biologically implementable, keeping certain transients or attractors. We here approach this question with an autonomous Boolean network model with underlying continuous dynamics, that has been proven useful in simulating biochemical stochasticity in regulatory networks[1].

[1] S. Braunewell and S. Bornholdt, Superstability of the yeast cell-cycle dynamics: Ensuring causality in the presence of biochemical stochasticity, J. Theor. Biol. 245 (2007) 638-643.

BP 68: Networks - From Topology to Dynamics IV (Joint Session BP/SOE/DY)

Joint session with SOE and DY organized by BP.

Time: Thursday 16:45–17:45   Location: H43

BP 68.1   Thu 16:45   H43

Fluctuations and transients in the actin cytoskeleton of chemotactic amoeba — •Jose Negrete JR[1,2], Alain Pumir[3], Hsing-Fang Hsu[2], Christian Westendorf[4], Marco Tarantola[2], Carsten Beta[2,5], and Eberhard Bodenschatz[2,6,7] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Dynamics and Selforganization, Göttingen, Germany — [3]Ecole Normale Supérieure de Lyon, France — [4]University of Graz, Austria — [5]University of Potsdam, Germany — [6]University of Göttingen, Germany — [7]Cornell University, Ithaca, USA

Biological systems with their complex biochemical networks are known to be intrinsically noisy. Here we investigate the oscillatory dynamics in the actin cytoskeleton of chemotactic amoeboid cells. We show that the large phenotypic variability in the polymerization dynamics can be accurately captured by a generic nonlinear oscillator model in the presence of noise. The relative role of the noise is fully determined by a single dimensionless parameter, experimentally measurable, and whose distribution completely characterizes the possible cellular behavior. Also, we perturbed experimentally the oscillatory cytoskeletal dynamics by a short chemoattractant pulse and measured the spatio-temporal response of filamentous actin reporter, LimE, and depolymerization regulators Coronin1 and Aip1. After pulsing, we observed self oscillating cells to relax back to their oscillatory state after a noisy transient. Particularly long transients were observed for cells initially displaying highly correlated oscillations.

BP 68.2   Thu 17:00   H43

Distribution of pair-wise covariances in neuronal networks — •David Dahmen[1], Markus Diesmann[1,2,3], and Moritz Helias[1,3] — [1]Inst. of Neurosc. and Med. (INM-6) and Inst. for Advanced Simulation (IAS-6) and JARA BRAIN Inst. I, Jülich Research Centre, Germany — [2]Dept. of Psychiatry, Psychotherapy and Psychosomatics, Medical Faculty, RWTH Aachen University, Aachen, Germany — [3]Dept. of Physics, Faculty 1, RWTH Aachen University, Germany

Massively parallel recordings of spiking activity in cortical circuits show large variability of covariances across pairs of neurons [Ecker et al., Science (2010)]. In contrast to the low average, the wide distribution of covariances and its relation to the structural variability of connections between neurons is still elusive. Here, we derive the formal relation between the statistics of connections and the statistics of integral pairwise covariances in networks of Ornstein-Uhlenbeck processes that capture the fluctuations in leaky integrate-and-fire and binary networks [Grytskyy et al., Front. Comput. Neurosci. (2013)]. Spin-glass mean-field techniques [Sompolinsky and Zippelius, Phys. Rev. B (1982)] applied to a generating function representing the joint probability distribution of network activity [Chow and Buice, J. Math. Neurosci. (2015)] yield expressions that explain the divergence of mean covariances and their width when the coupling in the linear network approaches a critical value. Using these relations, distributions of correlations provide insights into the properties of the structure and the operational regime of the network. Partly supported by Helmholtz Association: VH-NG-1028 and SMHB; EU Grant 604102 (HBP).

BP 68.3   Thu 17:15   H43

Global stability reveals critical components in the structure of multi-scale neural networks — •Jannis Schuecker[1,4], Maximilian Schmidt[1,4], Sacha J. van Albada[1], Markus Diesmann[1,2,3], and Moritz Helias[1,3] — [1]Inst of Neurosci and Medicine (INM-6) and Inst for Advanced Simulation (IAS-6) and JARA BRAIN Institute I, Jülich Research Centre — [2]Department of Psychiatry, Psychotherapy and Psychosomatics, Medical Faculty, RWTH Aachen University — [3]Department of Physics, Faculty 1, RWTH Aachen University — [4]These authors contributed equally

One of the major challenges of neuroscience is the integration of the available experimental data into a coherent model of the brain. In this endeavor, the exploration of the inevitable uncertainties in anatomical data should be guided by physiological observations. To this end we devise a method based on a mean-field reduction of spiking network dynamics for shaping the phase space of large-scale network models according to fundamental activity constraints, prohibiting quiescence and requiring global stability. In particular, we apply this framework to a multi-area spiking model of macaque visual cortex and obtain plausible layer- and area-specific activity [Schuecker et al. 2015, arXiv:1509.03162] by controlling the location of the separatrix dividing the phase space into realistic low-activity and unrealistic high-activity states. The study systematically identifies modifications to the population-level connectivity within and between areas critical for the stability of the network. Partly supported by Helmholtz association: VH-NG-1028 and SMHB; EU Grant 604102 (HBP).

BP 68.4   Thu 17:30   H43

From Interactions to Topology: A Population Dynamics Approach to Network Formation — •Adrian Fessel and Hans-Günther Döbereiner — Institut für Biophysik, Universität Bremen, Deutschland

We present a mean-field model integrating interactions between pop-

ulations of nodes to mimic the evolution of transportation networks. Changes in network topology are partitioned in basic events representing, e.g., fusion or growth of network fragments. Local dependencies are reflected by rate constants modifying the frequency of occurence of a given event.

The model presented shows promising results when compared to the percolating network of the slime-mold *Physarum polycephalum* [*Phys. Rev. Lett.* **109**, 078103 (2012)].