AKB 200 Poster Session II

Zeit: Dienstag 17:00–19:00 Raum: Poster TU C

AKB 200.1 Di 17:00 Poster TU C

Probing of the proteasom-protein interaction with force-spectroscopy — •Mirjam Beuttler, Jens Schiener, and Reinhard Guckenberger — Max-Planck-Institut für Biochemie, 82152 Martinsried

Atomic force microscopy (AFM) is an established method to investigate biological samples in their physiological environment. In our group we are investigating the 20S proteasome from Thermoplasma acidophilum. Besides imaging we will focus on force-measuring.

The proteasome is a barrel-shaped enzyme of 15 nm height and 11 nm width with a small opening at both ends. Through these two entrances unfolded proteins can access the inner part of the proteasome with the catalytic centers in order to be degraded there. Our goal is to characterize the translocation mechanism, as the forces involved are currently unknown. First step is to immobilize the proteasomes in an upright position which is achieved in our case directly on mica. Imaging the samples ensures the right orientation and the density of the surface covering. Second step will be the investigation of the forces involved in the translocation mechanism. Therefore suitable proteins which are known to be degraded by the proteasome will be bound to the AFM-tip. The forces exerted on the proteins by the proteasomes are transmitted to the tip. While retracting the lever with the tip from the surface the deflection of the lever changes due to the forces. Similarly, when the lever is kept stationary it will be bent towards the sample when the protein is sucked into the proteasome. Such force-distance-curves are offering a promising route to a better understanding of the translocation mechanism.

AKB 200.2 Di 17:00 Poster TU C

Geometry of interface mediated interactions — •Martin Michael Müller[1], Markus Deserno[1], and Jemal Guven[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — [2]Instituto de Ciencias Nucleares, UNAM, Apdo. Postal 70-543, 04510 México D.F., Mexico

Soft interfaces can mediate interactions between particles bound to them. One example is the interaction of protein inclusions in a lipid membrane. Traditionally, this phenomenon is treated by calculating the total energy of the particle-interface-system as a function of particle positions. The forces between the bound particles can then be obtained via appropriate derivatives. Unfortunately, the intrinsic nonlinearity of the problem generally forces one to restrict to linear approximations of the energetics.

It is, however, possible to choose a different, covariant approach and gain some nonlinear results: The forces between the particles are mediated through the interface and are thus encoded in its geometry. In analogy to classical elasticity theory one can write them as integrals over the surface stress tensor, which itself depends in a transparent way on the interfacial energy density. For standard symmetric two-particle situations this approach yields exact formulas for the force in terms of the mid-plane geometry, the sign of which is sometimes evident.

AKB 200.3 Di 17:00 Poster TU C

Small angle scattering study of intermolecular interactions in protein solutions — •Marc Niebuhr und Michel H.J. Koch — European Molecular Biology Laboratory, Hamburg Outstation, EMBL c/o DESY, Notkestrasse 85, D-22603 Hamburg, Germany

The results a study of intermolecular interactions in protein solutions measured with small angle X-ray scattering are presented. According to the DLVO theory the main interactions between spherical particles are the hard-sphere interactions, a short range attraction, due to surface-surface forces, and a long range repulsion caused by the fact that the particles are charged. The most interesting finding is that structure factors of salt concentration series and their change upon addition of urea and TMAO are better described if the strength of the attractive potential decreases with increasing salt concentration. Previous work in the literature had relied on a constant attractive potential within a given series of measurements.

AKB 200.4 Di 17:00 Poster TU C

Hydrogen bonding vs. stacking interactions in DNA base pairs - a Diffusion Monte Carlo study — •M. Fuchs[1], C. Filippi[2], J. Ireta[1], L. Ismer[1], and M. Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Instituut Lorentz, Univ. Leiden (NL)

Diffusion Monte Carlo (DMC) calculations can provide accurate total energies of molecular systems. DMC is thus useful for benchmarking (computationally cheaper) calculations based on density functional theory where one is relying on approximations for the exchange-correlation functional. On the other hand DMC remains computationally feasible even for larger systems where conventional correlated approaches such as Configuration Interaction or Coupled Cluster are at present too demanding. Here we explore DMC to study hydrogen bonded and stacked conformations of adenine-thymine and methylated adenine-thymine. Our results for the intermolecular interaction energies show that DMC predicts both hydrogen bond strengths and stacking interactions in agreement with results from the Coupled Cluster [CCSD(T)] approach, confirming these where they differ from MP2 data. We further show that gradient corrected density functionals (GGA-DFT) can yield reasonable bond strengths of the hydrogen bonded complexes but fail to bind the stacked conformations. Adding empirical corrections for the missing dispersion (van der Waals) attraction in GGA-DFT [1] we find that the stacked conformations do bind, yet markedly too strongly when compared to our DMC results. [1] Q. Wu and W. Yang, J. Chem. Phys. 116, 515 (2002).

AKB 200.5 Di 17:00 Poster TU C

Spectroscopic characterization of individual light-harvesting 2 complexes reconstituted into model membranes — •Martin Richter, Clemens Hofmann, Jürgen Baier, Silke Oellerich, and Jürgen Köhler — Experimental Physics IV, University of Bayreuth

Membrane-embedded pigment-protein complexes are the major players in photosynthesis. For a detailed study of these complexes, they are usually extracted from their native membrane, isolated and purified. The native membrane environment of these proteins is mimicked by detergent molecules in order to stabilize the complexes. However, this artificial protein environment can strongly affect the structural and spectroscopic properties of the pigment-protein complexes. Therefore, we reconstituted light-harvesting 2 (LH2) complexes, a photosynthetic pigment-protein complex from purple bacteria, into model membranes of phospholipids to study the influence of the protein environment on the structure and function of these complexes.

AKB 200.6 Di 17:00 Poster TU C

Biofilms of phototrophic systems in the evanescent field of light guides — •Davor Kosanic, Sven Schlicher, Sven Verpoort, Diana Fragel, and Hilmar Franke — Physics department, university of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

The interaction of biological systems with light has to be investigated for optical biosensors and for bioreactors. Especially when working with optical light guides the interaction takes place via the evanescent field. Therefore the particular field distributions have to be known.

The growth of algae on optical fiber tips or optical sensors has been investigated by video microscopy and by plasmon-leaky mode spectroscopy. For the latter method suspension of green algae in water has been regarded as an optical medium with high absorption coefficients. Model experiments have been performed using rhodamine/ethanol solutions.

The conventional plasmon-leaky mode set-up has been modified towards a compact method for monitoring solutions and suspensions with high absorption coefficients in the range of 50000 1/m , realistic values in algae suspensions.

AKB 200.7 Di 17:00 Poster TU C

Supramolecular Interaction at the Single Molecule Level — •Rainer Eckel[1], Robert Ros[1], Björn Decker[2], Jochen Mattay[2], and Dario Anselmetti[1] — [1]Experimentelle Biophysik und Angewandte Nanowissenschaften, Universität Bielefeld, Universitätsstrasse 25, 33615 Bielefeld — [2]Organische Chemie, Universität Bielefeld, Universitätsstrasse 25, 33615 Bielefeld

In supramolecular systems, the tailored non-covalent interaction between designed organic host and guest molecules opens fascinating con-

cepts for the development of new materials for artificial molecular recognition, self-assembly and biosensor applications. We applied mechanical single molecule force spectroscopy to investigate the specific binding of individual resorc[4]arene-ligand host-guest complexes. The molecular binding forces, their dependence to external loading rates, the rate of dissociation, and its corresponding cavity length directly relate to the molecular properties of the supramolecular species and are consistent with an activated decay of a metastable bound state(1). This allows new insights into the mechanisms, kinetics and thermodynamics of intermolecular association in chemical and biological receptor systems.

(1) R. Eckel, R. Ros, B. Decker, J. Mattay, and D. Anselmetti, Angew. Chem. (in press).

AKB 200.8 Di 17:00 Poster TU C

Excitation beyond the monochromatic laser limit: Simultaneous 3-D confocal and multiphoton microscopy with a single white-light laser source. — •Daniel Koch[1], Timo Betz[1], Jörn Teipel[2], Wolfgang Härtig[3], Jochen Guck[1], Josef Käs[1], and Harald Giessen[2] — [1]Universität Leipzig, Fakultät f Physik und Geowiss., Linnéstr 5, 04103 Leipzig — [2]Universität Bonn, Institut f Angewandte Physik, Wegelerstr 8, 53115 Bonn — [3]Universität Leipzig, Paul Flechsig Institut f Hirnforschung, Jahnallee 59, 04109 Leipzig

Confocal and multiphoton microscopy are essential tools in modern life sciences. They allow fast and highly resolved imaging of a steadily growing number of fluorescence markers ranging from labeled antibodies and fluorescence proteins to quantum dots, used for the localization and quantitative detection of molecules within living cells and organisms. Up to now, only one physical limitation seemed to be unavoidable. Both confocal and multiphoton microscopy rely on lasers as excitation sources, and their monochromatic radiation allows only a limited number of simultaneously usable dyes. We have overcome this limitation by successfully replacing all excitation lasers in a standard confocal microscope with the pulsed 430 to 1300 nm white-light which is generated in a tapered silica fiber. With this easily reproducible method, simultaneous confocal and multiphoton microscopy was demonstrated. By developing a coherent and intense laser source with spectral properties comparable to a mercury lamp, we provide the flexibilty to excite any desired fluorophore combination.

AKB 200.9 Di 17:00 Poster TU C

Force Spectroscopy with a Novel Small Focus AFM — •Volker Walhorn[1], Joerg Martini[1], Rainer Eckel[1], Jeroen Steen[2], Tobias Kramer[2], Bjoern Decker[3], Robert Ros[1], Dario Anselmetti[1], Juergen Brugger[2], and Juergen Mattay[3] — [1]Department of Biophysics and Applied Nanosciences, University of Bielefeld, Germany — [2]Inst. de Microsystèmes, EPFL, Lausanne, Switzerland — [3]Department of Organic Chemistry, University of Bielefeld, Germany

Atomic force microscopy has become potent tool for investigating inter- and intramolecular interactions. Single molecule force spectroscopy on supramolecular guest-host-complexes reveal information about the depth of the binding pocket and thermal off-rates.

Sensitivity and resolution are immanently conntected to the cantilever's mechanical properties. The cantilever's thermal noise induced by Brownian Motion of the surrounding medium is a fundamental limit of resolution. As the Nyquist Theorem is valid for the thermal white noise of a cantilever, reduction of the viscous damping by downsizing the cantilever's dimensions is compulsory. Furthermore, the resonant frequency is increased which extends experimental bandwidth and thus enables high speed measurements. Unfortunately small cantilevers cannot be used with commercially available AFM, since the laserfocus is too large.

We present results of single molecule force spectroscopy measurements on Calixarene-Ammonium-Complexes acquired with our homebuilt small focus AFM. As predicted, small cantilevers show favourable properties as increased resonant frequency and lower viscous damping.

AKB 200.10 Di 17:00 Poster TU C

Peptide antibiotics: insights in membrane selectivity and interaction — •Regine Willumeit[1], Mont Kumpugdee[1], Sebastian Linser[1], Sergio Funari[2], Jörg Andrä[3], Thomas Hauss[4], and Raz Jelinek[5] — [1]GKSS-Forschungszentrum, Max-Planck-Str. 1, 21502 Geesthacht — [2]c/o HASYLAB, Notkestrasse 85, 22603 Hamburg — [3]Research Center Borstel, Parkallee 10, 23845 Borstel — [4]Hahn-Meitner-Institute, Glienicker Str. 100, 14109 Berlin — [5]Ben Gurion University, Beersheva 84105, Israel

The past decade has brought a worldwide resurgence of infectious diseases due to the evolution of antibiotic-resistant strains. As a potential class of novel antimicrobial agents antimicrobial peptides have recently emerged. These peptides are small molecules that are fast and lethal towards a broad spectrum of pathogens but quite inactive on eukaryotic cells. However, the interaction of antibacterial peptides with their target membrane is not well understood. One promising antibacterial peptide is NK-2. It corresponds to residues 39-65 of NK-lysin, exhibits low haemolytic activity and is devoid of cytotoxic activity against human cell lines. In this paper several approaches to investigate the interaction of antibacterial peptides with membranes are presented. These include especially scattering techniques (X-ray and neutron scattering) and colorimetric biosensors.

AKB 200.11 Di 17:00 Poster TU C

Vibrational imaging of cholesterol enriched micro-domains in the Stratum corneum model system by CARS microscopy — •A. Kovalev[1], N. Patincharath[1], M. Köhler [2], and A. Volkmer[1] — [1]3rd Institute of Physics, University of Stuttgart, 70550 Stuttgart — [2]Roswell Park Cancer Institute, Buffalo, NY 14263, USA

For cellular components that either do not fluoresce or cannot tolerate the toxicity associated with staining and the photo bleaching of fluorophores, their intrinsic chemical properties can be used as contrast mechanisms through coherent anti-Stokes Raman scattering (CARS) microscopy. The CARS signal is resonantly enhanced when the difference in photon energies of the pump and the Stokes pulses coincides with the frequency of a Raman resonance. CARS microscopy has been demonstrated to exhibit high sensitivity, spatial and temporal resolution, noninvasiveness, and three-dimensional sectioning capability with sub-micron resolution. In this work, the application of CARS microspectroscopy to the study of a model system of Stratum corneum, the topmost barrier on the epidermis that prevents the penetration of external reagents through the skin is reported. Electroporation combined with application of vesicles formed by positively charged lipids makes the stratum corneum transparent for chemicals. This effect, which is important in transdermal drug delivery research, is not yet well understood. Investigations are carried out on model lipid mixtures consisting of ceramides, stearic acid and cholesterol, the three main lipid species of stratum corneum. A multiplex CARS scheme was employed for imaging and fast acquisition of CARS spectra revealing cholesterol-rich regions.

AKB 200.12 Di 17:00 Poster TU C

Imaging the interactions of functionalized, structured surfaces — •Peter Seitz, Ernst Stelzer, and Alexander Rohrbach — European Molecular Biology Laboratory (EMBL), Meyerhofstr. 1, 69117 Heidelberg

Functionalized surfaces can affect (bio-) chemical reactions and control spatially the affinity for various binding partners (receptor-ligand, antibody-antigene, etc.). These usually short-range interactions are initiated by long range electrostatic, electrodynamic and entropic interactions. We investigate the influence of long-range interactions on structured surfaces with Photonic Force Microscopy, where an optically trapped bead (probe) is scanned across the surface. The change of the bead's fluctuations encodes the interaction with the surface. The fluctuation traces are recorded interferometrically in three dimensions with nm-resolution and at scan-rates of several hundred kilohertz with a quadrant photodiode. Interactions can be imaged in the sub-piconewton range. The optical phase changes induced by the surface structure (e.g. an adhering cell) on the probing laser beam can be extracted from the signal of the trapped probe. In this way the extracellular matrix of biological cells not in contact with the coverslip can also be investigated.

AKB 200.13 Di 17:00 Poster TU C

NAD(P)H autofluorescence - an approach to cellular metabolism — •Bülent Peker, Raluca Niesner, and Karl-Heinz Gericke — IPC @ TU-Braunschweig, Hans-Sommer-Str. 10, D-38106 Braunschweig

The 2-Photon-excitation based Fluorescence Lifetime Imaging (FLIM) proved to be an excellent method for subcellular research in biological samples in the last few years. It is now a seminal method for "ex vivo" and "in vivo" non invasive visualisation research in extensive united cell structure and tissue with high resolution. The options given by these method like monitoring a reply to a stimulus were unfortunately deadlocked by too long data interpretation. Our technique of FLIM-Analysis allows an on-line monitoring by implementing a non-iterativ method. In addition

to multiexponential NAD(P)H- Analysis successful applications in pH-, η- and τ-imaging in artificial skin constructs show the capability of our method.

AKB 200.14 Di 17:00 Poster TU C

Subcellular parameter probing using TPM based FLIM — •Stefan Quentmeier, Raluca Niesner, Bülent Peker, and Karl-Heinz Gericke — IPC @ TU-Braunschweig, Hans-Sommer-Str. 10, 38106 Braunschweig

Two-photon scanning microscopy (TPM) combined with fluorescence lifetime imaging (FLIM) provides an excellent method for probing cellular parameters on subcellular level. Depending on the dye used different parameters like pH, ionic strength, CO_2 and O_2 concentration and viscosity can be monitored in high resolution. FLIM gives us a non-invasive technique at hand possessing high intrinsic 3D resolution, large penetration depth, low photodamage and simple experimental setup as sample preparation is limited to simple staining. As fluorescence lifetime is not affected by experimental parameters the instrumental stability of standard intensity based TPM experiments is easily outperformed by FLIM. We performed FLIM for pH, n and viscosity mapping in artificial skin constructions (ASC) and genuine human skin.

AKB 200.15 Di 17:00 Poster TU C

Single cell manipulation in microfluidic networks by optical tweezers — •Kai Leffhalm, Andy Sischka, Wibke Hellmich, Thanh Tu Duong, Katja Tönsing, Robert Ros, Alexandra Ros, and Dario Anselmetti — Experimental Biophysics, Physics Department, Bielefeld University, Germany

Control and manipulation of single cells gain importance as a tool to better understand the migration behaviour of living cells in vivo and for single cell analysis. Microfluidic networks provide dimensions small enough to navigate and steer single cells with optical tweezers to different areas of an artificial network where the flow properties can be controlled by electrophoresis and electroosmosis.

Potential applications include microproteomics and monitoring of the expression level of individual cells, which can be stimulated or suppressed by changing the velocity of the flow or the concentration of substances, e.g. cytokines or (cytostatic) drugs, in the culture medium.

We will present our experimental setup and our first test experiments where a cell is captured between two electrodes where it can be destroyed by an electric field, i.e. an electric pulse. This is an initial point for future single cell analysis.

AKB 200.16 Di 17:00 Poster TU C

Model of intracellular Ca^{2+} oscillations due to negative feedback — •Peter Borowski[1], Jürgen Reidl[2], Anke Sensse[3], Martin Zapotocky[1], Jens Starke[2], and Markus Eiswirth[3] — [1]Max Planck Institute for Physics of Complex Systems, Dresden — [2]Institute of Applied Mathematics, University of Heidelberg & WIN-Research Group of Olfactory Dynamics, Heidelberg Academy of Science and Humanities — [3]Fritz-Haber-Institute of the Max Planck Society, Berlin

We present a mathematical model for calcium oscillations and fast adaptation in the cilia of olfactory sensory neurons. Stoichiometric network analysis is used for analysing the kinetic equations and finding the oscillatory regime. The underlying mechanism is based on direct negative feedback and does not require any autocatalysis such as calcium-induced calcium release. Results of the model using physiological parameter values agree quantitatively with experiment, both with respect to oscillations and to fast adaptation. The bifurcation diagram of the model is calculated to make predictions regarding the occurence of oscillations.

AKB 200.17 Di 17:00 Poster TU C

Study of Energy-Transfer Processes in Metallo-Porphyrin Artificial Light-Harvesting Molecules — •Joachim Zeller[1,2], Robert Hauschild[1], Gernot Riedel[1], Teodor S. Balaban[2,3], Heinz Kalt[1,2], N. Berova[4], and K. Nakanishi[4] — [1]Institut fuer Angewandte Physik, Universitaet Karlsruhe (TH), 76131 Karlsruhe — [2]Centrum fuer Funktionelle Nanostrukturen, Universitaet Karlsruhe (TH), 76131 Karlsruhe — [3]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe — [4]Columbia University, New York, USA

Artificial light harvesting molecules mimic photosynthesis in which light is transformed into chemical energy. They consist of an antenna, which absorbs light and acts as an energy donor, and an energy trap, to which the excitation is transferred. We investigated energy transfer in 3 conformationally different metallo-porphyrins using time-resolved fluorescence spectroscopy. They consist of a Zn-TPP moiety (antenna/energy donor) and a free-base-TPP moiety (energy trap) which are linked with a covalent steroidal bridge. An analysis of the time-resolved fluorescence spectra using the method of decay-associated spectra (DAS) reveals energy transfer between the Zn-TPP energy donor and the free-base-TPP energy trap with transfer times 0.91 ns, 0.99 ns and 1.1 ns for the 3 different molecule conformations. A comparison of the measured transfer times to the values expected from Foerster theory shows only limited agreement. These results will be compared to the energy transfer dynamics in H-bonded supramolecular porphyrin complexes.

AKB 200.18 Di 17:00 Poster TU C

Density Functional Theory Study on the Stability of left-handed alpha-Helix Polyalanine — •Franziska Grzegorzewski, Lars Ismer, Joel Ireta, and Matthias Scheffler — Fritz Haber-Institut der Max Planck-Gesellschaft, Faradayweg 4-6, 14193 Berlin

The left-handed α-helix, α_L, is an unusual conformation in proteins and, if observed, mainly built with glycine, a non-chiral amino acid. The discrimination of α_L-helix has been attributed to unfavorable repulsive interactions between the side chain and the backbone atoms (steric effect). In order to provide a deeper insight on the factors influencing the relative stability of α_L-helix we performed systematic ab-initio calculations for polyalanine in different left-handed helical conformations using density functional theory (DFT) in the PBE approximation to the exchange-correlation functional. The potential energy surface of the left-handed polyalanine was explored for numerous configurations using different helix twists and varying the increment along the helix axis per residue. We find three minima corresponding to π_L-, α_L-, and 3_{10L}-helix. Based on an harmonic vibrational analysis, we find that only considering the loss of vibrational entropy in addition to the steric effect, DFT-PBE predicts that a fully extended structure will not fold spontaneously into α_L-helix in vacuum at room temperature

AKB 200.19 Di 17:00 Poster TU C

Anomalous Dynamics of Action Potential Initiation in Cortical Neurons — •Björn Naundorf[1], Maxim Volgushev[2], Theo Geisel[1] und Fred Wolf[1] — [1]Max-Planck Institut für Strömungsforschung and Fakultät für Physik, Universität Göttingen, 37073 Göttingen — [2]Abteilung Neurophysiologie, Ruhr-Universität Bochum

Action potential (AP) initiation in neurons is fundamental to information processing in the brain. In most neurons, AP initiation is mediated by the activation of fast, voltage-dependent sodium channels, canonically described by Hodgkin-Huxley (HH) type equations. Here we describe features of the dynamics of AP initiation which differ qualitatively from the predictions of the HH theory. We show that APs from neocortical neurons recorded *in vivo* and *in vitro* initiate much more rapidly than predicted by the steady state sodium activation curve, while at the same time APs are emitted in a very large voltage range. We then show that the two effects are mutually exclusive in HH type models and can not be resolved within the framework of the HH theory.
Using a phenomenological model, we further demonstrate that the observed AP onset dynamics has important consequences for the information processing capabilities of neocortical neurons. Rather than, as commonly believed, acting as a low pass filter, the model suggests that cortical neurons are specifically tailored to support highly transient signals, while suppressing slowly varying inputs.

AKB 200.20 Di 17:00 Poster TU C

Calculation of solvent entropies from MD simulations — •Friedemann Reinhard and Helmut Grubmüller — MPI für biophysikalische Chemie, Abteilung 070 – Theoretische und computergestützte Biophysik, Am Fassberg 11, 37077 Göttingen

Solvent entropy is the main contribution to the hydrophobic effect. Its computation from molecular dynamics simulations however proves difficult. First, due to the diffusive motion of the solvent molecules, the configuration space is much too large to be sampled sufficiently. Second, the typically very shallow energy landscapes generate phase space densities with quite complex topology.

We address both problems by exploiting the permutation symmetry of the solvent molecules. For every ensemble element generated by the simulation, the water molecules are relabeled such that the permutated configurations fall into a compact volume in phase space. Thereby we greatly enhance sampling without affecting any thermodynamic quantities. Thus the established entropy estimation methods for proteins should

become applicable to the relabeled solvent molecules too.

This expectation is confirmed by test calculations on simple model systems. Furthermore, the compactified phase space densities show comparatively simple topology, such that also the second problem is alleviated significantly. What remains to be done is to develop more elaborated density estimates, which is the subject of our current work.

AKB 200.21 Di 17:00 Poster TU C

Effect of receptor-ligand distance on adhesion cluster stability — •Thorsten Erdmann and Ulrich S. Schwarz — Max Planck Institute of Colloids and Interfaces, Theory Division, 14424 Potsdam

Cells in multicellular organisms adhere to the extracellular matrix through two-dimensional clusters of adhesion bonds. Single adhesion bonds have finite lifetimes and open and close stochastically. For many common receptor-ligand systems, the ligands are tethered to the substrate via polymeric spacers so that adhesion cluster stability crucially depends on receptor-ligand distance. Experimentally, the distance-dependent interplay of rupture and rebinding in adhesion clusters can be studied *in vitro*, e. g. by atomic force microscopy, the biomembrane force probe, or the surface force apparatus. In order to study this effect theoretically, we introduce a one-step master equation for the stochastic dynamics of parallel bonds. Binding requires stretching of the polymeric tether, which leads to a distance-dependent binding rate. Closed bonds correspond to stretched tethers and exert force on the receptors, which is counteracted by the elastic stiffness of the force transducer. This force accelerates unbinding, but it is also shared equally by all closed bonds. The formation of new bonds reduces receptor-ligand distance and increases the probability for further binding. These effects make receptor-ligand binding in adhesion clusters a cooperative and self-reinforcing process. A bifurcation analysis of a deterministic differential equation for the average number of closed bonds reveals the existence of a bistable region in which a bound and an unbound state coexist. In the stochastic treatment, the system continuously jumps between these two macrostates.

AKB 200.22 Di 17:00 Poster TU C

Tension-induced titin kinase activation studied by force-probe molecular dynamics simulations — •Frauke Gräter[1], Jianhua Shen[2], Hualiang Jiang[2], and Helmut Grubmüller[1] — [1]MPI fuer Biophysikalische Chemie, Am Fassberg 11, 37077 Goettingen — [2]Shanghai Insitute of Materia Medica, Zuchongzhi Lu 555, Zhangjiang Hi-Tech Park, 201203 Shanghai, China

The conversion of mechanical stress into a biochemical signal in a muscle cell requires a force sensor. Titin kinase, the catalytic domain of the muscle protein titin, has been suggested as a candidate. Its activation requires major conformational changes resulting in the exposure of its active site.

Force probe molecular dynamics simulations were used to obtain insight into the tension-induced activation mechanism. Our results suggest the rupture of two terminal beta-sheets as the primary unfolding steps. The low force resistance of the C-terminal relative to the N-terminal beta-sheet is found to be due to their different topology. A subsequent movement of the auto-inhibitory tail is seen to lead to the exposure of the active site, as is required for titin kinase activity. Thus, our reults support the hypothesis of titin kinase as a force sensor.

AKB 200.23 Di 17:00 Poster TU C

Use of carboxylic acids for the monitoring of anaerobic fermentation processes — •Dieter F. Ihrig[1], H. Michael Heise[2], Ulrich Brunert[1,2], Alexander Moor[2], Ruediger Kuckuk[2], and Martin Poschmann[1] — [1]University of Applied Sciences Suedwestfalen, Iserlohn, Germany — [2]ISAS - Institute for Analytical Sciences, Dortmund, Germany

We are studying anaerobic fermentation processes that involve a thermophilic first bioreactor stage and a mesophilic second stage. The developed anaerobic process is very efficient, but also rather unstable. For achieving a better process management, it is necessary to understand the interdependencies between process engineering parameters (for example, the hydraulic turn-over time or the organic biomass burden as characterized by the Chemical Oxygen Demand (COD) parameter) and biochemical variables such as the concentration of carboxylic acids. Results from the determination of carboxylic acids using steam extraction and Reversed-Phase-HPLC are discussed. Furthermore, activities were started using infrared spectroscopy for quasi-continuous process monitoring. Goal of the project is the development of an on-line sensor system based on infrared attenuated total reflection (ATR) measurements. For gathering practical experience, we constructed a micro-flow system for on-site spectroscopic measurements. The analytical results were compared to concentration values obtained by HPLC and to pH-readings of the bioreactor broth media. The project was funded by the German Federal Ministry for Education and Research (BMBF).

AKB 200.24 Di 17:00 Poster TU C

Molecular recognition of chemically structured substrates in a lattice model — •Thorsten Bogner, Andreas Degenhard, and Friederike Schmid — Condensed Matter Theory, Fakultät für Physik, University of Bielefeld, Universitätsstraße 25, E5 [5th floor]

We investigate the adsorption of polypeptides on a planar substrate by means of a coarse grained model on a lattice. The chemical composition of both, the peptide and the substrate, is modeled explicitly.

In particular we are interested in the emergence of specificity within the adsorption process. Despite its simplicity, we expect our model to exhibit the basic properties that lead to molecular recognition in 'real world' experiments. By analyzing the results of the simulations using methods from statistical data analysis, we find the small-scale structures of the peptide sequence to be a particular important factor regarding specificity. This is in qualitative agreement with existing binding experiments.

AKB 200.25 Di 17:00 Poster TU C

Membrane dynamics and membrane binding events investigated by photonic force microscopy — •Holger Kress, Ernst H. K. Stelzer, Gareth Griffiths, and Alexander Rohrbach — European Molecular Biology Laboratory (EMBL), Meyerhofstrasse 1, D-69117 Heidelberg, Germany

Optical tweezer based photonic force microscopy is used to study the binding of particles to the plasma membrane of macrophage cells. Macrophages are specialized cells that ingest particles such as bacteria or synthetic objects (e.g. latex beads) and enclose them into intracellular organelles. Optically trapped latex beads are moved to the plasma membrane of cells. The fluctuations of the trapped particle during the binding to the cell membrane and the following mechanical response of the membrane are tracked interferometrically. The tracked position fluctuations are measured in three dimensions with a precision of a few nanometers and a temporal resolution of 100 μs. The tracked position fluctuations encode information about the dynamics of the binding process itself and the following mechanical response of the cell to this stimulus.

AKB 200.26 Di 17:00 Poster TU C

Neuronal signal transmission in reconstructed neuronal networks on microfluidic Si-based devices: Towards an artificial chemical synapse chip — •Yulia Mourzina[1], Petra Schulte[1], Dmitri Kaliaguine[2], Simone Böcker-Meffert[1], and Andreas Offenhäusser[1] — [1]Institute of Thin Films and Interfaces, Research Center Jülich, Germany — [2]Faculty of Chemistry, St. Petersburg State University, Russia

Chemical synaptic transmission, the elementary interaction event between neuronal cells, is fundamental to understanding learning and memory. In order to perform long term studies about neuronal interactions in reconstructed neuronal networks, we intend to form an 'artificial chemical synapse' with spatially and temporally resolved non-invasive chemical stimulation and detection methods.

We reconstruct the defined synaptical connections of cortical neuronal cells on microfluidic Si-based chips and align the reconstructed neuronal networks with microapertures connecting the microfluidic compartments. Natural conditions of chemical synapses are simulated by means of providing localized chemical stimuli to the cells with neurotransmitters via microfluidics. Cell response is characterized by means of electrophysiological recordings. Further on, we intend to develop a non-invasive recording of the synaptic events in neuronal networks by means of electrochemical methods.

AKB 200.27 Di 17:00 Poster TU C

In situ Synthesis of DNA Chips — •Thomas Naiser, Timo Mai, Wolfgang Michel, and Albrecht Ott — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth

DNA-Chips are biosensors for measuring gene activity on a genome wide scale. They have become an important tool in Biological Sciences. The underlying principle is the duplex formation of nucleic acids (hybridization), which is highly sequence-specific and can therefore be used to determine the composition of nucleic acid mixtures extracted from bi-

ological specimens. We have built a photolithographic micro-projection setup to manufacture high density DNA-Chips in a photochemically controlled synthesis process. Virtual lithography masks, generated with a Digital Micromirror Device (a spatial light modulator commonly used in video projectors), allow local control of the synthesis, so that we can produce an array of closely spaced spots (10-15 micron in size), each one containing a different sequence of single stranded DNA. The whole chip comprises up to 10^5 freely programmable sequences (15-25mers) on an area of $10mm^2$. We present results from hybridization assays performed to investigate the physics underlying DNA-Chip technology.

AKB 200.28 Di 17:00 Poster TU C

Local Distribution of Silica in Equisetum hyemale — •Lanny Sapei[1], Sandra Lehmann[2], Robert Nöske[3], Peter Strauch[3], and Oskar Paris[1] — [1]Max Planck Institute of Colloids and Interfaces, Biomaterial Department, Research Campus Golm, 14424 Potsdam — [2]UP TRANSFER GmbH, Gesellschaft für Wissens- und Technologietransfer an der Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam — [3]Potsdam University, Chemistry Department, K-Liebknecht-Str. 24-25, 14476 Potsdam

Horsetail (Equisetum) is known as one of the strongest accumulators of silicon among higher terrestrial plants (up to 25% dry weight), mostly in the form of amorphous silica. This makes this plant an interesting candidate as a renewable resource of silica for the synthesis of biomorphous ceramics. We have examined the 3D Si-distribution in Equisetum hyemale using X-ray microtomography, supported by quantitative analysis with EDX mapping and Raman microscopy. The silica distribution within the plant tissue is quite heterogeneous, showing strong Si-accumulations in particular knobs at the epidermis. Scanning small-angle X-ray scattering (SAXS) with 0.1 mm spatial resolution reveals a strong scattering signal in these regions, quite different from the well known SAXS signal from cellulose in plant cell walls. This suggests that the silica is present in the form of nanoparticles.

AKB 200.29 Di 17:00 Poster TU C

Potential-Energy Surface of Infinite Helical Polypeptides — •Joel Ireta and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft

The potential-energy surfaces of infinite polyalanine and polyglycine chains in helical conformation are studied using density-functional theory in the Perdew, Burke and Ernzerhof approximation to the exchange-correlation functional (DFT-PBE). Minima associated to a π-helix, α-helix and 3_{10}-helix conformations are identified for both polypeptides. For polyalanine the α-helix minimum is the lowest in energy. However for polyglycine π-helix and α-helix minima are degenerated within the DFT accuracy. The α-helix is found to undergo structural transitions to a π- or 3_{10}-helix when the length of the helix is strainend by more than 10%. The barriers for the structural transitions mainly associated to the breaking of the hydrogen bonds are considerably affected by the side group in polyalanine. We find this effect can not be solely attributed to repulsive interactions between the side group and the helix backbone but to sizeable changes in covalent bonds in the peptide unit of polyalanine with respect to polyglycine.

AKB 200.30 Di 17:00 Poster TU C

Synthesis and Characterization of De Novo Designed Peptides Modeling the Binding Sites of [4Fe-4S] Clusters in Photosystem I — •Mikhail Antonkine[1,2], Christoph Breitenstein[2], Boris Epel[2], Eckhard Bill[2], Wolfgang Gärtner[2], John Golbeck[3], and Wolfgang Lubitz[2] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany. Tel.: 49 30 838 53047, Fax: 49 30 838 56081. — [2]Max-Planck-Institut für Bioanorganische Chemie, Stiftstrasse 34-36, Mülheim an der Ruhr, D-45470, Germany. — [3]Department of Biochemistry and Molecular Biology, The Pennsylvania State University, University Park, PA 16802,USA.

Photosystem I (PS I) is a membrane-bound pigment-protein complex found in photosynthetic organisms. It converts the energy of light into chemical energy. The terminal electron transfer cofactors in PS I are three [4Fe-4S] clusters named Fx, Fa, Fb. The PsaC subunit of PS I harbors binding sites of Fa and Fb clusters. We modeled the binding sites of the [4Fe-4S] clusters Fa and Fb of PsaC by preparing sixteen amino acid peptides. Model peptides incorporate the consensus iron-sulfur binding motif and amino acids from the environment of the respective iron-sulfur cluster. The [4Fe-4S] clusters were successfully incorporated into these model peptides, as shown by their optical absorbance, EPR and Mössbauer spectra. We compare continuous wave and pulsed EPR, Electron Spin Echo Envelope Modulation (ESEEM) and Mössbauer spectra of the model [4Fe-4S] clusters with the respective spectra of Fa and Fb in unbound PsaC and in the fully assembled PS I.

AKB 200.31 Di 17:00 Poster TU C

Electron Transfer Rates at Low Temperatures Using Wilsons Renormalization Group — •Sabine Tornow, Ning-Hua Tong, and Ralf Bulla — Theoretische Physik III, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Electron transfer in biomolecules is the key process in photosynthesis, oxidative phosphorilation or DNA damage repair. In the biomolecule complexes electrons are tunneling between donor and acceptor sites which leads to their particular function. The latter is affected by the structure of the protein through the coupling between protein motion and electron transfer. To calculate the transfer rate taking into account this coupling the spin boson model provides a well established description. While limiting cases are well understood in certain parameter regimes non-perturbative methods are needed, e.g., in the crossover from the nonadiabatic to the adiabatic regime. We present a theoretical non-perturbative study of the electron transfer using Wilsons Numerical Renormalization Group method and calculate the thermal rate constant at low temperatures.

AKB 200.32 Di 17:00 Poster TU C

Towards a Combined Approach of Single Molecule Tracking and Fluorescence Correlation Spectroscopy — •Stephan Schäfer — Biotechnological Centre, TU Dresden

Wide-Field Microscopy based on CCD detection and tracking of single fluorescently labelled molecules (SMT) in lipid bilayer membranes has proved to be a promising tool for a deeper understanding of biologically active lipid- and protein molecules. However, tracking of single molecules with a high mobility remains difficult due to limitations in the camera read-out rate and signal collection time. Using giant unilamellar vesicles (GUVs) which have been proven to be a suitable and reliable model for biological lipid membranes restricting diffusive motion to their 2D membrane surface. Besides SMT we employes Fluorescence correlation spectroscopy (FCS) as a time-averaging fluctuation analysis of small molecular ensembles. Comprising maximum sensitivity and high statistical confidence, FCS is especially well suited for investigations within cellular membranes. We present first results of a comparative study on SMT and FCS performed on the lipid bilayer membrane of GUVs. There is strong indication of a purely Brownian diffusion for the investigated composition (50

AKB 200.33 Di 17:00 Poster TU C

Organophosphonate monolayers as functionalisation for silicon based biosensing devices — •Karin Buchholz[1], Michael D. Carolus[2], Jeffrey Schwartz[2], Marc Tornow[1] und Gerhard Abstreiter[1] — [1]Walter Schottky Institut, TU München, 85748 Garching, Germany — [2]Department of Chemistry, Princeton University, Princeton, New Jersey 08544-1009

Planar semiconductor sensing devices based on silicon-on-insulator (SOI) substrates have immense potential for applications such as label-free, fast, and time resolved detection of biomolecule binding events due to their great sensitivity to surface potential changes via the field effect [1].

Phosphonate films are easy to apply and provide for stable silicon surface derivatization because they give dense, self-assembled monolayers that bond strongly to the native silicon oxide and that can be modified with tailored, substituted end groups [2].

We investigated the stability and current blocking properties of different alkylphosphonate layers over time by cyclic voltammetry and impedance spectroscopy. A maximum current blocking of 97 per cent at the reductive peak voltage of a reference sample was observed for samples coated with layers of hydroxyundecylphosphonic acids.

Concepts for biofunctionalisation of SOI sensors via Phosphonate acid monolayers will be discussed.

[1] M. G. Nikolaides et al., ChemPhysChem, vol. 4, 1104-1106 (2003)
[2] K. S. Midwood et al., Langmuir, vol. 20, 5501-5505 (2004)

AKB 200.34 Di 17:00 Poster TU C

Diamond-based biosensors — •Andreas Härtl[1], Jorge Hernando[1], Philipp Achatz[1], Tahmineh Pourrostami[1], Stefan Walter[2], Jose Garrido[1] und Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, Germany — [2]Institut für Organische Chemie und Biochemie, Technische Universität München, Germany

Diamond is known to be a per se biocompatible material, consisting just of carbon atoms. Other interesting properties are a large electrochemical potential window, low thermal background currents, fouling resistance, and chemical inertness. Together with the existance of a quasi-two-dimensional conductive layer at the surface of hydrogen terminated diamond, this suggests the use of diamond as an active substrate which can interact with biomolecules immobilized on it.

In this contribution we report on the functionalization of diamond surfaces with various biomolecules and on diamond based ion sensitive field effect transistors (ISFET). We have studied the immobilization of different proteins on the surface of single crystal and nanocrystalline diamond substrates, showing that covalent bonding can be achieved. Moreover, we have confirmed that the immobilized proteins retain their biological activity. First amperometric sensor applications have been realized and will be presented.

We also have fabricated ISFETs on single crystalline and polycrystalline H-terminated diamond substrates and have investigated their pH sensitivity.

AKB 200.35 Di 17:00 Poster TU C

Optical conductivity of wet DNA — •Arnd Hübsch[1], Robert G. Endres[2], Daniel L. Cox[1], and Rajiv R. P. Singh[1] — [1]Department of Physics, University of California, Davis, CA 95616 — [2]NEC Laboratories, Princeton, NJ 08540

DNA has attracted much attention in view of its possible application to nano-devices. Despite extensive efforts, however, the experimental results of the conductivity of DNA are still rather controversial. Motivated by recent optical experiments [1] we have studied the optical conductivity of DNA in its natural environment containing water molecules and counter ions. Our DFT calculations using the SIESTA code suggest a thermal activated doping of the DNA which leads to an electronic low-frequency absorption. The main contributions to the doping result from the DNA ends, breaks, or nicks.

[1] E. Helgren, A. Omerzu, G. Gruner, D. Mihailovic, R. Podgornik, and H. Grimm, cond-mat/0111299.

AKB 200.36 Di 17:00 Poster TU C

Covalent immobilisation of recombinant fusion proteins with hAGT for single molecule force spectroscopy — •Stefan Kufer and Hermann E. Gaub — Amalienstr.54(I); 80799 München

A genetically modified form of the human DNA repair protein O6-alkylguanine-DNA-alkyltransferase (hAGT) was used to immobilize different recombinant hAGT fusion proteins covalent and selective on gold and glass surfaces. Fusion proteins of hAGT with Glutathione S-Transferase (GST) and with tandem repeats of Titin Ig domains, were produced and anchored via amino-polyethylene glycol (PEG)-benzylguanine (BG). Anchoring was characterized and quantified with surface plasmon resonance (SPR), atomic force microscope (AFM) and fluorescence measurements. Individual fusion proteins were unfolded by single molecule force spectroscopy corroborating the selectivity of the covalent attachment.

AKB 200.37 Di 17:00 Poster TU C

Simulation of Fluorescence Anisotropy Experiments: Probing Protein Flexibility — •Gunnar Schröder[1], Ulrike Alexiev[2], and Helmut Grubmüller[1] — [1]MPI biophysik. Chemie, Göttingen — [2]Freie Universität, Berlin

Fluorescence anisotropy experiments in combination with site-directed fluorescent labeling offer the chance to locally probe protein conformation and dynamics. To study how information on the protein dynamics can be extracted from the fluorescence anisotropy of a bound dye, we performed molecular dynamics simulations of an Alexa488 dye covalently bound to the loop connecting the A- and B-helix of bacteriorhodopsin. The fluorescence anisotropy decay predicted by the simulation agrees well with the experimental results. The simulation revealed two depolarization processes with a rotational correlation time of about one nanosecond, which are due to the loop flexibility and slow conformational dye dynamics and which cannot be separated by experiment alone. Analysis of the correlation between the dye and the protein motions provides an atomistic description of the part of the protein dynamics, that is actually observed in the experiment. Furthermore, comparison of simulations with and without bound dye enabled us to test the inevitable assumption that in the experiment the influence of the dye on the protein dynamics is negligible. Indeed, only minor deviations in the loop flexibility were seen, thus providing solid theoretical grounds for the usual interpretation of the measurements.

AKB 200.38 Di 17:00 Poster TU C

Scanning Probe Microscopy Investigations of the Oriented Attachment and Membrane Reconstitution of His-tagged Cytochrome c oxidase to a Gold Electrode — •Dirk Mayer[1], Andreas Offenhäusser[1], Kenichi Ataka[2], and Joachim Heberle[2] — [1]Forschungszentrum Jülich, ISG-2: Institute for Bio and Chemosensors, Jülich, Germany — [2]Forschungszentrum Jülich, IBI-2: Structural Biology, Jülich, Germany

Many of the vital functions of cells are maintained by membrane proteins, which for instance selectively control the transfer of ions, biological signal molecules and energ. The high complexity of biological transmembrane machineries with respect to their structure (consisting of many subunits), the reduced periodicity (scalablility) and the multistep reaction paths makes the assignment of structure and function a challenging task. Monolayers of reconstituted membrane proteins supported by solid surfaces can be applied to modern surface analyzing methods. We are giving an account of a novel approach, combining the modification of a metal surface by attaching a Ni- NTA moiety with the reconstitution of the oriented and detergent solubilized proteins in a lipid bilayer. We employed surface-enhanced infrared absorption spectroscopy and scanning probe techniques for deriving a detailed description of the whole solid surface supported immobilization and reconstitution reaction path.

AKB 200.39 Di 17:00 Poster TU C

Near-field-THz-Imaging with high power cw-radiation — •Bruno Gompf, Michael Gerull, Tobias Müller, and Martin Dressel — 1.Physikalisches Institut, Universität Stuttgart

There is an increasing interest in THz-imaging especially of biological and medical samples. But until now, most of the work done in this field is based on time-domain techniques using ultrafast laser pulses. The inherent disadvantages of this broadband method are the low intensity and poor energy resolution. In combination with a near-field arrangement time-domain techniques have the additional problem that small apertures always act as high pass filters on broad-band radiation. We have developed a near-field spectrometer operating in the THz-range between 30 GHz and 1.4 THz, where we use backward-wave oscillators (BWO) as continuous-wave sources, which supply highly monochromatic ($\Delta\nu/\nu = 10^{-6}$) and coherent radiation with an output power of up to 300 mW. This instrument allows to record THz-images with a high spatial and spectroscopic resolution with an acquisition time of about 10 ms/pixel.

AKB 200.40 Di 17:00 Poster TU C

Development of a biosensor device on functionalized Silicon on Insulator (SOI) structures for the specific detection of proteins — •Simon Lud, Cornelia Neunteufel, Petra Neff, Michael Nikolaides, M. Fischer, and Andreas Bausch — Lehrstuhl für Biophysik E22, TU München, 85747 Garching, Germany

To handle the vast number of possible interactions between different molecules, detection systems must be able to screen many different interactions in parallel. Further on, in order to account for the different physical properties of the involved molecules, the detector must have a tunable sensitivity.

We present a device based on standard semiconductor technology which enables the selective and quantitative detection of biomolecular interactions. The sensor is based on hydrophobized Silicon-On-Insulator (SOI) substrates and is functionalized by a monolayer of lipids with incorporated metal chelate lipids. Both reversible charging of the chelate headgroup with divalent nickel ions and the specific binding of proteins was detected In addition, it was possible to detect charge differences between both peptides and proteins quantitatively. The sensor response is modelled within the standard Poisson-Boltzman theory and thus an average effective charge of different peptides and proteins can be determined. As the device is based on standard semiconductor technologies the SOI based Biosensor is well suited for parallelization needed in high throughput applications.

AKB 200.41 Di 17:00 Poster TU C

A Simple Scheme for Rapid 3D Orientation Determination of the Emission Dipole of Single Molecules — •Johannes Hohlbein[1] and Christian G. Hübner[2] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle — [2]Martin Luther University Halle-Wittenberg, Department of Physics, Hoher Weg 8, 06120 Halle

One of the unique features of single molecule absorption and emission is their anisotropy due to the well-defined transition dipole(s) for both processes allowing the determination of the molecule's orientation. While polarization-resolved techniques are usually capable to detect only a projection of the transition dipole, several methods have been proposed in order to determine the full three-dimensional orientation. Here, we report on a new detection scheme that allows for a shot-noise limited determination of the emission dipole orientation utilizing an annular mirror, a polarizing beam splitter in conjunction with three detectors in a scanning confocal optical microscope.

AKB 200.42 Di 17:00 Poster TU C

Molecular dynamics simulations of aquaporin channels — •Jochen Hub und Bert de Groot — Max-Planck-Institut für biophysikalische Chemie, Computational Biomolecular Dynamics Group, Am Fassberg 11, 37077 Göttingen

Aquaglyceroporins (AQPs) constitute a large family of integral membrane proteins that facilitate efficient and specific passive permeation of water and/or small alcohols across biological membranes in response to osmotic gradients. Members of these channels have been found in organisms ranging from bacteria to mammals. In humans they are expressed in tissues as diverse as kidney, red blood cells, brain, and eye lens.

Within the last years substantial progress has been made in understanding the permeation mechanism through AQPs, however questions regarding their selectivity for different solutes remain challenging.

We present "real time"molecular dynamics simulations of permeation through a recently discovered AQP channel in the malaria parasite Plasmodium falciparum (PfAQP). PfAQP shows the unusual behavior of high water *and* glycerol permeation which makes it an interesting target to investigate the molecular mechanisms of channel selectivity.

Since glycerol uptake via PfAQP is essential for the biogenesis of the parasite's glycerolipids, the long term focus is the design of a specific inhibitor for PfAQP as a novel potential anti-malaria agent.

AKB 200.43 Di 17:00 Poster TU C

Wirkung von Funkwellen auf Bäume und andere Pflanzen — •Jette Dröse und Irene Pundt — Institut für Umweltphysik, Universität Heidelberg, INF 229, 69120 Heidelberg

In Deutschland werden und wurden in den letzten 10 Jahren mehr als 80000 Mobilfunksendeanlagen aufgestellt. Europaweit führt die Intensivierung der bisherigen Mobilfunk Netze sowie des zukünftigen UMTS-Netzes zu einer deutlichen Erhöhung der gepulsten Mikrowellenstrahlung in der Atmosphäre. Gleichzeitig sind in den meisten Ländern Europas zunehmende Waldschäden zu beobachten. In Italien, Spanien und Frankreich ist der Anteil der gesunden Bäume in den letzten 10 Jahren um 30 Prozent gesunken auf nur noch 20 Prozent in Italien und Spanien bzw. 35 Prozent in Frankreich (Europäischer Waldschadensbericht, 2004, http://www.icp-forests.org/Reports.htm). Als Ursachen für die sog. neuen Waldschäden werden der Saure Regen, Ozon, der Klimawandel sowie verschiedene Kleinstlebewesen (Borkenkäfer) genannt. Es wird vielfach vermutet, dass auch Mikrowellenstrahlung (Rundfunk, Radar, Richt-, Mobilfunk) für Waldschäden mitverantwortlich ist. Wir geben einen Überblick über Ergebnisse bisheriger Untersuchungen, die sich mit dem Einfluss von Mikrowellen auf Bäume und Pflanzen beschäftigen.

AKB 200.44 Di 17:00 Poster TU C

Kinetics of Solid-Phase DNA Hybridization — •Timo Mai, Thomas Naiser, Wolfgang Michel, Philipp Baaske, and Albrecht Ott — Physikalisches Institut, Universität Bayreuth, 95440 Bayreuth

Solid-phase hybridization of DNA oligonucleotides is of growing importance because of the advances in DNA microarray technology.

We apply two distinct strategies both commonly used in DNA microarray experiments: Immobilization of pre-fabricated oligonucleotides and light directed in-situ synthesis. We investigate kinetics of hybridization on glass substrates using evanescent field excitation and fluorescence labelling of oligonucleotides. A FRET technique is used to account for contributions of nonspecific adsorption to the substrate during the hybridization process. We discuss the impact of these different methods of immobilization on hybridization kinetics.

AKB 200.45 Di 17:00 Poster TU C

Einkopplung externer elektrischer Pulse in Hefezellkulturen zur gezielten Beeinflussung des Stoffwechsels — •A. Reiher[1], S. Günther[1], A. Krtschil[1], H. Witte[1], A. Krost[1], C. Warnke[2], T. Mair[2] und S.C. Müller[2] — [1]Inst. für Exp. Physik, Abt. Halbleiterepitaxie, Universität Magdeburg, PF 4120, 39016 Magdeburg — [2]Inst. für Exp. Physik, Abt. Biophysik, Universität Magdeburg, PF 4120, 39016 Magdeburg

Wir zeigen, wie mittels einer elektrischen Stimulation über eine planare Mehrelektroden-Anordnung gezielt das Stoffwechselgleichgewicht von Hefezellen beeinflusst werden kann, was sich durch eine Verringerung eines detektierten NADH-Fluoreszenzsignals nachweisen lässt. Die Elektroden-Anordnung besteht aus zwei in sich greifenden Gold- Titan-Elektroden auf einem Glassubstrat. Es werden die Einkoppeleigenschaften für systematisch variierte Spannungspulse in die Hefezellkultur (bei Variation der Form, Dauer und Höhe der Spannungspulse, isolierte oder metallische Elektrode) untersucht. Die genutzte Elektrodenanordnung weist einen optimalen Puls- höhenbereich von 10 V bis 15 V auf, wobei die Einsatzspannung für die induzierten Stoffwechselveränderungen zwischen 4-5 V liegt. Diese Abhängigkeiten werden systematisch für verschiedene Elektrolyten (variierte Molarität bzw. pH-Wert) aufgezeigt, um die Physik der Pulsübertragung und -einkopplung in die Zellen zu verstehen.

AKB 200.46 Di 17:00 Poster TU C

Biochemical synthesis of periodic DNA nanotemplates — •Stefan Beyer und Friedrich C. Simmel — Department Physik, LMU München, Geschwister-Scholl-Platz 1, 80539 München

Rolling circle amplification (RCA), a biochemical method established in genetics and biosensing, can be used to produce DNA building blocks for the self-assembly of nanostructures. In RCA, small circular single-stranded oligonucleotides serve as templates for the polymerization of the complementary strand. The polymerase (phi29 DNA polymerase) used for this process has a unique strand displacement activity. This allows it to continue with the polymerization process after the completion of one cycle without unbinding from the substrate. After one polymerization cycle the leading strand is removed and another cycle begins. The result of many of such cycles is a long single DNA strand with a repetitive sequence. Such a strand can be functionalized by hybridization with biotinylated DNA strands complementary to the repetition unit. The resulting DNA nanotemplate can be used to align biotin-binding nanoparticles (streptavidin or anti-biotin conjugates) into one-dimensional arrays. The constructs are analyzed by atomic force microscopy, scanning electron microscopy, gel electrophoresis and fluorescence microscopy. RCA proves to be a very simple, efficient and inexpensive way to create long periodic DNA sequences which can serve as templates for linear structures composed of nanoobjects.

AKB 200.47 Di 17:00 Poster TU C

Osmotically induced water permeation through gramicidin and derivatives studied by computer simulations. — •Guillem Portella and Bert L. de Groot — Max Plank Institute for Biophysical Chemistry, Computational Biomolecular Dynamics Group Am Faßberg 11, 37077 Göttingen, Germany

Full atomistic molecular dynamics simulations provides deeper understanding of the microscopic energetic and structural determinants underlying permeation through molecular membrane channels. Gramicidin A has been used as a model channel extensively both experimentally and computationally. Here, we focus particularly on the efficient simulation of an osmotically induced water flux. So far, different methods have been developed to derive permeation rates from simulations: continuous-time random model aproximation from equilibrium simulations or external forces acting on molecules as a result of the osmotic gradient. We chose to explore a method that attempts to mimick the true situation in vitro or in vivo as closely as possible, namely by introducing a true osmotic gradient. This is achieved by a solute concentration gradient across the membrane. As membrane simulations are usually carried out using periodic boundary conditions, this creates a challenge to the simulation of osmotic gradients, as they would normally be balanced by diffusion across the periodic boundaries. In order to alleviate this problem, we created two different water compartments (with different solute concentrations)

by simulating two bilayers, which allows to efficiently study osmotically induced permeation, as has recently been demonstrated for carbon nanotubes.

AKB 200.48 Di 17:00 Poster TU C

Mapping the Thermoplasma proteome - structural proteomics studies by free-flow electrophoresis and cryo-electron tomography — •Christine Kofler, Istvan Nagy, Stephan Nickell, Marius Boicu, and Wolfgang Baumeister — Max Planck Institut für Biochemie, Molekulare Strukturbiologie

Thermoplasma acidophilum is a thermoacidophilic archaeon whose genome is completely known. To carry out proteomic analysis on this organism we use cell lysates which are fractionated using free-flow electrophoresis (FFE). The FFE separates the cytoplasmic proteins according to their isoelectric point. Single fractions are then investigated by means of cryo-electron tomography (cryo-ET) which allows to obtain three-dimensional (3-D) structural information of vitrified biological specimens at a resolution of 2-4 nm. Additionally, the contents of the single fractions are characterised by polyacrylamide gel electrophoresis and mass spectrometry. The knowledge of the 3-D structure and the determination of the identity of different proteins will enable us to generate a library of templates which is used as an input for pattern recognition algorithms designed to search electron tomograms of whole ice-embedded cells. The final aim of these studies is to locate and quantify the different macromolecular assemblies within 3-D reconstructions of intact *T. acidophilum* cells.

AKB 200.49 Di 17:00 Poster TU C

Solid State 31P-NMR Investigations of Different Calcium Phosphates — •Inderchand Manjubala[1], Sergey Maltsev[2], Christian Jaeger[2], and Peter Fratzl[1] — [1]Max-Planck Institute for Colloids and Interfaces, Department of Biomaterials, 14424 Potsdam, Germany — [2]Bundesanstalt für Materialforschung und -prüfung, Projektgruppe I.3903, Richard Willstaetter Str. 11, D-12489 Berlin, Germany

Synthetic hydroxyapatite and carbonated apatite have been used widely as bone substitute ceramic material as they resemble the natural bone apatite. In this study in-situ formation of biphasic calcium phosphate ceramic consisting of a mixture of hydroxyapatite and tricalcium phosphate in various ratios is synthesized under microwave irradiation. The amount of TCP increases as the Ca/P ratio decreases. 31P solid-state nuclear magnetic resonance (NMR) with magic-angle spinning (MAS) was used to determine the structure of the various synthetic calcium phosphates in comparison with X-ray diffraction. The XRD study reveals biphasic structure with hydroxyapatite and tricalcium phosphate phase and the amount of TCP increases as Ca/P ratio decreases. The Ca/P was also estimated from EDAX analysis.

AKB 200.50 Di 17:00 Poster TU C

Fluorescence spectroscopy of DNA nanodevices — •Andreas Reuter and Friedrich C. Simmel — CeNs und Department für Physik, Geschwister-Scholl-Platz 1, 80539 München

DNA tweezers consist of three branches of single stranded DNA, one of which is labelled with a fluorescence resonance energy transfer (FRET) pair. The three single strands form two double-stranded arms of 18 base pairs or roughly 6.1 nm length connected by a short hinge. The two duplex arms can be pulled together by the addition of a fourth single stranded DNA. In this case the dyes are in close proximity and FRET is very efficient. For the open configuration of the tweezers the average distance between the dyes was determined to be around 6 nm which corresponds to a mean opening angle between the duplex arms of 60°. However this value represents an average value over many possible configurations.

We perform single pair FRET experiments on three different configurations of the tweezers: fully stretched, where the dyes are separated by 40 base pairs, opened and closed. The width of the distribution of FRET efficiencies contains important information about the flexibility of the DNA nanodevice.

AKB 200.51 Di 17:00 Poster TU C

Complex and dynamic estrogen receptor-α interactions in living cells revealed by diffusion-time distribution analysis — •Michael Prummer, Hanna Jankevics, Paulina Izewska, Horst Pick, Kirsten Leufgen, and Horst Vogel — Laboratory of Physical Chemistry of Polymers and Membranes, Institute of Chemical Sciences and Engineering, Swiss Federal Institute of Technology (EPFL), CH-1015 Lausanne, Switzerland

Specific binding of ligands induce characteristic mobility patterns of human estrogen receptor-α (ER) in living breast cancer cells. These patterns were determined by analyzing the distribution of diffusion times obtained from fluorescence correlation spectroscopy experiments of ER conjugated to yellow fluorescent protein (YFP). The highly mobile ER in untreated cells slowed down in the presence of agonist and partial antagonist. The reduced mobility was accompanied by the formation of multiple discrete states in a broad distribution of diffusion times, where different states were observed for different ligands. This new finding reveals that ER forms a limited number of complexes with different mobility and varying population by dynamic interaction with many other nuclear components with well defined interaction times. Our approach to examine ER interactions at native expression levels opens up new routes to elucidate hormone-dependent transcription regulation and allows for the detection and distinction of pharmacologically and toxicologically active compounds. Diffusion time distribution analysis has the potential to become a general approach to monitor physical properties of biochemical networks in living cells.

AKB 200.52 Di 17:00 Poster TU C

Monitoring individual odorant receptors in cultured mammalian cells — •Michael Prummer, Valerie Jacquier, Horst Pick, and Horst Vogel — Laboratory of Physical Chemistry of Polymers and Membranes, Institute of Chemical Sciences and Engineering, Swiss Federal Institute of Technology (EPFL), CH-1015 Lausanne, Switzerland

The olfactory system is a highly specialized chemo-sensor recognizing a myriad of compounds at very low concentrations. Human odorant receptors (ORs) constitute a multi-gene family of G-protein coupled receptors with about 450 members. Although many putative ORs have been cloned, the expression in heterologous systems has been complicated by the failure of these proteins to translocate efficiently to the plasma membrane. Here, single-molecule detection is an appropriate tool allowing for the investigation of single ORs in the membrane of living cells. Human OR17-40 was enzymatically labeled with Cy5 and expressed in HEK293 cells where ligand-induced Ca-signaling and internalization proved its structural integrity and the existence of a functional secondary messenger system. Single-molecule tracking wide-field microscopy was utilized to record trajectories of ORs, which were analyzed in terms of the microscopic diffusion coefficient of each molecule, and the probability distribution of the mean-square displacement, averaged over many molecules. Current investigations are focused on how the mobility of ORs is influenced by ligand activation. The ultimate goal is to monitor the fate of individual ORs from their resting state through ligand binding until desensitization occurs.

AKB 200.53 Di 17:00 Poster TU C

The effect of biological variability on spatiotemporal patterns in a chain of biochemical oscillators: numerical simulations and Eigenvalue analysis — •Tetyana Morokhovska and Marc-Thorsten Hütt — Bioinformatics Group, Department of Biology, Darmstadt University, Schnittspahnstr. 3-5, D-64287 Darmstadt

Noise has an important effect on spatiotemporal patterns in biological systems. In contrast to noise, biological variability (or disorder) is a static system property. Nevertheless it can have dynamical implications, as the magnitude and the statistical properties of the biological variability influence the capabilities of the elements to synchronize or form patterns. We study such influences in a chain of coupled nonlinear oscillators, each of which can be thought of as a simple form of oscillating biochemical reaction. In addition to numerical simulations, where spatiotemporal patterns are quantified with methods from information theory, we also present results on Eigenvalue distributions, which arise from biological variability in the system's parameters.

The simulations show that under certain conditions an increase in variability can induce spatial waves and complex spatiotemporal patterns. In particular, it is seen that the mutual information quantifying the complexity of the spatiotemporal patterns can depend resonantly on variability.

Eigenvalues for this system are studied both numerically and with algebraic methods based on Sturm sequences and the Routh-Hurwitz criterion. We show that certain aspects of the spatiotemporal patterns can be understood qualitatively on the level of Eigenvalue distributions.

AKB 200.54 Di 17:00 Poster TU C

Watching conformational changes of pigment-protein complexes by optical single-molecule spectroscopy — •Silke Oellerich[1,2], W.P.F. de Ruijter[2], R.J. Cogdell[3], J. Köhler[1], and T.J. Aartsma[2] — [1]Experimentalphysik IV, Universität Bayreuth — [2]Dept. of Biophysics, Leiden University, The Netherlands — [3]Dept. of Biochemistry, University of Glasgow, Scotland

Pigment-protein complexes of photosynthetic purple bacteria are an interesting model system for studying pigment-pigment interactions as well as pigment-protein interactions. These interactions strongly affect the spectral properties of the complex. Changes or even fluctuations in these interactions result in spectral changes, which can be followed by optical single-molecule spectroscopy. Low-temperature fluorescence-excitation spectra of individual bacterial light-harvesting 3 complexes (LH3), which consists of 27 bacteriochlorophyll a pigments, provide a detailed picture about the influence of locally restricted changes in the pigment-protein interaction on the spectral properties of the entire complex.

AKB 200.55 Di 17:00 Poster TU C

Theoretical investigations of radiation damage in protein crystals produced by X-rays — •Melanie Zehnder, Ivan Vartaniants, and Edgar Weckert — HASYLAB at DESY, Notkestrasse 85, 22607 Hamburg

The data quality and the achievable resolution in X-ray crystal-structure analysis of protein crystals is limited by radiation damage in many cases. The aim of the investigation is a better quantitative understanding of the damage caused by the absorbed photon and the subsequent processes in proteins by Monte-Carlo simulations.

The dominating inelastic interaction for X-ray photons of usual energies with an atom in the protein is the photo-effect, in which photo-electrons with nearly the incoming photon energy and low energy Auger-electrons are created. At higher energies the Compton scattering becomes more and more dominant. In this case an electron of few keV is produced and most of the energy is kept by the photon. For normal protein crystal sizes of around 0.3 mm this photon interacts in general just once. In contrast, the produced electrons have a high inelastic cross-section, so that the resulting electron cascade has a high damage-potential.

By means of a Monte-Carlo approach the electron cascade and the spatial distribution of ions and excited atoms produced by inelastic interactions are analyzed in order to obtain more quantitative information of the damage. Furthermore, the average time for a cascade produced by each photon is evaluated. One of the aims of these investigations is to find the optimum data collection energy dependent on a given chemical composition.

AKB 200.56 Di 17:00 Poster TU C

Modelling the Structure and Optical Properties of the Rhodopsin Chromophore — •Minoru Sugihara[1], Marko Schreiber[2], Peter Entel[1], and Volker Buss[2] — [1]Theoretical Physics, University of Duisburg-Essen — [2]Theoretical Chemistry, University of Duisburg-Essen

Modelling the Rhodopsin Chromophore with QM/MM: Four available X-ray structures of rhodopsin show a considerable variety of the chromophore geometry despite the similarity of the chromophore binding pocket. Based on the recent two crystal structures obtained by Okada [1,2], we have re-investigated the chromophore geometry applying QM/MM methodology. Our results show that the different chromophore geometries converge to practically one identical structure, which shows strong bond alternation and is twisted, in addition to the ionone ring, in the region undergoing photoisomerization [2].

Calculation of the Optical Properties with Ab-Initio Method: (CASPT2) Using the calculated chromophore geometry inside the binding pocket the absorption maximum of the chromophore was calculated. Two factors were considered: the internal distorsion and the presence of the counterion. We find that the first excited state is weakly red-shifted (ca. 20nm) due to the deformation of the chromophore and is strongly blue-shifted (ca. 100nm) in the presence of the counterion [3].

[1] T. Okada, et al. Proc. Natl. Acad. Sci. USA, 99 (2002) 5982. [2] T. Okada, et al. J. Mol. Biol. 342 (2004) 517. [3] M. Schreiber, et al. J. Chem. Phys. 23 (2003) 12045

AKB 200.57 Di 17:00 Poster TU C

Analysis of spatio-temporal patterns of the energy metabolism in a yeast extract by Karhunen - Loève decomposition — •Satenik Bagyan, Ronny Straube, Thomas Mair, and Stefan Müller — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung Biophysik, Universitätsplatz 2, 39106 Magdeburg, Germany

Glycolytic degradation of sugar is the primary pathway for the generation of energy in living cells and shows non-linear, oscillatory reaction kinetics, which is mediated by an autocatalytic reaction. Coupling of non-linear reaction kinetics with diffusion leads to the formation of glycolytic waves. We used an open spatial reactor to investigate the spatio-temporal pattern formation during glycolysis in the yeast extract. The dynamics of glycolytic waves in the open spatial reactor is changing over time from ordered (circular- or spiral- shaped waves) to more complex structures. To elucidate the mechanisms leading from ordered to complex behaviour, we analysed the dynamics of the spatio-temporal patterns with a Karhunen-Loève decomposition. We found that the early behavior of the patterns can be reconstructed with only 2 modes, but the later states require more modes for reconstruction. This indicates that during the initial states the patterns are dominated by periodic forces whereas at later states some kind of spatial desynchronization takes place.

AKB 200.58 Di 17:00 Poster TU C

Electric field induced perturbation of the energy metabolism of living yeast cells — •Ch. Warnke[1], T. Mair[1], S.C. Mueller[1], A. Reiher[2], A. Kritschl[2], H. Witte[2], and A. Krost[2] — [1]Otto-von-Guericke Universität Magdeburg, Inst.Exp.Phy., Abt.Biophysik — [2]Otto-von-Guericke Universität Magdeburg, Inst.Exp.Phy., Abt.Halbleiterepitaxie

Electric fields are often used for biophysical or biomedical treatment of biological cells, e.g. cell fusion or killing of cells. Despite these important applications, there are only a few data about the possible mechanisms that determine the electrosensitivity of biological cells. Since electrostimulation always induces depolarization of biomembranes, an impact of the energy metabolism is obvious due to the regeneration of electrochemical gradients by the expenditure of cellular energy. We have constructed a new electrical interface for local stimulation of biological cells with variable duration and amplitude. When applying short lasting electrical pulses to yeast cells, we find a direct response of the energy metabolism (measured by NADH-fluorescence) to these pulses. A sudden and fast decrease in NADH is followed by a slower recovery of the fluorescence signal. We attribute these changes to the immediate break down of ATP as a consequence of the regeneration of the membrane potential (AT-Pases) and the slower regeneration of ATP by glycolysis and respiration. We present a first kinetic analysis of this behaviour and basic characterization of the phenomenon.

AKB 200.59 Di 17:00 Poster TU C

Characterization of Cellular Protein Distributions Using *Karhunen-Lòeve* Decompositon — •Ronny Straube[1], Stefan C. Müller[1], Ronald Koop[2], and Walter Schubert[2] — [1]Abteilung Biophysik, Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany — [2]MelTec GmbH, Leipziger Str. 44, 39120 Magdeburg, Germany

Immuno-fluorescence microscopy is a widely used technique to visualize the location of proteins on a cellular level. This method is based upon the interaction of fluorochrome labeled antibodies with antigens. In general, it is limited by the number of simultaneously usable fluorochrome labeled antibodies due to problems concerning the spectral separability of the fluorescence signals.

Recently, this limitation has been overcome by using a repetitive method (called *MELK* [1]) where many different antigens can be visualized on the same sample of cells. Thereby, it becomes now possible to study combinatorial patterns of protein distributions based on series of fluorescence intensity images of a high spatial resolution.

We use the *Karhunen-Lòeve* decomposition to characterize the cellular distributions of 18 human surface antigens on an ensemble of peripheral blood leukocytes (PBL's). By analyzing the mode structure we find that some antigens tend to aggregate while others prefer to separate. We also investigate the reproducibility of the *MELK* patterns.

[1] Patentnummer (Deutschland): 197 09 348.5-52, W. Schubert, "Automatisches Multi-Epitop-Ligand-Kartierungsverfahren", MelTec GmbH, 1997

AKB 200.60 Di 17:00 Poster TU C

Potential and limitations of DNA microarrays from a single-molecule point of view — •Beate Sick and Keith Harshman — DNA Array Facility, Universitaet Lausanne, CH-1015 Lausanne

DNA microarrays are a high-throughput technology which provide a snapshot of the transcriptome of some ten thousand genes in parallel. Since the native RNA expression levels in a cell can span a range of 6 orders of magnitude, it is desirable to cover the same dynamic range in one microarray experiment. In order to approach this goal several components in a microarray experiment have still to be optimized. In this contribution we assess physical limitations of DNA microarray experiments and include technical boundaries and biological variability. We discuss the observed limited reproducibility and dynamic range of typical microarray data from homemade spotted arrays and from commercial platforms (Affymetrix). The ultimate lower detection limit is reached when a single target gene transcript binds to a probe feature, provided the instrumentation has single-molecule sensitivity. On the other hand, the total number of binding sites for transcripts on each feature, which is determined for instance by the feature size, defines the ultimate upper detection limit. From these theoretical considerations the accessible dynamic range is evaluated for different existing platforms. In an outlook the impact of further miniaturization of microarrays on the dynamic range will be discussed.

AKB 200.61 Di 17:00 Poster TU C

Response of ion currents across the cell membrane to excitation with high-frequency electrical fields — •Michael Olapinski[1], Andrea Brüggemann[2], Michael George[2], Stephan Manus[1], Niels Fertig[2], and Friedrich C. Simmel[1] — [1]Sektion Physik and Center for Nanoscience, Universität München, Geschwister-Scholl-Platz 1, 80539 München — [2]Nanion Technologies GmbH, Pettenkoferstr. 12, 80336 München

Due to the intrinsically large RC time constants of the measurement setup, classical patch-clamp techniques are limited in time resolution. They are therefore not suitable for the application of high-frequency (HF) electrical signals and for the study of fast processes coupling to the ion transport dynamics.

Our setup combines a patch-clamp on-a-chip system with an open-end coaxial probe that is positioned a few tenths of a millimeter above the investigated cells. Ion currents through the cell membrane are measured in whole-cell configuration while high-frequency fields are applied at frequencies between 100 MHz and 50 GHz and at power levels up to +25dBm.

Preliminary results obtained on rat basophil leukaemia (RBL) cells containing potassium channel $K_{ir}2.1$ suggest that the ion current is sensitive to the applied HF field in specific frequency ranges and depends on the presence of potassium ions and the applied membrane potential. Temperature measurements of the solution do not show any significant temperature rise.

AKB 200.62 Di 17:00 Poster TU C

Nanomechanical Cantilevers: Versatile, Label-free Biosensors — •Joachim Köser and Felice Mauro Battiston — Concentris GmbH, Davidsbodenstrasse 63, CH-4056 Basel, Switzerland

Nanomechanical cantilever sensors are a promising, label-free technology for the detection of biomolecules and the measurement of biomolecular interactions. They allow the real-time study of processes occurring at biological interfaces. Cantilevers are small silicon beams, which are fixed to a solid support at one end and move freely at the other end. They support two complementary sensing principles: While their resonance frequency depends on the mass load, changes in surface stress are reflected by the bending of the cantilevers. Surface stress can forces from conformational changes upon ligand binding or nucleic acid hybridization as well as protein denaturation or misfolding. Further biophysical properties, such as repulsion/attraction of molecules at the sensor surface, or binding of substances from the analyte can be monitored with the appropriate equipment.

We will present novel instrumental developments, which allow reliable, user-friendly measurements with cantilever sensors and open the door for a wider range of applications of this technology in basic research and biochemical analysis. Recent data obtained with our new cantilever sensor platform "Cantisens Research"will be presented.

AKB 200.63 Di 17:00 Poster TU C

Design of Novel GaAs/Peptide Hybrids Using Molecular Dipole Engineering — •Klaus Adlkofer[1], Tomoyuki Morita[2], Daniel Gassull[1], Shunsaku Kimura[2], and Motomu Tanaka[1] — [1]Lehrstuhl für Biophysik E22, Technische Universität München, James-Franck-Strasse, D-85748 Garching, Germany — [2]Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Japan

Combination of low-dimensional semiconductors and bio/organic molecular constructs includes a large potential towards the design of new functional material. The primary aim of this study exists in design of novel hybrid materials by combination of GaAs semiconductors and functional peptide helices with a large macromolecular dipole. The quality of the optimized monolayers was examined by measuring the film thickness with ellipsometry. When LipoL16B was grafted on GaAs, the film showed a lot of defects, which can be attributed to the weaker reactivity of disulfide coupling group. However, grafting of the peptides with thiol coupling groups (AcSL8B and AcSL16B) resulted in film thickness which agrees very well with the length of the peptide helices. Topography of the engineered surface was studied by AFM, confirming that the peptide monolayer is as smooth as the native GaAs surfaces. Furthermore, the orientation of the helical peptides was evaluated by FTIR. The established functionalization protocols can be transferred onto near-surface semiconductor nano-structures with GaAs cap layers such as quantum dots (QDs) and two-dimensional electron gases (2DEGs).

AKB 200.64 Di 17:00 Poster TU C

Multi-Frequency EPR studies on Quinoprotein Ethanol Dehydrogenase:Characterization of the novel PQQ cofactor — •Robert Bittl[1], Christopher Kay[1], Bina Mennenga[2], and Helmut Görisch[2] — [1]Institut für Experimentalphysik, Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Fachgebiet Technische Biochemie, Institut für Biotechnologie, Technische Universität Berlin, 13353 Berlin, Germany

Pyrroloquinoline quinone (PQQ) is one of several quinone cofactors utilized in a class of dehydrogenases, known as quinoproteins. The quinoprotein methanol dehydrogenase (MDH) is among the best-characterised PQQ-dependent enzymes thus far. MDH has an $\alpha 2\beta 2$ tetrameric structure with each β-subunit folded around the surface of an α-subunit. The PQQ cofactor is bound to a Ca2+ ion and sandwiched between a tryptophane residue and an unusual eight-membered disulfide ring structure formed from adjacent cysteine residues.

Here we describe the first detailed characterization of the enzyme-bound PQQ in both wild type and mutant proteins lacking the disulfide ring, using multi-frequency/resonance EPR methods. Thus, we have determined the principal values of the rhombic g-tensor [1], and from pulsed ENDOR experiments at X-Band and W-Band, supported by DFT calculations, we have determined and assigned many of the proton hyperfine couplings. From HYSCORE experiments, the hyperfine couplings from the two nitrogens in the cofactor could be determined.

[1] C. W. M. Kay, B. Mennenga, H. Görisch and R. Bittl, FEBS Lett 564 (2004) 69-72.

AKB 200.65 Di 17:00 Poster TU C

A grating based detection platform for multi-color fluorescence correlation spectroscopy — •Markus Burkhardt, Katrin G. Heinze, and Petra Schwille — Biotec/TU Dresden, Tatzberg 47-51, 01307 Dresden, Germany

Fluorescence Correlation Spectroscopy (FCS) is based on time dependent fluorescence intensity fluctuations of labeled biomolecules as they enter and leave a diffraction-limited optical detection volume via Brownian diffusion. From these fluctuations, concentrations, diffusion and binding coefficients are easily obtained. Simultaneous monitoring of biomolecular species, labeled with spectrally distinct fluorophores, has proven to reveal inter- and intramolecular mechanisms both in vitro and in vivo.

We have developed a continuously tunable, filterless multi-color detection unit for FCS. Our tailored platform, using a grating instead of the classical dichroic mirror cascade, allows for accommodation of up to 15 detection channels covering the entire visible spectral range. As a proof of principle, we successfully demonstrate simultaneous FCS of four distinct fluorescent quantum dots being mixed in aqueous solution. Grating-based detection allows for spectral high-resolution FCS and is a feasible tool for quantitative investigation of complex biomolecular dynamics on a single molecule level.

AKB 200.66 Di 17:00 Poster TU C

Design of functional carbohydrate clusters for control of dynamic cell adhesion — •Jochen Oelke[1], Andreea Banu[1], Richard R. Schmidt[2], Achim Wixforth[3], and Motomu Tanaka[1] — [1]Dept. Phys. E22, TU München, D-85748 Garching, e-mail: mtanaka@ph.tum.de — [2]Dept. Chem., Univ. Konstanz, D-78457 Konstanz — [3]Dept. Phys., Univ. Augsburg, D-86135 Augsburg

The general goal of this work is the design of functional micro- and nano-clusters of ligands through controlled self-assembling processes at the interface, and their use as a new platform to control adhesion of bacteria under defined shear stresses.
As functional ligands, we synthesize a new class of fluorinated glycolipids bearing mannose or gal(1→4)-α-gal moieties. The fluorocarbon segment is used in order to induce de-mixinig due to the immicibility with the hydrocarbon segment, whereas the sugar part is responsible for the recognition with bacteria (for example mannose for enteroaggregative bacteria). As the first step, formation of these clusters was studied at the air/water interface, followed by deposition onto solid surfaces. The strength of bacterial adhesion, we determine the critical shear field required for the cell detachment (dissociation rate) by coupling the functionalized surface to two micro-fluidic systems: (a) conventional capillary flow chambers, and (b) "flat-fluidics" using surface acoustic waves (SAWs).

AKB 200.67 Di 17:00 Poster TU C

Characterization of High-K Coatings on Silicon Chips in Electrolyte for Capacitive Stimulation of Nerve Cells — •Frank Wallrapp und Peter Fromherz — Max Planck Institute of Biochemistry, Martinsried, Germany

Non-invasive capacitive stimulation of neurons is commonly achieved from silicon chips insulated by a thin layer of SiO_2. Higher capacitances of the chips however would facilitate stimulation. We therefore replaced SiO_2 by the high-k materials HfO_2 and TiO_2. Capacitance and leakage current were measured in an electrolyte-insulator-silicon (EIS) configuration. Considering leakage current and biocompatibility, HfO_2 and TiO_2 both proved to be as suitable for neuronal stimulation as SiO_2. Due to the higher capacitance, TiO_2 is superior in applications. For all materials, the dielectric constant, interfacial layer thickness and charge trapping properties were examined. The capacitance vs. voltages (CV) curves of SiO_2 and HfO_2 were explained by standard metal-insulator-semiconductor (MIS) theory. Those of TiO_2 exhibited some unique features which we were able to rationalize by treating the TiO_2 explicitly as a wide band-gap semiconductor. The new high-k coated chips have opened up the way to new applications, e.g. opening voltage-gated channels in HEK293 cells and stimulating rat brain slices.

AKB 200.68 Di 17:00 Poster TU C

Capacitive stimulation of recombinant voltage-gated Na^+ channels on a silicon chip — •Ingmar Schön and Peter Fromherz — Dept. Membrane and Neurophysics, MPI of Biochemistry, Martinsried, Germany

To understand and optimize capacitive excitation of neurons from silicon microstructures, it is necessary to study the response of defined voltage-gated ion channels to voltage transients applied to a chip.

The model system comprises HEK293 cells stably transfected with $rNa_V1.4$ sodium channels. The cells were cultured on a silicon chip insulated with a thin layer of hafnium oxide and coated with fibronectin. Voltage transients were applied to the chip. They were chosen such that capacitive coupling gave rise to a stationary negative voltage in the narrow extracellular space between chip and cell. The resulting changes of sodium current through the attached membrane were recorded at constant intracellular voltage using whole-cell patch clamp.

We succeeded in capacitive gating of $rNa_V1.4$ channels. The evoked sodium current was sensitive to pharmacological agents LqhαIT (slowed inactivation) and TTX (channel blocking). Numerical simulations were in good agreement with the experiments. However, sufficient coupling strength required an electrolyte with rigorous reduced conductance.

AKB 200.69 Di 17:00 Poster TU C

A versatile two-photon fluorescence laser scanning microscope for single molecule applications — •Zdeněk Petrášek and Petra Schwille — Biotechnologisches Zentrum der TU Dresden; Institut für Biophysik; Tatzberg 47 - 51; 01307 Dresden; Germany

An imaging system with optical beam scanning, two-photon excitation and fluorescence detection has been constructed. The setup consists of a Ti:Sapph laser and a commercial inverted microscope to which a home-built scanning and detection unit is attached. The fluorescence signal can be detected in two channels with the light separation based on wavelength or polarization. The time-resolved detection allows simultaneous measurement of fluorescence decay kinetics (sub-ns timescale) and FCS (sub-μs to $>s$ timescale) with the access to the complete photon sequence. The combination of imaging, pulsed excitation and fast detection allows fluorescence lifetime imaging (FLIM) to be performed.

The design focus has been on the freedom of control over the scan mirror movement. An arbitrary scanning pattern can be programmed, thus allowing scanning-FCS techniques to be employed. Scanning-FCS is especially suitable for investigation of slowly diffusing or stationary chromophores (FCS, cross-correlation). Since it is the laser beam and not the sample stage that is being moved, mechanical stability of the sample is maintained.

AKB 200.70 Di 17:00 Poster TU C

Acute Brain Slices on Silicon Chips: From Capacitive Stimulation to Recording with Field Effect Transistor Array — •Christian Stangl and Peter Fromherz — Max Planck Institute of Biochemistry, Dept. Membrane- and Neurophysics, Am Klopferspitz 18, D-82152 Martinsried

Silicon chips with arrays of capacitive stimulators and field effect transistors provide a novel approach in investigating the brain. Previous studies demonstrated the non-invasive stimulation and recording on cultured brain slices. Now for the first time acutely dissected brain slices have been used to record evoked neuronal field potentials.

Dead cell layers on the surface of acute slices, caused by the cutting procedure, complicate both capacitive stimulation and coupling with transistors. We treated this problem by simulating the distribution of evoked field potentials within the slice. The calculated profiles fit to data from conventional extracellular microelectrode measurements.

Capacitive stimulation and recording with field effect transistors are possible with the use of acute brain slices in spite of the dead cell layers. With this novel non-invasive approach we could probe neuronal projections in hippocampal slices as well as the neuronal plasticity of the hippocampus.

AKB 200.71 Di 17:00 Poster TU C

Single Molecule Anisotropy Measurements in Lipid Bilayers — •Jakob C. Schweizer, Zdeněk Petrášek, and Petra Schwille — Biotechnologisches Zentrum der TU Dresden; Institut für Biophysik; Tatzberg 47-51; 01307 Dresden; Germany

Fluorescence widefield microscopy was combined with polarization optics in order to study the fluorescence polarization of single biomolecules. The fluorescence emission was split by a wollaston prism, providing spatially displaced images for the parallel and perpendicular polarization components, respectively. From these images, fluorescence anisotropy values were calculated.

A common cause for fluorescence depolarization, among others, is rotational diffusion. Initial measurements were performed in which orientation and rotational diffusion of flourescent dyes in supported lipid bilayers in different membrane phases were investigated. In these systems, the orientation of transition dipoles of the used dyes was shown to be restricted to two dimensions. The Perrin equation for such a two-dimensional system was deduced. Fluorescence anisotropy values from ensemble measurements and single molecule-measurements were compared. The investigation of rotational diffusion on the single molecule level is expected to yield a deeper insight into the structure and dynamics of biological systems.