

AKB 40 Poster Session II

Time: Wednesday 16:30–19:30

Room: P3

AKB 40.1 Wed 16:30 P3

Effects of Eye-phase in DNA unzipping — ●SANJAY KUMAR — Department of Physics, BHU, Varanasi, India — MPIPES, Noethnitzer str. 38 01187, Dresden Germany

The onset of an “eye-phase” and its role during the DNA unzipping is studied when a force is applied to the interior of the chain. The directionality of the hydrogen bond introduced here leads to a saw-tooth like behaviour which was earlier seen in the protein unfolding experiments. The effects of intermediates (hairpins) and stacking energies on the melting profile can also be studied.

AKB 40.2 Wed 16:30 P3

Macroscopic crystallographic structure of *Strongylocentrotus purpuratus* and *spisula solidissima* by pole figure analysis — ●SIMONE HERTH¹, JEREMY K. BIGNESS², and ROBERT H. DOREMUS^{1,2} — ¹Rensselaer Nanotechnology Center, Rensselaer Polytechnic Institute, Troy, NY, USA — ²Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY, USA

The shells of sea animals, such as the sea urchin *Strongylocentrotus purpuratus* and the clam *spisula solidissima*, provide strong protection against enemies while retaining low weight. In *Strongylocentrotus purpuratus* the high toughness of the skeleton is achieved by the combination of a strong, but 50% porous backbone made of the mineral calcite and proteins, which distribute stress concentrations. In contrast, the shell of *spisula solidissima* consists of the mineral aragonite and has a very low porosity. However, little is known about the macroscopic texture of these surprisingly strong composites, which was studied by a pole figure analysis of an oral and an aboral piece of the sea urchin skeleton and a small part of the clam shell. The sea urchin exhibits a strong texture in only a few crystallographic directions indicating a preferred macroscopic orientation of the calcite planes. The orientation of the planes in the aboral part is slightly more symmetric with about the same degree of texture. In contrast, the texture of the clam shell is very weak.

AKB 40.3 Wed 16:30 P3

Simulation studies of lipid bilayer around a conical inclusion and mediated interactions between inclusions. — ●GREGORIA ILLYA and MARKUS DESERNO — MPI Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present a mesoscopic model for lipid bilayers with embedded conical inclusions, which is investigated using a solvent free coarse-grained simulation technique [1].

Above the gel-fluid transition temperature, i.e., in the fluid phase, the lipids are not in a spontaneously tilted phase. Inserting a conical object into the membrane will impose a local tilt on the surrounding lipids and also bend the membrane. The tilt of the lipids will decay with some characteristic decay length [2]. We measure this lipid tilt decay length for an almost flat membrane where the inclusion only imposes a tilt on the lipids and for a membrane where the inclusion also bends it.

Since transmembrane inclusions can deform the membrane, these deformations will generate interactions between the inclusions. We are currently investigating the force between two inclusions mediated by the tilt field and the membrane deformation, and compare the results with the theoretical prediction [2].

[1] Cooke, I. R., Kremer, K., and Deserno, M., Physical Review E, 72, 011506, 2005. [2] Mueller, M. M., Deserno, M., and Guven, J., to appear in Phys. Rev. E.

AKB 40.4 Wed 16:30 P3

Conformational properties of semiconductor-binding synthetic peptides — ●GÖKHAN GÖKOĞLU^{1,2}, MICHAEL BACHMANN¹, TARIK ÇELİK², and WOLFHARD JANKE¹ — ¹Institut für Theoretische Physik, Universität Leipzig, Germany — ²Fizik Mühendisliği Bölümü, Hacettepe Üniversitesi Ankara, Turkey

We investigate thermodynamic properties of three 12-residue synthetic peptides with generalized-ensemble Monte Carlo simulations [1]. In recent experiments [2,3] it was found that these peptides, although similar in their amino acid content, adsorb with noticeably different strength to a GaAs (100) surface. In our study, we analyze the differences of the characteristic helix-coil transitions observed in our simulations employing an all-atom model based on the ECEPP/2 force field in vacuum and implicit

solvent. Here we primarily focus on the folding channels as seen in the free-energy landscape, where the free energy is expressed as a function of a suitably defined overlap parameter [4].

- [1] G. Gököğlü, M. Bachmann, T. Çelik, W. Janke, to be published.
 [2] S. R. Whaley, D. S. English, E. L. Hu, P. F. Barbara, A. M. Belcher, Nature **405**, 665 (2000).
 [3] K. Goede, P. Busch, M. Grundmann, Nano Lett. **4**, 2115 (2004).
 [4] U. H. E. Hansmann, M. Masuya, Y. Okamoto, Proc. Natl. Acad. Sci. USA **94**, 10652 (1997).

AKB 40.5 Wed 16:30 P3

Traction Force Microscopy on Elastic Layers of Finite Thickness — ●RUDOLF MERKEL, CLAUDIA CESA, BERND HOFFMANN, and NORBERT KIRCHGESSNER — Institute of Thin Films and Interfaces 4, Research Centre Jülich, Germany

Most living cells adhere to solid substrates and apply sizeable mechanical forces to them. Such forces are applied predominantly at focal adhesion sites which are micron sized protein complexes in the adhesion zone. In recent years traction force microscopy was introduced as a technique to discern the force contributions of different focal adhesion sites of one cell [1,2]. Here cells are cultivated on very soft films that are deformed by cell forces. The resulting deformation fields are measured by tracking microstructures on the film surface. Data evaluation relies on the fact that forces and displacements are connected by the mechanical Greens' tensor. Here we present expressions for the Greens' tensor of an elastic film of finite thickness bonded to a rigid substrate. These results show distinct deviations from the Greens' tensor of an elastic half space that has been exclusively used in this technique up to now. Moreover, we validated these results experimentally.

- [1] Dembo and Wang, Biophys. J. **76** (1999) 2307.
 [2] Balaban et al., Nature Cell Biol. **3** (2001) 466.

AKB 40.6 Wed 16:30 P3

Competition of Diffusion and Driven Motion in Lattice Gases — ●HAUKE HINSCH¹, PAOLO PIEROBON^{1,2}, and ERWIN FREY¹ — ¹Arnold Sommerfeld Center and CeNS, Department of Physics, LMU München, Germany — ²Hahn-Meitner-Institut, Abteilung Theorie, Berlin, Germany

Driven and diffusive lattice gases have proved useful as model systems for a variety of biological transport processes like ribosomal mRNA transcription or the motion of molecular motors along microtubules. Furthermore, they have attracted interest as a paradigm of non-equilibrium systems in statistical physics which exhibit a surprisingly rich phase behavior. Recently, the total asymmetric exclusion process (TASEP) has been extended by equilibrium bulk ad- and desorption dynamics resulting in interesting competitive effects (Parmeggiani, PRL 90, 2003). We study the competition of driven and diffusive motion on two one-dimensional lattices. An investigation with mean-field theory and Monte Carlo techniques reveals novel behavior and limitations of mean-field theory.

AKB 40.7 Wed 16:30 P3

Two-Dimensional Dynamics of a Semiflexible Polymer in Flow — ●TOBIAS MUNK and ERWIN FREY — Arnold-Sommerfeld-Center, LMU München

In this poster we address the question how a single stiff polymer moves in a viscous fluid environment. The model system we refer to is the bio-polymer F-actin. The polymer is represented by a continuous two-dimensional space curve with a fixed length and a curvature-dependent bending energy. Furthermore we account for the constraint of inextensibility by introducing a Lagrange multiplier into the hamiltonian. By invoking suitable eigenfunctions we obtain a system of coupled first order stochastic differential equations of Langevin type, which can be solved numerically.

We present results for the polymer's motion in two simple flow fields: In a shear flow, the semiflexible filament periodically tumbles. Each of these tumbling events induces a transient buckled conformation, induced by the interplay of elastic, viscous and stochastic forces. In a toggled elongational flow, we observe the dynamics of the force extension and tension propagation.

Our numerical results nicely complement recent experiments with DNA in flow. Furthermore, they predict some behaviour specific to F-actin,

which is considerably stiffer than DNA, to be observed in future experiments.

AKB 40.8 Wed 16:30 P3

Vasculature remodeling in tumor-induced angiogenesis – a stochastic model — ●RAJA PAUL¹, KATALIN BARTHA², and HEIKO RIEGER³ — ¹BIOMS, IWR, Ruprecht-Karls-University Heidelberg, D-69120 Heidelberg, Germany — ²Department of Medical Biochemistry, Semmelweis University, Budapest, Hungary — ³Theoretische Physik, Universität des Saarlandes, D-66041 Saarbrücken

Based upon a recently introduced model[1] for vascular network remodeling via vessel cooption, regression and growth in tumors[2] we study a dynamically evolving two-dimensional biconnected network incorporating the effect of probabilistic neo-vascularization and vessel collapse. The morphology of a regular vasculature is drastically changed in the presence of an expanding tumor. Independent vessel collapse results in a percolation transition of the network, flow correlated collapse stabilizes the network in the tumor center at a non-vanishing microvascular density (MVD). MVD, blood flow and shear force has been computed for a wide range of parameters and found to be in good qualitative agreement with experimental data[3] for human melanoma.

[1] K. Bartha and H. Rieger, q-bio.TO/0506039.

[2] D. Hanahan and J. Folkman, Cell, **86**, 353 (1996).

[3] B. Döme, S. Paku, B. Somlai and J. Tímár, J. Path., **197**, 355 (2002).

AKB 40.9 Wed 16:30 P3

Influence of lipid rafts on cell signalling — ●STEFAN SEMRAU and THOMAS SCHMIDT — Biophysics, University Leiden

Heterogeneities such as lipid rafts are believed to play a major role in cell signalling by influencing the diffusion and localization of proteins in the plasma membrane. Colocalization of proteins seems to be crucial at the beginning of the signal transduction pathway. Lipid rafts, whose existence in living cells is suggested by many experiments, are cholesterol and sphingolipid enriched membrane domains in which the lipid phase is probably different from that of the environment. We study lipid rafts in controllable model systems that are much less complex than living cells but suitable to mimic lipid rafts: structured supported lipid bilayer membranes and giant unilamellar vesicles (GUVs) from lipid mixtures. The influence of e.g. the size, shape, boundary behaviour and composition of membrane domains on the diffusion of fluorescently labelled proteins or lipids is studied by single-molecule tracking and Monte-Carlo simulations.

AKB 40.10 Wed 16:30 P3

Topological correlations enhance pattern formation in reaction-diffusion processes on scale-free networks — ●SEBASTIAN WEBER¹, MARC-THORSTEN HÜTT², and MARKUS PORTO¹ — ¹Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany — ²Theoretische Biologie und Bioinformatik, Technische Universität Darmstadt, Schnittspahnstr. 3, 64287 Darmstadt, Germany

We study the reaction-diffusion processes $A + A \rightarrow \emptyset$ and $A + B \rightarrow \emptyset$ on uncorrelated, disassortative, and assortative scale-free networks. A method to suitably compare the pattern formation on these different networks is developed. We apply this method to quantify the residual pattern formation occurring on uncorrelated networks. The analogous analysis of disassortative and assortative networks shows that degree correlations substantially alter the dynamical behavior and that such topological correlations yield an enhanced pattern formation.

[1] S. Weber, M.-Th. Hütt, and M. Porto (submitted)

AKB 40.11 Wed 16:30 P3

Prediction of site-specific amino acid distributions and limits of divergent evolutionary changes in protein sequences — ●MARKUS PORTO¹, UGO BASTOLLA², H. EDUARDO ROMAN³, and MICHELE VENDRUSCOLO⁴ — ¹Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 8, 64289 Darmstadt, Germany — ²Centro de Biología Molecular 'Severo Ochoa', Cantoblanco, 28049 Madrid, Spain — ³Dipartimento di Fisica, Università di Milano Bicocca, Piazza della Scienza 3, 20126 Milano, Italy — ⁴Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK

We derive an analytic expression for site-specific stationary distributions of amino acids. The stationary distributions that we obtain have a Boltzmann-like shape, and their effective temperature parameter, measuring the limit of divergent evolutionary changes at a given site, can be predicted from a site-specific topological property. These analytic re-

sults, obtained without free parameters, are in very good agreement with the site-specific amino acid distributions obtained from the Protein Data Bank.

[1] M. Porto, H.E. Roman, M. Vendruscolo, and U. Bastolla, Mol. Biol. Evol. **22**, 630 (2005); 1156 (2005).

[2] U. Bastolla, M. Porto, H.E. Roman, and M. Vendruscolo, Gene **347**, 219 (2005).

AKB 40.12 Wed 16:30 P3

Elastic properties of viral capsids — ●MATHIAS PUHLMANN and PETER LENZ — AG Komplexe Systeme, Philipps-Universität Marburg, Renthof 6, 35032 Marburg

Empty viral shells have astonishing elastic properties. Recent experiments on bacteriophage $\phi 29$ [1] have shown that these nano-containers withstand nano-newton forces. Their elastic response to applied point forces is nonlinear and varies across the surface. To elucidate these phenomena we study numerically discrete elastic models. Our simulations reveal the connection between the geometry of viral capsids and their mechanical properties. The numerically determined distribution of elastic spring constants agrees well with the experimental findings. By measuring the stress distribution we are able to predict the rupture probabilities across the capsid surface.

[1] I.L.Ivanovka et al., PNAS 101(20):7600 (2003)

AKB 40.13 Wed 16:30 P3

Supramolecular organization of photosynthetic complexes in model membrane systems — ●TOBIAS PFLOCK¹, MANUELA DEZI², GIOVANNI VENTUROLI², JÜRGEN KÖHLER¹, and SILKE OELLERICH¹ — ¹Experimentalphysik IV, Universität Bayreuth, D-95445 Bayreuth — ²Dept. of Biology, University of Bologna, Italy

A common feature of biological membranes is the supramolecular organization of proteins within the membrane to functional units. This process involves a close interaction between the membrane lipids and proteins. Therefore, it is of particular interest to understand the role of lipids for the spatial membrane organization of the proteins. In order to direct this question in a fundamental way, we chose to reconstitute proteins into model membrane systems. This approach allows to sensitively control the membrane lipid composition as well as the lipid-protein ratio. An interesting system for these studies is the photosynthetic unit of purple bacteria, consisting of the reaction centre (RC) and the light-harvesting complexes LH2 and LH1. These pigment-protein complexes organize very efficiently to highly functional units within the natural photosynthetic membrane. The spatial organization of these proteins in model membranes as a function of the membrane composition can be studied by using "Giant unilamellar vesicles" (GUV). These vesicles allow a direct observation of protein diffusion and clustering within the membrane by the use of fluorescence wide-field imaging, which can be employed with a sensitivity down to the single-molecule level. For these studies, we succeeded in establishing a protocol for the efficient preparation of GUVs over a wide range of lipid-protein ratios.

AKB 40.14 Wed 16:30 P3

Pumping Nanofluidics Optically along Freely Defined Patterns — ●FRANZ WEINERT and BRAUN DIETER — Noether Group on Dissipative Microsystems, Applied Physics, Ludwig Maximilians Universität München, Amalienstr. 54, 80799 München, Germany

Liquid is pumped in thin films by nonlinear thermal expansion. The flow geometry is not defined by channels, but by the focus movement of an infrared laser scanning microscope. The fluid follows the laser path in reverse direction. Pumping matches a theory based on temperature dependent viscosity. For decreasing chamber thickness, pump speed rises quadratically, reaching 20 $\mu\text{m/s}$ for 2.5 μm . Highly viscous liquids are pumped equally well. The technique frees micro- and nanofluidics from the load of channel lithography, delicate interfacing and complex pump design.

AKB 40.15 Wed 16:30 P3

Conductivity of unordered denatured and hybridized DNA — ●THOMAS KLEINE-OSTMANN¹, CHRISTIAN JÖRDENS¹, KAI BAASKE¹, THOMAS WEIMANN², MARTIN HRABE DE ANGELIS³, and MARTIN KOCH¹ — ¹Inst. f. Hochfrequenztechnik, Schleinitzstr. 22, 38106 Braunschweig — ²Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — ³GSF National Research Center for Environment and Health, Ingolstädter Landstr. 1, 85764 Neuherberg

The electronic properties of DNA remain highly controversial. Depending on the technique and the experimental conditions, a variety of - some-

times contradictory - results have been obtained. They are of paramount importance for two visionary technologies: self-assembled nanoelectronics and marker-free gene tests. Here, we report on the conductivity of natural DNA under ambient conditions. We examined both single-stranded and double-stranded herring DNA in buffer solution that consists of 120-3000 nucleotides. It was spotted and dried on Au nanocontacts deposited on oxidized Si with a gap size of 100 nm. I-V curves are obtained in a sealed measurement chamber that allows for the adjustment of the ambient relative humidity in a wide range from 10 to 100 percent. We find an exponential humidity dependence of the conductivity that is identical for single- and double-stranded DNA within the measurement accuracy. While the small conductivity of dry DNA is comparable to that of a large band-gap semiconductor, we attribute the increased conductivity of DNA at high humidity levels to water molecules accumulated at the phosphate backbone. We observe s-shaped I-V curves that can be well explained by the dissociation of water attached to the DNA molecules.

AKB 40.16 Wed 16:30 P3

The Stress of Leaves in our Climatic Environment — ●AGNIESZKA KROL-OTWINOWSKA, KARL HIEBLE, and MARGRET GIESEN — Institut für Schichten und Grenzflächen, ISG 4, Forschungszentrum Jülich, D 52425 Jülich

Climatic changes as well as industrial pollution may have a dramatic effect on the health condition of plants. Our goal is to gain a new understanding of the correlation between the functionality of plant leaves and environmental factors from a surface scientist's point of view. For that purpose we introduce for the first time measurements of the surface stress of cuticular wax layers under climatic realistic conditions. The origin of surface stress is the local polarization of the electron charge density due to the chemical bonding of adsorbates. Using the laser deflection method (1) surface stress changes of the order of 0.01 N/m are detectable. Changes in the surface stress are hence sensitive indicators for interaction-induced charge changes and structural surface relaxations. We present studies of the surface stress of wax layers from cherry laurel (*Prunus Laurocerasus*) and apple leaves (*Golden Delicious*) as a function of climatic relevant parameters (e.g. gas dose, air humidity, pH, temperature, UV-light). (1) *Rev. Sci. Instrum.* 66(9), (1995), 4734

AKB 40.17 Wed 16:30 P3

The effect of differentiation on the deformability of cells — ●FRANZISKA LAUTENSCHLÄGER, S. SCHINKINGER, M. JUNGNITSCH, J. SCHWARZ, and J GUCK — Universität Leipzig, Abteilung Physik der weichen Materie, Linnéstr. 5, 04103 Leipzig, Germany

From molecular biology it is known that during differentiation there are characteristic changes in the three main constituents of the cytoskeleton-microtubules, actin, and intermediate filaments. Since the cytoskeleton is the main structural element in cells these changes should be reflected to varying degrees in their mechanical properties. To test this hypothesis, we investigated the impact of differentiation and specific toxins on cell elasticity with the Optical Stretcher. In our experiments we used human neural precursor cells (HPCM) which were differentiated into glia cells, GABAergic, and dopaminergic neurons as well as hematopoietic precursor cells (NB4 cells) treated with retinoic acid (ATRA) to differentiate them into mature blood cells. Our results show an increasing stiffness and a decreasing variance during differentiation. This suggests using deformability as a new cell marker for stem cell characterization and sorting.

AKB 40.18 Wed 16:30 P3

Probability for specific bond formation for a Brownian particle in linear shear flow above a wall — ●CHRISTIAN KORN^{1,2} and ULRICH S. SCHWARZ^{1,2} — ¹University of Heidelberg, Im Neuenheimer Feld 293, D-69120 Heidelberg, Germany — ²Max Planck Institute of Colloids and Interfaces, D-14424, Potsdam, Germany

Cohesion in biological systems and biotechnological applications is usually provided by specific bonds between receptors and ligands. The formation of these bonds requires a physical transport process which brings receptors and ligands to sufficient proximity for binding.

As a non-trivial example here we study the motion of a rigid spherical Brownian particle in linear shear flow carrying receptors for ligands covering a planar boundary wall. This situation is relevant for the binding of white blood cells to blood vessel walls, which can be studied quantitatively in flow chambers. The appropriate mobility matrix follows from the Stokes equation and is position-dependent due to the presence of the wall. This leads to a non-trivial multiplicative noise term in the corre-

sponding Langevin equation.

We determine the mean time for receptor-ligand encounter as a function of the Péclet numbers, which describe the transition from diffusive to deterministic transport. We also show in quantitative detail how the results are influenced by the values of receptor and ligand coverage.

AKB 40.19 Wed 16:30 P3

Towards surface-based model systems of the pericellular coat — ●RALF RICHTER^{1,2} and JOACHIM SPATZ^{1,2} — ¹University of Heidelberg, Department of Biophysical Chemistry, INF 253, D-69120 Heidelberg — ²Max-Planck-Institute for Metals Research, Department New Materials & Biosystems, Heisenbergstrasse 3, D-70569 Stuttgart

The pericellular coat of many cell types constitutes an intriguing self-organized system with multiple roles in cell division, migration, adhesion and signaling. The polysaccharide hyaluronan is a vital structural component of this strongly hydrated matrix. The nature of hyaluronan and its interaction with hyaluronan binding proteins determine the mechanical properties of the coat which are intimately related to its biological function.

Due to the complexity of living cells, the understanding of self-organization and mechanical properties of the pericellular coat in vivo or in vitro constitutes a considerable challenge. Complementary to investigations on living cells, simplified model systems can help to address specific questions in a controlled manner.

In our work, we aim to create models of the pericellular coat on flat supports. Our approach allows for the application of a whole range of surface sensitive label-free characterization techniques. The immobilization of hyaluronan on a solid-supported lipid membrane is an example of the envisaged bottom-up approach that allows the creation of models of increasing complexity that mimic various aspects of the pericellular coat. With these models we expect to gain information about the relationship between composition, structure and mechanics of the pericellular coat.

AKB 40.20 Wed 16:30 P3

Statistics of local sequence alignments — ●STEFAN WOLFSHEIMER and ALEXANDER K. HARTMANN — Institut für theoretische Physik, Göttingen, Germany

Sequence alignment is a tool used for comparison in protein and DNA databases. Widely used algorithms are e.g. BLAST and FASTA. Knowledge about the distribution of gaped optimal subalignment scores of random sequences is essential in order to distinguish relevant alignments from alignments that occurred by chance[1]. Analytical solutions are only available for the ungaped case, and yield the Gumbel distribution. Nevertheless, for database applications gaped alignments schemes are much more relevant.

Here we use a method to obtain regions of the distribution on a wide range, including the rare event tail down to $p \sim 10^{-40}$. This is similar to the problem of obtaining the density of states of a complex physical system, like spin glasses and therefore methods from statistical mechanics could be adopted [2]. The optimum alignment score corresponds to the ground state of the physical system. By simulated annealing techniques and using the sequences as dynamic variables, rather than the alignments, the distribution of scores is obtained. We study different BLOSUM and PAM scoring matrices and quantify in each case the deviations in the rare event tail from the Gumbel distribution.

[1] S.F. Altschul and W. Gish, *Methods in Enzymology*, **266**, 460

[2] A.K. Hartmann, *Phys. Rev. E* **65**, 056102 (2002)

AKB 40.21 Wed 16:30 P3

Light scattering measurements on single cells in a dual beam laser trap — ●MORITZ KREYSING, KORT TRAVIS, and JOCHEN GUCK — Institute for Soft Matter Physics, Universität Leipzig, Linnéstr. 5, 04103 Leipzig

The principle aim of this work is the development of an easy to handle fast working method to measure light scattering properties of single cells in aqueous media. Therefore we made use of the high symmetry of cells lying directly on the axis of a dual beam laser trap. Additionally to the common setup of this trap laser light in the visible range is emitted by one of the fibers, scattered by the cell and is then partly coupled into the opposite fiber. Measuring this recoupled light while varying the position of the cell by modifying the trapping lasers power allows to calculate the scattered light's intensity as a function of the angle. Comparing this to standards measured with a confocal microscope and models based on Mie theory provides information about average refractive index, size, and deformation of the cell, for example caused by using the setup as optical

stretcher. Further insights into the dielectric properties of cell organelles and surface morphology can be obtained. This could eventually be utilized in cell sorting applications.

AKB 40.22 Wed 16:30 P3

Phase behaviour of DMPC and farnesol mixtures — ●MARIA HANULOVA and SERGIO S FUNARI — HasyLab at Desy, Notkestr. 85, D-22603 Hamburg

Farnesol is a 15carbon polyisoprenol derived from the mevalonate pathway. It regulates the cell cycle, post-translationally attaches to proteins and so helps protein sorting in cell membranes, inhibits neural channels, enhances drug penetration and sensitizes bacteria to antibiotics.

We studied the phase behaviour of DMPC (dimyristoyl phosphatidylcholine) and farnesol mixtures in the temperature range 5-80°C using X-ray diffraction and polarized optical microscopy. The mixtures were prepared in water or in buffer (10mM HEPES, 100mM NaCl, 1mM EDTA, pH 7.4).

Farnesol itself does not form ordered structures and does not mix with water, but incorporates into lipid membranes. DMPC + farnesol mixtures form lamellar phases at low temperatures. The gel-fluid transition is broader than in DMPC and occurs at lower temperatures. The DMPC ripple phase is suppressed. In the fluid state, we usually observed two coexisting lamellar phases, probably farnesol-rich and farnesol-poor domains.

In mixtures with farnesol contents up to 50 mol%, the lamellar phase persists till 80°C. Interestingly, at higher farnesol content the lamellar phase vanishes at 40-45°C and new ordered structures assemble on further heating. At about 60°C a cubic phase occurs and an additional hexagonal phase is seen above 70°C. The thermal behaviour nearly does not change for mixtures with 60 to 95 mol% farnesol.

AKB 40.23 Wed 16:30 P3

Cell rheology at high stress — ●PHILIP KOLLMANNBERGER, JOHANNES PAULI, CLAUDIA MIERKE, CARINA RAUPACH, and BEN FABRY — Zentrum für Medizinische Physik und Technik, Henkestr. 91, 91054 Erlangen

Rheology measurements in many cell types have established that cells exhibit a power-law creep modulus, or equivalently, a weak frequency dependence of the storage and loss moduli according to a power-law. These findings indicate that cell rheology is governed by multiple processes that play out on vastly different time scales. Previous measurements, however, were carried out in the linear regime, where stress and strain are related by a simple linear relationship, and the superposition principle holds. Here we measured the displacement of CSK-bound superparamagnetic beads in a feedback-controlled magnetic field gradient at high forces up to > 10 nN for which linearity, superposition and time scale free behavior of responses have not been established. At all forces, bead displacement d during during the on-phase (creep) and off-phase (relaxation) was well described by a power law: $d(t) = a \cdot (t/t_0)^b$. For forces less than 2 nN, power-law parameters during creep and recovery were identical. At higher forces, however, the recovery became progressively incomplete (a decreased) and faster (b increased). These results suggest that at higher forces, stable, long-lived stress-bearing structures within the cytoskeleton are disrupted. Subsequent structural rearrangements are then expected to contribute to a speed-up of relaxation processes.

AKB 40.24 Wed 16:30 P3

Controlling the Surface Density of DNA on Au by Electrically Induced Desorption — ●KENJI ARINAGA^{1,2}, ULRICH RANT², JELINA KNEŽEVIĆ², ERIKA PRINGSHEIM², MARC TORNOW², SHOZO FUJITA¹, NAOKI YOKOYAMA¹, and GERHARD ABSTREITER² — ¹Fujitsu Laboratories Ltd., 10-1 Morinosato-Wakamiya, Atsugi 243-0197, Japan — ²Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

Self-assembled DNA layers on solid surfaces have been of great interest and widely introduced to various techniques for bio-molecular investigations. Recently, we have investigated the active electrical manipulation of oligodeoxynucleotides on Au, employing optical means. We showed that the packing density within the DNA layer crucially determines the free mobility (rotatability) of individual molecules on the surface [1]. While this parameter bears a particular significance, very few investigations have been reported that address methods for controlling the surface density of DNA on Au. In this contribution, we discuss the adsorption mechanisms of thiolated DNA on gold as well as desorption properties under controlled substrate potentials. The adsorption strongly depends

on the diffusion of DNA and the ionic strength of electrolyte. On the other hand, we show in situ and in real time that electrochemically induced desorption can efficiently be controlled by tuning the magnitude and application-time of the substrate voltage. As a result, it is demonstrated that this method of electrical desorption provides effective means to adjust the surface density of DNA on gold surfaces.

[1] U. Rant, K. Arinaga et al., Nano Letters 2004, 4, 2441.

AKB 40.25 Wed 16:30 P3

Modelling cell-population growth of in-vitro monolayers — ●MICHAEL BLOCK¹, DIRK DRASDO², and ECKEHARD SCHÖLL¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin — ²IZBI University Leipzig, Härtelstrasse 16-18, 04107 Leipzig, Germany

Which mechanisms determine the growth kinetics and phenotypes of tumors is still largely unknown and - due to unknown influences - can even in cell cultures often not be clearly re-solved. We here present computer simulations of growing monolayers that permit a systematic analysis of the effect of migration, cell-cell adhesion, apoptosis, the cell cycle time distribution, biomechanical influences, mutations and medium properties on the bulk and surface growth dynamics. For this purpose we consider a kinetic Monte Carlo approach on a random lattice on which, as we explicitly show, lattice artifacts are eliminated. The model is calibrated according to off-lattice models that represent kinetic and bio-physical parameters explicitly ([1]). We compare our simulation results quantitatively with experimental findings by Bru et. al. ([2]), propose alternative mechanisms for their explanation and predict how it may be possible to distinguish between them by suitable experiments.

[1] Drasdo, D. and Höhme, St., Phys. Biol. 2, 133-147 (2005).

[2] Bru et al., Biophys J. 85, 2948-61 (2003).

AKB 40.26 Wed 16:30 P3

Counterion profile at a planar charged interface by anomalous x-ray reflectivity — ●KLAUS GIEWEKEMEYER and TIM SALDITT — Institut für Röntgenphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The distribution of counterions in the vicinity of charged surfaces is a theoretically well-studied subject with high relevance for biological problems like protein adsorption to membranes, membrane fusion etc. Although theoretical research on the subject has produced very detailed results that go far beyond the mean field approach (e.g. ion-ion correlation effects, particle volumes), accurate experimental evidence even for the historic Poisson-Boltzmann (PB) mean field result is rare and not completely satisfying. Here an approach to the problem is made by studying the simplest, in the PB theory still analytically solvable case of a planar charged surface at the solid liquid interface. As an experimental realization of this system a DODAB (Di-Octadecyl-Dimethyl-Ammonium-Bromide) monolayer adsorbed to an OTS (Octadecyl-Trichloro-Silane) monolayer bound to a Silicon substrate is chosen. The distribution of the systems Bromide counterions in aqueous solution has been probed with resonant small angle x-ray reflectivity. Furthermore, the variation of the Gouy-Chapman length of the counterion cloud has been studied by changing the charge density of the amphiphilic layer on top of the OTS by mixing the cationic DODAB with zwitterionic DPPC (Di-Palmitoyl-Phosphatidyl-Choline). Selected results and their analysis from an experiment at ESRFs ID 1 beamline are presented.

AKB 40.27 Wed 16:30 P3

Control of Single Nanocrystal Fluorescence Emission in a combined TIRFM/AFM Setup — ●RAINER ECKEL¹, VOLKER WALHORN¹, CHRISTOPH PELARGUS¹, THOMAS NANN², DARIO ANSELMETTI¹, and ROBERT ROS¹ — ¹Experimental Biophysics and Applied Nanosciences, Faculty of Physics, Bielefeld University, Universitaetsstr. 25, 33615 Bielefeld, Germany — ²Freiburg Materials Research Center (FMF), Stefan-Meier-Str. 21, 79104 Freiburg, Germany

Optomechanical switching and local energy transfer between individual nanoobjects are concepts of growing importance for investigating and manipulating matter at the nanoscale. We report on a new possibility to switch the fluorescence emission of a single semiconductor nanocrystal (quantum dot) by external, optomechanical intervention of an AFM tip. The experimental setup combines atomic force microscopy (AFM) and total internal reflection fluorescence microscopy (TIRFM) in a way that enables laser induced fluorescence imaging of single fluorophores and their simultaneous mechanical addressing with an AFM probe. The flu-

orescence quenching of an individual semiconductor quantum dot could be controlled mechanically, using an AFM tip functionalized with gold nanoparticles as the quenching agent. It was possible to repeatedly switch the fluorescence emission from the bright (blinking) state to the dark (quenched) state. This opens fascinating possibilities for future simultaneous force spectroscopy and fluorescence resonant energy transfer measurements on single biomolecular complexes.

AKB 40.28 Wed 16:30 P3

Highly oriented liquid water within the cationic lipid DODAB — ●LYDIA WOITERSKI¹, JOSEF A. KÁS¹, DAVID W. BRITT², and CARSTEN SELLE¹ — ¹Institute of Experimental Physics I, University of Leipzig, Linnestraße 5, D-04103 Leipzig, Germany — ²Department of Bioengineering, University of Utah, Salt Lake City, UT, 84112, USA

Cationic lipid membranes spontaneously form complexes with DNA. Therefore, cationic synthetic lipids are widely used for the preparation of gene transfection systems.

We performed a fundamental attenuated total reflection (ATR) Fourier-Transform infrared (FTIR) spectroscopic study on the phase behavior and hydration properties of the cationic lipid dioctadecyldimethylammonium bromide (DODAB).

A unique shape of the $\nu(\text{OH})$ -absorption band was detected that arises from liquid water in the vicinity of the polar lipid headgroup. Six subbands of the OH-absorption can be assigned to different populations of highly oriented water molecules. Furthermore, the spectroscopic properties of the headgroup bound water were observed to be strongly sensitive to the halide counterion present.

Another newly found feature of DODAB is a drastic change in the $\nu(\text{CNC})$ -absorption which is attributed to a strong conformational alteration in one of the alkyl chains when the water is completely removed.

AKB 40.29 Wed 16:30 P3

An Intestinal Drug Transport Model — ●NIKO KOMIN and RAÚL TORAL — IMEDEA, Palma de Mallorca, Spain

Drug absorption in the intestinal tract happens due to two different processes: passive diffusion proportional to the concentration difference and active transport via a molecular pump. The active transport is usually described as a Michaelis-Menten process.

Little is known about the number and location of the pumps (inside/outside the intestine) and its governing parameters. Experiments and nonlinear parameter regression try to know more about the process, but a deeper understanding of the underlying process would facilitate the experimentators work and help on the drug development, meaning less experiments, safer and maybe more specific drugs.

In this work differential equations describing the continuous concentration transport are analysed. Long term and short term solutions are desired. Besides we try to explain the variability in the measurements, introducing variability or noise into the equations.

AKB 40.30 Wed 16:30 P3

Purification and characterisation of nacre proteins and their interaction of nacre proteins with CaCO_3 at the molecular scale — ●LAURA TRECCANI, FABIAN HEINEMANN, and MONIKA FRITZ — Institut of Biophysics, University of Bremen, Germany

Nacre (mother of pearl) of certain molluscs furnishes an elegant model to investigate biomineralizing processes. Nacre is a polymer-ceramic composite material consisting mainly of CaCO_3 and biomolecules (chitin and proteins). It shows a highly ordered hierarchical structure consisting of parallel layers of aragonite tablets (500 nm thickness) alternated with layers of organic material (10 nm thickness). Nacre has a high mechanical strength and resistance against corrosion in seawater that far exceeds the properties shown by the inorganic CaCO_3 mineral. Organic molecules are necessary for a controlled nucleation and growth of the material. The role of several water-soluble proteins purified from nacre of *H. laevigata* has been investigated. Crystallization experiments were performed with the AFM (Atomic Force Microscope) in aqueous solution on a calcite surface and with the ammonium carbonate method. It has been elucidated that each protein influences the crystal growth in a different way. Some proteins can act as nucleators, where others can act as inhibitors. Recently small proteins directly incorporated into the mineral phase have been detected. The characterisation of the single biomolecules and their roles in self-organizing mechanisms of nacre formation could lay the basis for a better understanding of biomineralization and the development of new synthetic biomaterials.

AKB 40.31 Wed 16:30 P3

Orientation of the Membrane-Active Peptide Gramicidin S within Model Membranes — ●STEFAN SURBER — Universität Leipzig, Lehrstuhl für die Physik Weicher Materie, Fakultät für Physik und Geowissenschaften, Linnestr. 5, D-04103 Leipzig

S. Surber, J.A. Käs and C. Selle

The amphipathic peptide gramicidin S (GS) attacks the integrity of membranes but the detailed mode of action is still unclear. In order to unravel the orientation of GS within models for bacterial and mammalian membranes - which is considered crucial for fundamental interactions between GS and membrane lipids - we performed an attenuated total reflection (ATR) Fourier transformed infrared (FTIR) spectroscopic study. For this purpose, mixtures from GS and phospholipid from neutral and anionic phospholipids representing bacterial and mammalian membrane components were used. The effect of varied hydration on the peptide-lipid interactions was also investigated. For the first time, the orientation of GS within model membranes was directly measured utilizing the related amide I IR spectroscopic absorptions. First results on the orientation of GS in Langmuir-Blodgett transferred lipid monolayers are also presented.

AKB 40.32 Wed 16:30 P3

Electrostatic Interactions modulated within Monolayers of charged Amphiphilic Peptide — ●ANN FALK, STEFAN SURBER, LYDIA WOITERSKI, JOSEF KÁS, and CARSTEN SELLE — Universität Leipzig, Fakultät Physik & Geowissenschaften, Exphysik I, PWM

We performed a fundamental investigation on the effect of the antimicrobial peptide gramicidin S (GS) on the properties of lipid monolayers as membrane mimics. As a first step, pure GS monolayers on subphases of physiologic ionic strength were characterized at room temperature ($I \sim 0.19 \text{ M}$). Pressure-area isotherms of GS monolayers were recorded indicating a phase transition from a liquid to a solid phase in two dimensions that was dependent on the subphase pH. This variation can be explained by pH-dependent basic amino acid side group charges of GS. Brewster-Angle-Microscopy was used to monitor the solid-phase domain growth during the 2D phase transition. We observed that the shape of the solid domains is surprisingly sensitive to pH alterations over ten orders of magnitude. X-ray reflectivity and grazing incidence diffraction measurement were performed under analog conditions. First results of experiments on the interactions of GS with various phospholipids representing bacterial and mammalian membrane components are also presented.

AKB 40.33 Wed 16:30 P3

Dynamics of the denaturated protein Ribonuclease A — ●RALF BIEHL¹, BERND HOFFMANN², MICHAEL MONKENBUSCH¹, AUREL RADULESCU¹, BELA FARAGO³, RUDOLF MERKEL², and DIETER RICHTER¹ — ¹Institut fuer Festkoerperforschung, Forschungszentrum Juelich, Germany — ²Institut fuer Schichten und Grenzflaechen, Forschungszentrum Juelich, Germany — ³Institut Laue-Langevin, Grenoble, France

The protein folding and function is strongly coupled to the structure and the thermal equilibrium fluctuations. In view of the macromolecule energy landscape the protein folding follows a path from the unfolded state at high energy to the low energy state at the final configuration with intermediate states in between. Thereby the secondary and ternary structure is determined. Catalytic activities or transport mechanisms follow transitions between intermediate states in the energy landscape. All involve configurational changes on length scales from single amino acids to sizes of complete α helices or β sheets and the total size of the protein. Timescales reach from picoseconds to microseconds. A way to explore the energy landscape at equilibrium is to observe thermal fluctuations of the protein. By changing environmental parameters e.g. temperature the level of energy is changed. We present here measurements on bovine Ribonuclease A by means of SANS and Neutron Spin Echo Spectroscopy together with DLS measurements. The protein dynamics was examined under conditions providing the possibility of refolding to the natural state. We compare our experimental results with simple and more complex protein models to reproduce the observed dynamics.

AKB 40.34 Wed 16:30 P3

Self-assembled phagosome crystal structures in fibroblasts — ●VAMSI KODALI^{1,2}, JOACHIM SPATZ^{1,2}, and JENNIFER CURTIS^{1,2} — ¹Max-Planck-Institute for Metals Research, Department New Materials & Biosystems, Heisenbergstr. 3, D-70 569 Stuttgart. — ²University of Heidelberg, Department of Biophysical Chemistry.

During phagocytosis, cells actively deform their plasma membranes to engulf foreign objects. The engulfed object (phagosome) is then actively transported towards the nucleus by dynein motors in a process called retrograde motion. In this study we present the surprising observation that fibroblast cells ingest large numbers of latex microspheres and arrange them in beautiful 2D crystals with hexagonal order in the perinuclear region. We study the process of the crystallization which occurs for bead sizes ranging from 750 nm up to at least 6 microns, where the upper limit has not been fully explored. We also consider the influence of the crystallization of the beads on normal cell processes such as cell proliferation and study the impact of this massive volumetric intrusion on the organelles and the cytoskeleton of the fibroblasts. It was also found that there is an area limitation for the crystal structures in the cell and this limited area depends on the cell size and is independent of the bead size. Finally, we present the counterintuitive observation that mixed sizes of microspheres tend to phase separate with the large spheres moving to the center even under biased initial conditions.

AKB 40.35 Wed 16:30 P3

Transport along freely suspended actin cortex models in a controlled microfluidic environment — ●SIMON SCHULZ^{1,2}, TAMAS HARASZTI^{1,2}, WOUTER ROOS², CHRISTIAN SCHMITZ^{1,2}, JENS ULMER^{1,2}, STEFAN GRAETER^{1,2}, and JOACHIM P. SPATZ^{1,2} — ¹Max-Planck-Institute for Metals Research, Department New Materials & Biosystems, Heisenbergstr.3, D-70569 Stuttgart — ²University of Heidelberg, Department of Biophysical Chemistry, INF 253, D-69120 Heidelberg

Arrays of microfabricated pillars are constructed to serve as a template for mimicking the actin cortex of cells. The 3D template surface prevents interaction of the actin filaments hanging between pillars. A special flow-cell design enables applying flow around a network of actin freely suspended between polydimethylsiloxane pillars. This opens new possibilities to study the biomechanics of two-dimensional actin networks as a function of actin-crosslinkers, to observe the active diffusion of molecular motors operating on pending networks and to investigate the alternations in the transport of microscopic particles, coated by different proteins and molecular motors, along these actin cortex models under the drag of flow.

Additionally, actin filaments act as tracks for guiding passive and active transport of cargo such as organelles or microspheres by molecular motors like myosin-V. The stiffness of the F-actin can be tuned by bundling through various cross-linkers.

These transport problems are biomimetic studies of tracks and external driving force on a statistical process of two-dimensional networks isolated from the complicated and undetermined cellular environment.

AKB 40.36 Wed 16:30 P3

Effect of cholesterol on the collective dynamics of phospholipid membranes — ●BEATE BRÜNING^{1,2}, TIM SALDITT², ARNO HIESS¹, and MAIKEL C. RHEINSTÄDTER¹ — ¹Institut Laue-Langevin, B.P. 156,6 rue Jules Horowitz, 38042 Grenoble, France — ²Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Phospholipid membranes often serve as simple model systems to understand basic properties of their far more complex biological counterparts. Only recently, the collective short wavelength dynamics in a model membrane system (DMPC), i.e., the corresponding dispersion relation, were investigated by inelastic neutron scattering techniques [1]. The insertion of the membrane-active molecule cholesterol, which is known to regulate membrane fluidity, membrane permeability and the lateral mobility of proteins, is now a first step towards the understanding of coherent dynamics in physiologically relevant membrane systems.

While the structure of phospholipid/cholesterol systems is well studied, their short scale dynamics are so far largely unknown. We have studied the influence of cholesterol to the collective short wavelength fluctuations of the phospholipid acyl chains using inelastic neutron scattering. The measurements were carried out with thermal as well as cold neutrons on the three-axis spectrometers IN12 and IN8 at the high flux reactor of the ILL in Grenoble, France. We were able to determine the dispersion relations within the plane of the membranes in the fluid and the liquid ordered phases of samples with two different cholesterol contents, namely 3% and 35%.

[1] M.C. Rheinstädter *et al.*, Phys. Rev. Lett. 93, 108107 (2004).

AKB 40.37 Wed 16:30 P3

Approximation of localised calcium fluxes — ●KAJETAN BENTELE and MARTIN FALCKE — Hahn Meitner Institut Berlin, Glienickestrasse 100, 14109 Berlin, Germany

To model spatially resolved intracellular calcium-dynamics, it is necessary to investigate the calcium current through a single channel. An open channel can be modelled as a pore connecting an intracellular calcium store, the endoplasmic reticulum (ER), with the cytosol. The radius of such a channel is about 6 nanometres in contrast to the diameter of the cell ranging from 10 to 100 micrometres. Opening of such a channel leads to a localised increase of the cytosolic calcium concentration nearby the channel. This process is the fundamental building block in the concentration dynamics of global events such as calcium waves and oscillations.

We present a quasi-steady state approximation of the single-channel current with a simplified dynamics. The approximation is based on the observation that the channel current exhibits multiple time scales: infinitely many fast time scales and a long time-scale that can be up to 5 orders of magnitude larger. The former play a prominent role in building up the concentration-peak around the channel. The slow time scale is determined by the average concentration in the ER and therefore can be mimicked by a quasi steady state approximation. This approximation will be used in simulations to eliminate spatial dynamics in the ER.

AKB 40.38 Wed 16:30 P3

DNA elasticity and specific binding — ●NILS BECKER and RALF EVERAERS — MPI Physik Komplexer Systeme, Dresden

In essential biological processes, DNA interacts with proteins in an indirect way. In some complexes the double helical structure of DNA remains intact, but is strongly deformed. Binding then depends on the deformability of the DNA. This indirect readout mechanism allows for binding to specific sequences based on their elasticity and structure.

An understanding of this kind of specific interaction requires detailed information about sequence-dependent DNA elasticity. Modeling DNA as a chain of rigid elements, the base pairs, this information can be encoded in elastic potentials between each step of two base pairs. Harmonic base pair step potentials have been determined in rather dissimilar ways from high-resolution structural data [1] and by molecular dynamics computer simulation of oligonucleotides [2].

We examine the relation of these two parametrizations. On this basis we give a measure for estimating how much the elastic deformation of a given base pair contributes to sequence specificity in a given complex. As a test case, we show results for the bacteriophage 434 repressor, a well-studied such complex [3], in which some base pairs are not contacted by the protein but still when mutated, greatly modify binding affinity.

[1] W. Olson *et al.*, PNAS 95(19), 11163, 1998

[2] F. Lankas *et al.*, Biophys J 85(5), 2872, 2003

[3] G.B. Koudelka *et al.*, PNAS 85(13), 4633, 1988

AKB 40.39 Wed 16:30 P3

Molecular Dynamics Study of the Chromophore Binding pocket in Rhodopsin — ●MINORU SUGIHARA^{1,2}, MARKUS GRUNER², PETER ENTEL², and VOLKER BUSS¹ — ¹Theoretical Low-Temperature Physics — ²Theoretical Chemistry, University of Duisburg-Essen

The 11-cis retinal protonated Schiff base (pSb) is the chromophore in rhodopsin, the black/white photoreceptor in the vertebrate eye. The chromophore is covalently attached to Lys296 via a pSb and has a salt-bridge with the negatively charged counterion, Glu113. The first crystal structure of bovine rhodopsin [1] has revealed that the chromophore is fixed in the pocket by hydrophobic interaction at the β -ionone ring and polar interaction, in particular by a salt-bridge. Upon illumination with light, the chromophore photoisomerizes from 11-cis to all-trans. The first intermediate, bathorhodopsin, stores 32-35 kcal/mol of the photon energy in the twisted all-trans form. The starting model of the chromophore binding pocket (534 atoms) was taken from the crystal structure [2]. In this study, the chromophore conformation inside the pocket, the origin of the twisted conformation, and the stability of the protonation state [3] will be discussed. For molecular dynamics study, the plane wave code, VASP [4] was used. The calculations were carried out on the IBM BlueGene/L at the Reseach Center Jülich. [1] Palczewski, K., Okada, T. *et al.* Science 289 (2002) 739. [2] Okada, T., Sugihara, M. *et al.* J. Mol. Biol. 342 (2004) 571. [3] Buss, V. Chirality 13 (2001) 13. Sugihara, M., Buss, V. *et al.* Biochemistry 41 (2002) 15259. Sugihara, M., Buss, V. *et al.* J. Phys. Chem. B 108 (2004) 3673. Sugihara, M., Hufen, J. Biochemistry in press. [4] Kresse, G., Furhermüller J. Phys. Rev. B 54 (1996) 11169.

AKB 40.40 Wed 16:30 P3

DNA Melting in Aggregates: Impeded or Facilitated? — ●ANDREY CHERSTVY¹ and ALEXEI A. KORNYshev² — ¹Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — ²Department of Chemistry, Faculty of Physical Sciences, Imperial College London, SW7 2AZ, London, United Kingdom

How does DNA melt in columnar aggregate relative to its melting in diluted solution? Is the melting temperature increased or decreased with the aggregate density? Have DNA-DNA interactions, predominantly of electrostatic nature, an effect on the character of the melting transition? In attempt to answer these questions, we have incorporated the theory of electrostatic interactions between DNA duplexes [1,2] into the simplest model of DNA melting. The analysis shows that the effect of aggregate density is very different for aggregates built of homologous (or identical) DNA fragments relative to the case of DNA with random base pair sequences. The putative attraction between homologous DNA helices hampers their melting and increases the melting temperature and can even dramatically change the character of the transition [3]. In the aggregate of nonhomologous DNAs, the pattern of electrostatic interactions is more complicated, and their effect could be opposite; in some cases we may even expect electrostatically induced melting [3]. These findings define new directions for melting experiments in dense DNA assemblies.

[1] A. A. Kornyshev and S. Leikin, J. Chem. Phys., 107 3656 (1997). [2] A. G. Cherstvy, A. A. Kornyshev, and S. Leikin, J. Phys. Chem. B, 106, 13362 (2002); *ibid.*, 108, 6508 (2004). [3] A. G. Cherstvy and A. A. Kornyshev, J. Phys. Chem. B, 109, 13024(2005).

AKB 40.41 Wed 16:30 P3

Optical manipulation of neuronal cells in 3D scaffolds — ●ANDREAS CHRIST and JOCHEN GUCK — Institut für Physik weicher Materie, Universität Leipzig, Linnéstraße 5, 04103 Leipzig

Control of neuronal outgrowth is an important objective in neuroscience, cell biology and medicine. It already has been shown that this is possible in 2D by surface patterning or optically by gradient forces and in 3D environments by chemical gradients.

The aim of our research is to optically influence growth of neurites in a 3D scaffold. For this purpose we grow neuronal cells (NG-108) in fibrin gels and direct a non-focused low-power laserbeam into the region of cell growth. The gradient force exerted by the laser should pull the growth cone of neurites into the beam. The radiation pressure exerted by the laser on the growing neurite will then tend to direct the neurite into the direction of the beam propagation. This is confirmed by Confocal Laser Scanning Microscopy of the GFP-transfected cells.

AKB 40.42 Wed 16:30 P3

Study of DNA/RNA strand interactions using lattice models — ●CHRISTIAN SIMM, SANJAY KUMAR, and RALF EVERAERS — Max-Planck-Institut für Physik komplexer Systeme, Dresden

Research in binding properties of DNA/RNA is key for the understanding of many biological processes - like hairpin formation in ssDNA and miRNA, RNA secondary structure, and bubble formation during DNA transcription. We study lattice models of DNA which account for base stacking and polarity of the DNA strands. We draw comparisons to simpler models without these features to get a better understanding of the effects of stacking and polarity. We use exact enumeration and Monte-Carlo simulation techniques to test assumptions of the nearest-neighbour model.

AKB 40.43 Wed 16:30 P3

Optimal Foraging Strategy: Angle Matters — ●UDO ERDMANN¹, SEBASTIAN GÖLLER¹, LUTZ SCHIMANSKY-GEIER¹, IGOR M. SOKOLOV¹, and FRANK MOSS² — ¹Institut für Physik, Humboldt-Universität zu Berlin — ²Center for Neurodynamics, University of Missouri at St. Louis

We report a theory to describe the motion of zooplankton. Into contrast to move just randomly like a classical Brownian particle, zooplankters like *Daphnia* or *Copepods* pick their turning angle from a distribution which is far from being Gaussian or equally distributed. This leads to different behavior in the motion compared to normal diffusion. The question which can be asked here is: Is there an evolutionary reason to forage for food in the aforementioned manner? The talk is planned to give an answer into that direction.

AKB 40.44 Wed 16:30 P3

Relating microstructure of biomaterials to mechanical properties — ●BORIS BREIDENBACH¹, ADRIAN SHEPPARD², ULRIKE WEGST³, and KLAUS MECKE¹ — ¹Institut für theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — ²Applied Mathematics, Australian National University, Canberra, Australia — ³Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

Although biomaterials like wood or nutshells consist mainly of cellulose, they exhibit a broad range of mechanical properties. As woods mainly consist of cellulose, the explanation for this behaviour lies in the microscopic structure of the pore space. We have studied the structure of wood using phase contrast X-ray tomography at a resolution of $0.3\mu\text{m}$ to resolve the fibrous structure.

Using parallel implementations of anisotropic diffusion and a region growing algorithm, we can extract the pore space of the 2000^3 voxel large data sets. For these structures we calculate the Minkowski valuations, a complete set of morphometric tensors which allow for a characterization of anisotropy in materials. The extracted wood structure can also be used to numerically measure the elasticity tensor. The aim is to relate the elastic properties of heterogeneous materials to Minkowski tensors.

AKB 40.45 Wed 16:30 P3

Investigation of ion channel function with a high frequency approach — ●MICHAEL OLAPINSKI¹, ANDREA BRÜGGEMANN², MICHAEL GEORGE², NIELS FERTIG², STEPHAN MANUS¹, and FRIEDRICH C. SIMMEL¹ — ¹Department für Physik, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München, Germany — ²Nanon Technologies GmbH, Pettenkoferstr. 12, 80336 München, Germany

Due to the limited bandwidth of the measurement setup, classical patch-clamp techniques cannot be used to study fast dynamical processes within ion channel proteins which may influence ionic transport. To overcome this limitation, chip-based methods are explored to study ion channel dynamics with the help of high-frequency (HF) techniques.

We present an approach, where a patch-clamp on-a-chip system is combined with an open-end coaxial probe that is positioned in close proximity to the cells under investigation. Ionic currents through the cell membrane are measured in whole-cell configuration while HF fields are applied at frequencies from MHz to 40 GHz. The ionic currents measured with rat basophil leukaemia (RBL) cells containing a potassium channel are sensitive to the applied HF field in specific frequency ranges and depend on the presence of potassium ions and the applied membrane potential. However, local heating of the buffer can be shown to play an important role in this case. Using a lock-in technique with a modulated HF excitation, it becomes possible to differentiate between thermal effects caused by the HF irradiation and intrinsic effects in which the field couples to membrane polarization and ion channel dynamics.

AKB 40.46 Wed 16:30 P3

Temperature dependent voltage-induced gating of OmpF — ●CATALIN CHIMEREL¹, LIVIU MOVILEANU², and MATHIAS WINTERHALTER¹ — ¹International University Bremen, Germany — ²Syracuse University, New York, USA

OmpF porin is a trimeric β -barrel channel from the outer cell wall of *E. coli*. A characteristic of the channel is its complete closure at transmembrane voltages (~ 130 mV at room temperature), which depend on the experimental conditions. We employed single-channel and macroscopic current recordings in planar lipid bilayers to examine the gating fluctuations leading to transient or permanent closure as a function of applied voltage in a temperature range between 2 and 72 °C. The OmpF single-channel conductance, the amplitude of the gating blockades, and the lifetime of the closure sub-states were strongly temperature-dependent. Increasing the temperature increases the number of short-lived fluctuations, their lifetime, and the OmpF single-channel conductance in a non-linear manner, but decreases the threshold transmembrane voltage above which a complete closure occurs. These data reveal different mechanisms for channel closure that are discussed.

AKB 40.47 Wed 16:30 P3

Nanoindentation studies of full and empty viral capsids and the effects of capsid protein mutations on elasticity and strength — ●IRENA L. IVANOVSKA¹, JEAN PHILIPPE MICHEL², M. M. GIBBONS³, W. S. KLUG³, C. M. KNOBLER², GJJS. J.L. WUITE¹, and CHRISTOPH F. SCHMIDT¹ — ¹Dept. Physics, Vrije Universiteit, Amsterdam, NL — ²Department of Chemistry and Biochemistry, University of California Los Angeles, Los Angeles, CA 90095-1569, USA — ³Department of Mechanical and Aerospace Engineering, University of California Los Angeles, Los Angeles, CA 90095-1597, USA

The elastic properties of capsids of the cowpea chlorotic mottle virus (CCMV) have been examined at pH 4.8 by nano-indentation measurements with an atomic force microscope. Studies have been carried out on wild-type capsids, both empty and containing the RNA genome, as well as on full capsids of a salt-stable mutant and empty capsids of the subE mutant. Full capsids resisted indentation more than empty capsids but all of the capsids were highly elastic. There was an initial reversible linear regime that persisted up to indentations varying between 20 and 30 % and applied forces of 0.6 to 1.0 nN; it was followed by a steep drop in force that was associated with irreversible deformation. A single point mutation in the capsid protein increased the capsid stiffness. The experiments are compared with calculations by finite element analysis of the deformation of a homogeneous elastic thick shell. These calculations capture the features of the reversible indentation region, and allow Young's moduli and relative strengths to be estimated for the empty capsids.

AKB 40.48 Wed 16:30 P3

Multifunctional liposomes: controlled permeability and micromanipulation — ●YANNIC RAMAYE¹, JOANA GOMES¹, TRISTAN RUYSSCHAERT², DIDIER FOURNIER², JÜRGEN FRITZ¹, and MATHIAS WINTERHALTER¹ — ¹International University Bremen, Germany — ²Institut Pharmacologie et Biologie Structurale, UMR5089, Toulouse, France

Enzymes are able to accelerate biochemical reactions by many orders of magnitudes and it is tempting to use them for biotechnological synthesis. However, instability, their low recovery during biocatalytic processes and their high cost make them commercially less advantageous. A possible method to protect proteins from hostile environment is via encapsulation in vesicles. We control the permeability of water soluble substance by reconstitution of natural or bio-engineered channel forming proteins. For example, Acetylcholinesterase is highly sensitive to pesticides and was engineered to become a tool for pesticide detection. We have shown that encapsulation into liposomes stabilizes the enzyme against dilution effect and protects it against proteolytic agents. High encapsulation yield was achieved using affinity to bind the free enzyme to the capsule surface. Vesicles with covalently bonded complementary strands were bound to the surface of a DNA-chip. This allows to functionalize a large number of capsules on specific areas. Magnetic liposomes are synthesized by swelling dried lipids with magnetic fluid based on maghemite citrated nanoparticles. The incorporation of these nanoparticles allows liposome manipulation by applying a magnetic field. To increase stabilization, vesicles can easily be coated with polyelectrolytes.

AKB 40.49 Wed 16:30 P3

Temperature dependence of X-ray photoreduction and EXAFS Debye-Waller factors suggest role of protein-specific dynamics — ●PAOLA LOJA — FU-Berlin

In oxygenic photosynthesis, driven by lights the Mn4-complex of Photosystem II (PSII) cycles through four semi-stable intermediate states denoted as S-states. As revealed by X-ray absorption spectroscopy (XAS, EXAFS), the S-state transitions are coupled to significant rearrangements of the nuclei of the tetra-manganese complex (Dau et al., 2000; Haumann et al., 2002). Nonetheless the energetic efficiency is extraordinarily high (small enthalpic losses) and the involved activation energies are surprisingly low. Are protein-specific dynamics of importance?

AKB 40.50 Wed 16:30 P3

Shear-dependency of von Willebrand factor measured in hydrodynamic flow and by micro-pipette aspiration technique — ●J. OPFER, A. WIXFORTH, and M. F. SCHNEIDER — Universität Augsburg

Von Willebrand factor (vWf) is a biopolymer, which is known to play an important role in hemostasis. Dysfunction entails severe bleeding disorders. Recently it was shown that vWf reactivity is increased by shear stress, which is presumably caused by a coil-fiber transition. On the other hand, a shear-induced loss of efficiency has been found. Hence the

correlation between shear forces and vWf effectivity is of great interest.

In order to study this correlation we mimic blood flow using novel designed bio-chips by means of surface acoustic waves (SAW), which are launched into the fluid containing vWf polymers and generate a laminar flow. The method allows sample volumes of only a few microliters, a wide spectrum of flow velocities and the imitation of any physiological relevant geometry.

Besides micro-pipette aspiration technique is applied for measuring homotypic interactions of vWf molecules, which have undergone different shearing forces. Mono-laminar phospholipid vesicles are coated with vWf and exposed to a vWf-covered wall. The vesicle's deformation reflects the magnitude of adhesive forces mediated by the polymer and permits observing its self-association kinetics.

AKB 40.51 Wed 16:30 P3

Interaction of the small G-protein Ms-Rac1 from *Medicago sativa* with GTP — ●DANIEL WESNER¹, MARTINA BRECHT², KARSTEN NIEHAUS², DARIO ANSELMETTI¹, and ROBERT ROS¹ — ¹Faculty of Physics, Experimental Biophysics & Applied Nanosciences, University of Bielefeld, 33615 Bielefeld, Germany — ²Faculty of Biology, Genetics, University of Bielefeld, 33615 Bielefeld, Germany

Small GTP-binding proteins are important molecular regulators in the signal transduction chains of eukaryotic cells. The protein Ms-Rac1 from *Medicago sativa* can switch from an active to an inactive state, controlled by the binding of the nucleotides GTP and GDP, respectively. We characterize the interaction of Ms-Rac1 with fluorescently labeled GTP by using fluorescence correlation spectroscopy (FCS). The labeled, protein-bound GTP can be competitively displaced by an excess of unlabeled GTP. The binding and dissociation of GTP and Ms-Rac1 are significantly accelerated by reducing the concentration of magnesium. The off-rates were determined to be $3.0 \times 10^{-4} \text{ s}^{-1}$ and $3.2 \times 10^{-3} \text{ s}^{-1}$ at a concentration of Mg^{2+} of 510 and $3.8 \mu\text{M}$, respectively. Moreover, we found a reduced hydrodynamic radius of the protein-GTP-complex with increasing salt concentration, indicating the formation of oligomers of approx. 25 subunits at low ionic strength. At higher ionic strength the fraction of bound GTP shows a hyperbolic dependence on the concentration of Ms-Rac1, where the reaction displays a pseudo-first order kinetics. In addition, the influence of guanine nucleotide dissociation inhibitors (GDI) on these interactions was quantified. Incubation of Ms-Rac1 with RhoGDI reduces the observed binding rate of labeled GTP by a factor of 1.7.

AKB 40.52 Wed 16:30 P3

Motion by Stopping: Brownian motors without asymmetric potential — ●SUSAN SPORER, CHRISTIAN GOLL, and KLAUS MECKE — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen, Germany

The Brownian motion of a particle in a liquid can be biased without thermal gradients or macroscopic force fields, if the shape of the particle is asymmetric and relaxation in equilibrium is prohibited by external force. In contrast to previous work the external potential does not need to be asymmetric, it is sufficient to arrest the particle at periodic intervals. We analysed by molecular dynamics simulations the dependence of the drift velocity on the particle shape and the fluid density. In the limit of a dilute gas an exact analytic calculation of the shape dependence is possible.

AKB 40.53 Wed 16:30 P3

Form follows function: how PufX-induced dimerization improves the efficiency of the light harvesting complexes of *Rb. sphaeroides* — ●TIHAMER GEYER — Zentrum für Bioinformatik, Universität des Saarlandes, D-66041 Saarbrücken

Lately there has been renewed interest in the "mystery" protein PufX, which occurs in the purple bacteria *Rb. sphaeroides* and *Rb. capsulatus*. It is responsible there for a dimerization of the light harvesting complexes of type I (LH1). Its key function seems to be to open the LH1 rings for eased diffusion of the quinones to the enclosed reaction centers (RC).

We show that the symmetry breaking induced by PufX also has an important effect on the main purpose of the LH1s, which is to help the RCs to absorb light. For this we extend a simple dipole model of the bacteriochlorophyll (Bchl) arrays of the LH1 and the RC [Hu et al., J. Phys. Chem 101 (1997) 3854] to calculate the absorption properties of the PufX induced LH1 dimers and their coupling to the special pair Bchls of the RCs. Comparison with the closed monomeric LH1/RC unit shows that the dimer has the same photosynthetically effective absorption cross section per monomer though it contains less Bchls. Additionally, the dimeric

setup reduces the statistical fluctuations in the photon rate for the two RCs, thus further increasing the efficiency of photosynthesis.

AKB 40.54 Wed 16:30 P3

Normal heart beat, alternans and fibrillation in a model for the rabbit ventricles — ●STEFFEN BAUER¹, GEORG RÖDER¹, and MARKUS BÄR — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin

Cardiac propagation is investigated by simulations of the modified Beeler-Reuter model using the geometry and muscle fibre orientation of the ventricles taken from the San Diego rabbit heart. Electrical excitation is introduced by a periodic pacing of the apex of the heart. Depending on the pacing frequency qualitatively different dynamics are observed namely normal heart beat, alternans and fibrillation at small, intermediate and large pacing frequencies, respectively. The simulated electric potential on the heart surface during normal heart beat agrees well with experimental data. The onset of alternans and fibrillation are in line with simulations of a one-dimensional model, where the corresponding instabilities are analyzed in more detail.

AKB 40.55 Wed 16:30 P3

SFM-Investigations on cell motility — ●C. BRUNNER¹, M. GÖGLER¹, A. EHRLICHER¹, B. KOHLSTRUNK¹, D. KNEBEL², and J. KÄS¹ — ¹Institute for Soft Matter Physics, University of Leipzig, Linnéstr. 5, 04103 Leipzig — ²JPK Instruments AG, Bouchéstr. 12, 12435 Berlin

A cell's ability to move is essential for various functions in nature, such as morphogenesis, immune response, and the invasiveness of cancer. On the molecular level, actin polymerization and molecular motors, such as myosin, are involved in cell motility, but the mechanism as a whole is not very well understood. We used a scanning force microscopy (SFM) technique to directly measure the forward forces actively generated at the leading edge, the cell body, and in lamellar fragments of fish keratocytes. We glued polystyrene beads with 2-3 μm radii to cantilever tips to provide a well-defined probe geometry and avoid puncturing the cell. The bead was positioned in front of a moving cell which pushed the bead out of its path and therefore bent the cantilever. The forward force was calculated using the detected vertical deflection of the cantilever in an elastic wedge model, which considers cellular deformation. To reveal more about the force generation machinery used during protrusion, we treated keratocytes with the drug cytochalasin D, which interrupts actin polymerization by capping the actin filaments. The cell's velocity decreases depending on the drug concentration. Comparison of the protrusion forces with and without cytochalasin D reveals the importance of actin polymerization in keratocyte motility.

AKB 40.56 Wed 16:30 P3

Two-photon scanning fluorescence correlation and cross-correlation spectroscopy — ●ZDENĚK PETRÁŠEK and PETRA SCHWILLE — Biotechnologisches Zentrum der TU Dresden; Institut für Biophysik; Tatzberg 47 - 51; 01307 Dresden; Germany

Fluorescence correlation and cross-correlation spectroscopy methods (FCS and FCCS) obtain information about molecular diffusion and inter- and intramolecular processes by analysing fluctuations of the fluorescence intensity reflecting the fluctuations of various physical parameters. The fluctuations are quantified by means of the autocorrelation function of the measured signal $F(t)$. In order for the autocorrelation to be representative of the investigated system the averaging in the autocorrelation calculation has to be performed over sufficiently high number of statistically independent events. This may be difficult to achieve when the diffusion of the fluorescent particles is slow, resulting in insufficient turnover of the particles in the measurement volume.

The scanning FCS (SFCS) combines the standard FCS with relative movement of the sample and the excitation beam. This improves the statistical accuracy by averaging over more independent locations within the sample. Furthermore, photobleaching effects can be reduced since the excitation dose is distributed over a larger part of the sample. We have employed a home-built two-photon laser scanning system to compare SFCS and SFCCS with their stationary counterparts, using several scanning patterns. The focus is on achieving a good signal-to-noise ratio and minimizing photobleaching effects while keeping the measurement time and the total light dose low.

AKB 40.57 Wed 16:30 P3

Transitions in a bistable model of the calcium/calmodulin-dependent protein kinase-phosphatase system in response to LTP and LTD protocols — ●MICHAEL GRAUPNER and NICOLAS BRUNEL — Laboratoire de Neurophysique et Physiologie, CNRS UMR 8119, Université René Descartes - Paris V, Paris, France

The calcium/calmodulin-dependent protein kinase II (CaMKII) plays a key role during induction of long-term post-synaptic modifications following calcium entry. The biochemical network involving CaMKII and its regulating protein signaling cascade has been hypothesized to be a bistable realization of such a switch. However, it is still unclear whether LTP/LTD protocols lead to transitions between these two states in realistic models of such a network. A detailed biochemical model of the CaMKII autophosphorylation and the protein signaling cascade governing the CaMKII dephosphorylation is presented. As reported by Zhabotinsky [Biophys J 2000; 79:2211], two stable states of such a system exist at resting intracellular Ca^{2+} concentration: a weakly-(DOWN) and a highly-phosphorylated (UP) state of the CaMKII. A transition from the DOWN to the UP state can be achieved by high calcium elevations. Intermediate Ca^{2+} concentrations enhance CaMKII dephosphorylation. This results in depotentiation - switching from the UP to the DOWN. Finally, it is shown that the CaMKII system can qualitatively reproduce results of plasticity outcomes in response to standard experimental induction paradigms of long-term modifications.

AKB 40.58 Wed 16:30 P3

DNA transport during bacterial transformation — ●MADELEINE LEISNER¹, MARTIN CLAUSEN², IRENA DRASKOVIC³, DAVE DUBNAU³, and BERENIKE MAIER² — ¹LMU, Department für Physik, LS Rädler, Munic, Germany — ²Institut für allgemeine Zoologie und Genetik, Westfälische Wilhelmsuniversität, Münster, Germany — ³Department of Microbiology and Molecular Genetics, University of Medicine and Dentistry of New Jersey, Newark, USA

Bacteria employ a variety of molecular motors near the cell envelope to move and communicate with their environment. We are particularly interested in the molecular machines that transport DNA through the bacterial envelope during transformation. Bacteria can acquire genetic diversity by horizontal gene transfer. Many bacteria are naturally competent for uptake of naked DNA from the environment in a process called transformation. Recently, we used optical tweezers to demonstrate that the DNA transport machinery in *Bacillus subtilis* is a force-generating motor, that processively transports macromolecular DNA through nanopores. Currently, we are investigating how the concentration of the single strand binding protein YwpH affects DNA transport properties and transformation efficiency.

AKB 40.59 Wed 16:30 P3

Fluorescence analysis of environmental stress response of single cells within a bacterial population — ●JUDITH LEIERSSEDER¹, KIRSTEN JUNG², and JOACHIM RÄDLER¹ — ¹Physik Department LMU — ²Biologie Department LMU

Gene regulatory networks play a crucial role for the survival of bacteria as they allow them adaptation to varying environmental conditions. In our study we investigate the dynamics of gene expression in bacteria monitored by quantitative and time resolved image processing of GFP-hybrid proteins. This allows the acquisition of time traces of distinct proteins produced in response to environmental stress, which are used as input data for mathematical models. The analysis of many traces in an automated procedure measures the distribution of gene expression in a bacterial population. It allows conclusions on the regulatory mechanism and resolves cell-to-cell variations within a population. As a model system we studied the gene encoding GFP under the control of the arabinose promoter in *E. coli*. The change in GFP content following the exposure to different concentrations of arabinose was measured.

AKB 40.60 Wed 16:30 P3

Structure and Stability of Thiol Containing Collagen Peptides — ●CHRISTIAN RENNER^{1,2}, ULRIKE KUSEBAUCH¹, SERGIO CADAMURO¹, and LUIS MORODER¹ — ¹Max-Planck-Institut für Biochemie, D-82152 Martinsried — ²School of Biomedical and Natural Sciences, Nottingham Trent University, Nottingham NG11 8NS, UK

Collagen is the most abundant protein in mammals and as a natural biomaterial confers stability and strength to tissue. The dominant structural element is the right-handed triple helix that consists of three left-handed poly proline II-like helices formed by the single amino acid

chains and coiled around each other. These trimeric super-helices build chemically cross-linked fibrils or networks that can associate to even larger structures. Cysteine residues are present in native collagens in non-triple helical portions where during maturation interchain disulfide knots are formed to crosslink the constituent three chains, but single cysteine residues of unknown structural and/or biological function are also found in triple-helical sequence portions. In the present study we have synthesized and analysed collagen peptides based on the regular structure (Gly-Pro-Hyp)_n (Hyp is (4R)-hydroxyproline) where one or two amino acids were exchanged for cysteine. The reactivity of the thiol groups thus introduced allows to crosslink peptide chains within the triple helix or link different triple helices for forming a stable biomaterial. Moreover, selective ¹⁵N-labeling of individual glycine residues was expected to allow monitoring of thermal unfolding of the triple helix at defined sites and thus to analyze with spatial resolution the structural stability of the overall rod-like collagen triple helix.

AKB 40.61 Wed 16:30 P3

Characterisation of the affinity improvement of antibody mutants with dynamic force spectroscopy — ●JULIA MORFILL and KERSTIN BLANK — Lehrstuhl für angewandte Physik, LMU München, Amalienstrasse 54, 80799 München

Many biotechnological and pharmaceutical applications require antibodies with high specificity and affinity. To optimise antibody-antigen interactions, a detailed knowledge of the structure of the binding pocket is useful. We investigated four different mutants of a recombinant antibody fragment with a known crystal structure specific for a peptide with single molecule force spectroscopy. The results of these measurements show a loading rate dependent unbinding force. For the clone with the highest affinity (KD = 5.2 pM) we achieved a spontaneous dissociation rate in the order of 10⁻⁴ 1/s and a potential width of 0.9 nm. The clone with the lowest affinity (KD = 2.6 nM) has a similar potential width and a dissociation rate in the order of 10⁻³ 1/s. Interestingly, the two clones only differ in a few amino acids, which do not directly interact with the antigen. In order to explain the affinity improvement, it is therefore necessary to have a more detailed look at the dynamics of the unbinding process.

AKB 40.62 Wed 16:30 P3

Close contact fluctuations: the seeding of signalling domains in the immunological synapse — ●AMIT CHATTOPADHYAY — Università degli Studi di Padova, Facoltà di Ingegneria, Dipartimento di Fisica G. Galilei, Via Marzolo 8, 35131 Padova, Italy

We study the effects of thermal membrane fluctuations on the size and density of regions of close contact in cell:cell contact interfaces. Such regions are vital for the generation of early signals in T-cell contact interfaces and for the stabilisation of the contact and development of an immunological synapse. Our calculations indicate that these regions are on the nanometer scale, while the corresponding density rapidly decays with membrane-membrane separation. Our method is a generalisation of probability of first crossing techniques to a system without reflection symmetry.

AKB 40.63 Wed 16:30 P3

Proton-driven rotation within the F₀-motor of ATP synthase — ●NAWID ZARRABI¹, MONIKA DÜSER¹, DAN J. CIPRIANO², S. DUNN², and MICHAEL BÖRSCH¹ — ¹3. Physikalisches Institut, Universität Stuttgart, Germany — ²Department of Biochemistry, University of Western Ontario, London, Canada

ATP formation by F₀F₁-ATP synthase requires conformational changes that are induced by the stepwise rotation of the γ and ϵ subunit. The opposite direction of rotation during ATP synthesis and hydrolysis was confirmed by single-molecule fluorescence resonance energy transfer (FRET) [1,2]. Rotation of γ and ϵ is coupled to the rotation of the c subunits of the ion-driven F₀ motor. ATP hydrolysis resulted in a three-stepped rotation of the c -ring of F₀ from a thermophilic bacterium. However, ATP synthesis by the sodium-translocating enzyme from *P. modestum* was associated with a multi-stepped rotation. To distinguish between the two mechanisms we have developed a single-molecule FRET assay to monitor the c -ring rotation in F₀. Our first data strongly support a stepwise movement of the c -ring during ATP synthesis and hydrolysis in contradiction to a quasi-continuous rotation. \Zitat{1}{Diez, M., B. Zimmermann, M. Börsch, M. König, E. Schweinberger, S. Steigmiller, R. Reuter, S. Felekyan, V. Kudryavtsev, C.A.M. Seidel, and P. Gräber: Nat. Struct. Mol. Biol.

11:135-142, 2004} \Zitat{2}{Zimmermann, B., M. Diez, N. Zarrabi, P. Gräber, and M. Börsch: EMBO J. 24:2053-2063, 2005} \Zitat{3}{Düser, M. G., Y. Bi, S. D. Dunn, and M. Börsch: Biochim. Biophys. Acta-Bioenergetics 1658:108 S Supplement, 2004}

AKB 40.64 Wed 16:30 P3

Surface-diffraction from proteins interacting with solid supported membranes — ●KIRSTIN SEIDEL¹, CHRISTIAN DANIEL², BERT NICKEL¹, and JOACHIM RÄDLER¹ — ¹Ludwig-Maximilians Universität, Department für Physik and Center for Nanosciences, München — ²Technische Universität München

We study the interaction of Annexin 2 with anionic lipid membranes using neutron and x-ray synchrotron scattering techniques. Annexin 2 interacts with negatively charged phospholipids in a calcium dependant manner. Furthermore annexin is able to bind two adjacent membranes. The solid supported membranes were achieved by spreading large unilamellar vesicles (100nm) of lipid mixtures of neutral (POPC) and negatively charged (POPS) phospholipids on silicon substrates. The protein was provided by B. Windschagl and C.Steinem, Universität Regensburg. The system was characterized by fluorescence microscopy the same samples were then measured with x-ray reflectivity at Hasylab (D4). With these methods we gained information about the homogeneity, fluidity and thickness of the underlying membrane. In future experiments we will use neutron reflectometry at FRM2 (REFSANS) to visualize the protein layer. Here we want to benefit from the possibility of contrast variation due to the scattering length density difference between deuterium oxide and water.

AKB 40.65 Wed 16:30 P3

Capacitive Stimulation of Neurons by Opening Na⁺ Channels with Silicon Chips — ●INGMAR SCHOEN and PETER FROMHERZ — Max Planck Institut für Biochemie, Abteilung Membran- und Neurophysik, 82152 Martinsried bei München

We demonstrate that opening Na⁺ channels by capacitive coupling with a silicon chip is a feasible, non-invasive method for neural stimulation in planar neuroelectronic devices.

Experiments were carried out with neurons from the pond snail *Lymnaea stagnalis* on silicon chips with HfO₂ as insulator. The cell was contacted with a patch pipette and ramps were applied to chip voltage. Capacitive coupling evoked an ionic current flow along the cleft in cell adhesion that led to an extracellular voltage drop therein. With a negative extracellular voltage, the adhesion membrane was depolarized. Voltage clamp experiments verified successful opening of ion channels and allowed for a detailed characterization of ionic currents and the optimization of Na⁺ influx. This charge inflow was capable of triggering action potentials in current clamp in a limited parameter range. In the case of positive extracellular voltage, the upper membrane was directly depolarized and sodium channel opening reliably led to action potentials.

This method provides a thorough understanding and control of stimulated neural excitation without malignant electroporation of the cell membrane or electrochemical reactions at the substrate surface.

[1] I. Schoen and P. Fromherz, *Appl. Phys. Lett.* **87**, 193901 (2005).

AKB 40.66 Wed 16:30 P3

Mesoscopic simulations of membrane protein diffusion and membrane-protein interactions — ●GERNOT GUIGAS and MATTHIAS WEISS — Cellular Biophysics Group (BIOMS), Deutsches Krebsforschungszentrum, Im Neuenheimer Feld 580, 69120 Heidelberg

We use dissipative particle dynamics (DPD) to study the diffusion of membrane proteins and how active proteins alter the membrane's (elastic) properties. We find that the size-dependent diffusion coefficient $D(R)$ of integral membrane proteins with radius R is best described by the Saffman-Delbrück relation. To our knowledge, this is the first computational confirmation of the logarithmic dependence of D on R . We further show that active proteins can considerably alter the membrane's (elastic) properties, e.g. phospholipase A₂ softens the membrane while cleaving phospholipids into lysolipids and fatty acids [1].

[1] Jakobsen, Mouritsen, Weiss, *J. Phys. Condens. Mat.* **17**, S4015 (2005).

AKB 40.67 Wed 16:30 P3

Imaging of Electrical Dynamics in Cultured Brain Slices by Multi-Transistor-Array (MTA) Recording — ●ARMIN LAMBACHER¹, MICHAEL HUTZLER¹, MARTIN JENKNER², BJÖRN EVERSOMANN², ROLAND THEWES², and PETER FROMHERZ¹ — ¹Max Planck Institute for Biochemistry, Department of Membrane and Neurophysics — ²Infineon Technologies, Corporate Research, München, Germany

Direct electrical interfacing of semiconductor chips with neuronal tissue may lead to novel experimental approaches in brain research and also give rise to hybrid computational devices. Here we report on a time-resolved imaging of the electrical activity in organotypic brain slices from rat hippocampus by multi-transistor-array (MTA) recording on an area of 1 mm² at a resolution of 7.8 μm and 0.5 ms. Brain slices were cultured on the inert titanium dioxide surface of silicon chips fabricated by an extended CMOS process. Upon stimulation in the CA3 region we observed fast propagating waves of negative field potentials which we assign to orthodromic and antidromic action potentials in the mossy fibers and slower transient field potentials of postsynaptic activity in CA3 and CA1 with negative sign in stratum radiatum and positive sign in stratum pyramidale. The transistor signals matched local micropipette recordings of electrical field potentials in amplitude and shape. Direct interfacing of an MTA chip provides a complete observation of neuronal signaling in an extended area of brain tissue. This technique is suitable to elucidate the functionality of planar neuronal systems at a high resolution.

AKB 40.68 Wed 16:30 P3

Adaptive Resolution Scheme for Efficient Multiscale Molecular Dynamics Simulations — ●MATEJ PRAPROTNÍK, LUIGI DELLE SITE, and KURT KREMER — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

A novel adaptive resolution method for efficient hybrid atomistic/mesoscale molecular dynamics (MD) simulations is presented. The unique feature of the method is that it allows for a dynamical change of the number of molecular degrees of freedom during the course of MD simulation by an on-the-fly switching between the atomistic and mesoscopic levels of detail. The new approach is general and can be applied to any molecular system of biological relevance, e.g., water, but at present tested on a model system of a liquid of tetrahedral molecules. The simulation box is divided into two regions: one containing only atomistically resolved tetrahedral molecules, the other containing only one particle coarse-grained spherical molecules. The molecules can freely move between the two regions while changing their level of resolution accordingly. The simulation results show that the hybrid and the corresponding all-atom systems have the same statistical properties.

AKB 40.69 Wed 16:30 P3

Diffusion along Microfluidic Channels — ●ANDREAS HEEREN¹, CHENG-PING LUO¹, GUENTER ROTH², ALEXANDER GANSER³, ROLAND BROCK³, KARL-HEINZ WIESMUELLER², WOLFGANG HENSCHERL¹, and DIETER KERN¹ — ¹Institute of Applied Physics, University of Tuebingen, 72076 Tuebingen, Germany — ²EMC microcollections GmbH, 72070 Tuebingen, Germany — ³Institute for Cell Biology, University of Tuebingen, 72076 Tuebingen, Germany

Living cells respond simultaneously to a variety of different stimuli. To achieve a specific cellular response a well defined mixture of stimuli or agents is required. However, in order to identify optimum mixtures of even few different compounds with respect to their relative and absolute concentrations, large numbers of biological tests are needed. Diffusion represents a highly efficient means for the generation of substance mixtures, namely continuously varying concentration profiles, with a minimum of pipetting steps. Here we present an array of microfluidic channels for the generation of binary substance mixtures with only two pipetting steps. For this purpose a microfluidic structure with a height of 500 μm was fabricated using the negative tone resist SU8. In a test diffusion of fluorescein dissolved in water was observed by fluorescence microscopy. The diffusion constant was determined by analyzing the fluorescence micrographs. Furthermore a procedure to detect unwanted flow in the channels was developed.