BP 26: Posters II

Time: Thursday 17:00–19:30 Location: Poster A

BP 26.1 Thu 17:00 Poster A

Fast $\mathcal{O}(N^2)$ Hydrodynamics for Brownian Dynamics Simulations — •Tihamér Geyer and Uwe Winter — Zentrum für Bioinformatik, Universität des Saarlandes, Saarbrücken, D–66041 Saarbrücken

In Brownian Dynamics (BD) simulations, the solvent molecules are replaced by a continuous solvent, thus greatly reducing the complexity and the required numerical effort. The polarizability of the solvent molecules is thereby taken into account by a shielded Coulomb interactions while the mechanical displacement of the solvent leads to hydrodynamic interactions (HI). Due to the many-body nature of this (effective) interaction, which introduces a correlation into the random motion of the particles, it is more complicated to evaluate. Effectively, HI is calculated from a factorization of the $6N \times 6N$ diffusion matrix, for which the runtime scales as $\mathcal{O}(N^3)$. This makes it prohibitive to include HI into BD simulations with more than a hundred particles.

Here we report on an approximation to the hydrodynamic interaction, which, at weak coupling, preserves the statistical moments of the correlated random motion of the particles. Due to this approximation, the hydrodynamic corrections to the particle displacements can be evaluated with a runtime $\propto \mathcal{O}(N^2)$, i.e., it scales as the evaluation of the direct interactions. With this form it is now possible to include HI into simulations with virtually arbitrarily many particles.

Here we present first test runs that show that the errors introduced through the approximation are negligible compared to the benefit of including the hydrodynamic corrections to the continuum solvent model.

BP 26.2 Thu 17:00 Poster A

Effect of high pressure on the global and internal dynamics of multimeric proteins studied by quasielastic neutron scattering experiment. — •Marie-Sousai Appavou[1], Sebastian Busch[2], Wolfgang Doster[3], Ana Gaspar[2], and Tobias Unruh[2] — [1]Forschungszentrum Jülich GmbH, IFF-JCNS, Garching, Germany — [2]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany — [3]Technishe Universität München, Physik Department E 13, Garching, Germany

Pressure is a physical parameter, which in contrast to temperature, allows to separate volume changes from entropic effects. Moreover, pressure is increasingly utilized in the sterilization and bio-conservation processes in food and pharmaceutical industries. In the range up to 2000 bar, essentially association-dissociation phenomena of biomolecular assemblies are observed. The unfolding of monomeric proteins typically requires pressures exceeding 3 kbar. Pressure can also be used to investigate the effect of density changes on molecular motions. Quasi-elastic neutron scattering allows exploring structural fluctuations of proteins on the pico-second time scale. In this contribution we present a series of neutron scattering spectra of hemoglobin and beta-casein as a function of pressure. For this project we have built a new scattering cell with high transmission, which can sustain pressures up to 2000 bar. Dynamic changes as a result of water reorganisation and subunit dissociation will be discussed.

BP 26.3 Thu 17:00 Poster A

Effective Connectivity profile: A Structural Representation that Evidences the Relationship between Protein Structures and Sequences — Ugo Bastolla[1], Angel R. Ortiz[1], Markus Porto[2], and •Florian Teichert[2] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 6-8, 64289 Darmstadt, Germany — [2]Centro de Biología Molecular "Severo Ochoa", (CSIC-UAM), Cantoblanco, 28049 Madrid, Spain

We recently defined the vectorial Effective Connectivity profile (EC) to describe protein structures [1] which is highly correlated with the average hydrophobicity profile (HP) of simulated proteins with stable native structure. We showed analytically that the optimally stable HP belongs to a family of profiles that we call the Generalized Effective Connectivity family (GEC), of which the EC is a distinctive member, as well as the previously defined revised PE profile [2]. This mathematical relationship unveils the close relationship between different vectorial representations derived from structural and from sequence data, as we could demonstrate. Finally, we show that structurally similar proteins have similar EC profiles, a property that we exploit to perform protein structure alignments [3].

[1] U. Bastolla, A.R. Ortíz, M. Porto, and F. Teichert, (submitted).
[2] F. Teichert and M. Porto, Eur. Phys. J. B **54**, 131-136 (2006).
[3] F. Teichert, U. Bastolla, and M. Porto, BMC Bioinformatics **8**, 425 (2007).

BP 26.4 Thu 17:00 Poster A

SABERTOOTH: Protein Structural Alignment Based on a Vectorial Structure Representation — •Florian Teichert[1], Ugo Bastolla[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Hochschulstr. 6-8, 64289 Darmstadt, Germany — [2]Centro de Biología Molecular "Severo Ochoa", (CSIC-UAM), Cantoblanco, 28049 Madrid, Spain

The task of computing highly accurate structural alignments of proteins in very short computation time is still challenging. We tackle this issue that arises mostly from the complexity of protein structures by representing a protein fold's topology in the form of a vectorial profile [1,2], consisting of only one real number per amino acid. Doing so, the alignment of spatial structures is carried out by maximizing the overlap of profile vectors. This simplification results in favourable scaling of computation time with chain length in comparison with other algorithms while we achieve an accuracy that is comparable to established alignment tools, like Dali, as we have shown [3]. The algorithm discussed is implemented in the 'SABERTOOTH' alignment server, freely accessible at `http://www.fkp.tu-darmstadt.de/sabertooth/`.

[1] F. Teichert and M. Porto, Eur. Phys. J. B **54**, 131-136 (2006).
[2] U. Bastolla, A.R. Ortíz, M. Porto, and F. Teichert, (submitted).
[3] F. Teichert, U. Bastolla, and M. Porto, BMC Bioinformatics **8**, 425 (2007).

BP 26.5 Thu 17:00 Poster A

Kinetic clustering analysis of protein (un)folding trajectories from molecular dynamics simulation — •Lothar Reich and Thomas R. Weikl — Max-Planck-Institute of Colloids and Surfaces, Wissenschaftspark Golm, 14424

Small fast-folding proteins reach their folded state within microseconds. In the past years, the folding dynamics of these proteins has become accessible by molecular dynamics (MD) simulations. Central questions are: Which partially folded or metastable states dominate the folding/unfolding process, and can we describe the folding/unfolding process on a network of such states? We have performed extensive MD simulations of the Pin WW Domain, a fast-folding three-stranded beta-sheet protein, and have analyzed the folding/unfolding trajectories with a novel kinetic clustering method, the Perron-Cluster-Cluster analysis (PCCA). Our analysis reveals a complex network of metastable states.

BP 26.6 Thu 17:00 Poster A

Stretching of a DNA/HU-protein complex in SMD simulations — •Carsten Olbrich and Ulrich Kleinekathöfer — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

The protein HU is a member of a family of prokaryotic proteins that interact with the DNA in a non-specific way [1]. Its major function is the binding, compaction and stabilization of DNA. We applied steered molecular dynamic (SMD) simulations to DNA which is bound to a HU protein. Using these all-atom simulations including explicit water and about 80 000 atoms in total, we are able to gain insight into the discrete disruptions events which occur when the DNA releases from the protein body. These disruptions were first observed in experiments performed with optical tweezers [2].

[1] R. Dame and N. Goosen, FEBS Lett. **529**, 151 (2006).
[2] M. Salomo, F. Kremer et al., J. Mol. Biol. **359**, 769 (2006).

BP 26.7 Thu 17:00 Poster A

Restrained Protein Folding Dynamics in the Tube Model — •Katrin Wolff[1], Michele Vendruscolo[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Department of Chemistry, University of Cambridge, UK

The study of protein folding dynamics through all-atom molecular dynamics requires significant computational efforts, and coarse-grained models are therefore of great interest. Here, we use the tube model [1], which has been shown to be computationally very effective in reproducing the folding behaviour of proteins [1,2,3]. In order to drive the folding dynamics towards a specific protein structure, we augment

the energy function with a term based on a structural profile. For single-domain proteins, this structural profile has been shown to contain sufficient information to reconstruct the contact map of the target structure [4]. When directly applied to folding, the use of the structural profile is conceptually very different from the use of the contact map, since the latter would result in a Gō-type model. By contrast, the structural profile entries contain global information about the protein structure rendering this approach similar to the actual protein folding process [5]. We show that by adopting this strategy we are able to fold several small to medium-size single-domain proteins.

[1] T.X. Hoang *et al.*, Proc. Natl. Acad. Sci. USA **101**, 7960 (2004).
[2] T.X. Hoang *et al.*, Proc. Natl. Acad. Sci. USA **103**, 6883 (2006).
[3] S. Auer *et al.*, Phys. Rev. Lett. **99**, 178104 (2007).
[4] M. Porto *et al.*, Phys. Rev. Lett. **92**, 218101 (2004).
[5] K. Wolff, M. Vendruscolo, and M. Porto, submitted.

BP 26.8 Thu 17:00 Poster A

Proteins under extreme conditions - new SAXS setup at beamline BL9 of DELTA synchrotron — •Christina Krywka[1], Christian Sternemann[1], Roland Winter[2], and Metin Tolan[1] — [1]Fachbereich Physik, Universität Dortmund, D-44221 Dortmund, Germany — [2]Fachbereich Physikalische Chemie, Universität Dortmund, D-44221 Dortmund, Germany

The biological activity and the chemical properties of proteins depend on the structure of the solvent and its thermodynamic parameters. Understanding the effects of cosolvents on the structure and dynamics of proteins is crucial for a deeper insight into protein stability, folding, aggregation and fibrillation processes. The latter play an important role in many conformational diseases, such as Alzheimer, Creutzfeldt-Jakob, and Parkinson. Recently, we could show that these fibrillation processes are strongly influenced by the type and concentration of cosolvents. In order to determine the effects of different types of cosolvents on the native and unfolded states of the model protein Staphylococcal Nuclease (SNase) we have performed Small-Angle-X-ray-Scattering (SAXS) measurements at temperature and pressure conditions where unfolding of the protein sets in. The experimental equipment which had to be developed in the course of the ongoing project comprises of a high-pressure, temperature controlled sample cell with the ability to perform SAXS-measurements at pressures up to 7 kbar in a wide temperature range (-15°C to 80°C). This contribution will provide an outline of recent high-pressure data of SNase and the experimental setup installed at the multi-purpose beamline BL9.

BP 26.9 Thu 17:00 Poster A

(Structure-) Mechanical properties of nanocoposite silk and wood at macro and molecular scales. — •Igor Krasnov[1], Imke Diddens[1], Tomasz Pazera[1], Sergio S. Funari[2], Richard Davies[3], Manfred Burghammer[3], and Martin Müller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel — [2]Hasylab at Dasy, Hamburg — [3]ESRF, Grenoble, France

Using an in situ combination of tensile tests and X*ray fiber diffraction, we have directly determined the mechanical roperties of both the crystalline and the disordered phase of the biological nanocomposite silk and wood.

The measurements at single fibers and bundels was done in controlled enviromental conditions such as temperature and humidity. We have adapted a model from linear viscoelastic theory, which fully accounts for the semicrystalline orphology of studying materials. The viscoelastic parameters (modulus, viscosity, relaxation times) were determined at a wide range of time scales.

The observed interplay of morphology, mechanical and enviromental properties will have strong impact on the design of novel high*performance nanocomposite fibers.

BP 26.10 Thu 17:00 Poster A

Mechanical properties of Wood investigated using X-Ray Scattering under defined humidity conditions — •Tomasz Pazera[1], Igor Krasnov[1], Imke Diddens[1], Florian Kunze[1], Henning Vogt[1], Richard Davies[3], Manfred Burghammer[3], Sergio S. Funari[2], and Martin Müller[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]HASYLAB at DESY, Hamburg — [3]ESRF, Grenoble, France

Wood is a composite material that mainly consists of stiff cellulose crystals surrounded by a softer, water adsorbing matrix. The mechanical properties of pine earlywood have been studied in combined X-ray diffraction and stretching experiments at defined humidity conditions. We observed explicit variations in both the crystal strain and the stress-strain curves of wood. The most radical discrepancy in the behaviour of the whole wood-fibre was estimated to happen between 85%-100% relative humidity. In this range, the matrix shows strong macerating effects. By stretching in direction of the fibre axis we received information about changes in the correlation of crystal strain and force transfer inside the fibre at different humidities. Furthermore, an investigation of single fibres shows explicit changes in the orientation of the microfibrils in the cell wall.

BP 26.11 Thu 17:00 Poster A

Nanotomography of Biomaterials — •Stephanie Röper[1], Christian Zeitz[2], Christian Dietz[1], Nadine Drechsel[1], Anke Bernstein[3], Nicolaus Rehse[1], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [2]Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken — [3]Experimentelle Orthopädie, Martin-Luther-Universität Halle-Wittenberg, D-06097 Halle/Saale

Biomaterials such as bone and teeth are nanocomposites of proteins and minerals. At the molecular length scale these materials have a stiff inorganic component (hydroxylapatite) that reinforces the soft organic matrix (type I collagen) through a recurring structural motif. To gather information of the nanometer scaled structure of these materials we use nanotomography. For this scanning probe microscopy (SPM) based method the specimen is ablated layer-by-layer by wet chemical etching and imaged with tapping mode SPM after each etching step. In our experiments we focus on cortical human bone (embedded and native) and human teeth. The stepwise etching is done in-situ in the SPM with an automated setup. We will present our latest volume images of human bone and teeth and discuss new concepts for adjusting the imaging parameters to maintain a good imaging quality.

BP 26.12 Thu 17:00 Poster A

The influence of pH and temperature on the self-assembly of amelogenin and its relevance for the biomineralization of enamel — •C. Gilow[1], B. Aichmayer[1], F.B. Wiedemann-Bidlack[2], H.C. Margolis[2], and P. Fratzl[1] — [1]Max Planck Institute of Colloids and Interfaces, D-14424 Potsdam, Germany — [2]The Forsyth Institute, Boston, MA 02115-3782, USA

In the early stages of dental enamel formation, amelogenin is the most abundant matrix protein. The self-assembly of amelogenin to so-called "nanospheres" is believed to control the growth and alignment of hydroxyapatite crystals in the developing enamel tissue. Previous studies [1] on the formation of these "nanospheres" and their subsequent temperature-induced aggregation showed that the interaction between the "nanospheres" is controlled by the hydrophilic C-terminus of the protein. Further studies by Wiedemann-Bidlack et al. [2] revealed that the pH-value is the dominant parameter which regulates the higher-order assembly of amelogenins. In the current study measurements with small-angle X-ray and neutron scattering techniques are used to elucidate the structure of these protein agglomerates, which - in spite of their commonly used name were found to strongly deviate from a spherical shape. Through a systematic study of the effects of temperature and pH as well as a more detailed characterisation of the shape of the "nanospheres" we hope to get a clearer understanding of the processes involved in the mineralization of dental enamel.

1.Aichmayer, B., et al., J Struct Biol, 2005. 151: 239.
2.Wiedemann-Bidlack, F.B., et al., J Struct Biol, 2007. 160: 57.

BP 26.13 Thu 17:00 Poster A

2-Photon laser scanning microscopy of cartilage materials — •Thorsten Bergmann[1], Jörg Martini[1], Maik Tiemann[1], Michael Dickob[2], Ronald Schade[3], Klaus Liefeith[2], Katja Tönsing[1], and Dario Anselmetti[1] — [1]Bielefeld University, Exp. BioPhysics & Appl. NanoSc., Bielefeld, Germany — [2]Orthopedic Surgery, Bielefeld, Germany — [3]IBA e.V., Department of Biomaterials, Heilbad Heiligenstadt, Germany

2-photon laser scanning microscopy (2PLSM) is a powerful tool for label-free investigation of living cells and strongly scattering tissue samples. In our experiments, strongly scattering native hyaline cartilage has been imaged with this technique using multifocal 2PLSM and analyzed in descanned and non-descanned detection mode. Intensity, wavelength and fluorescence lifetime sensitive detection methods were used for imaging the autofluorescence of the extracellular matrix (ECM) as well as the chondrocytes, the only cells within this tissue. Spectral and lifetime separation of chondrocytes from the ECM allow to quantify the chondrocyte density. The intensity and the structural differences of the detected fluorescence signal from the ECM can be

used for differentiation of arthritic and non-arthritic cartilage. Additionally, results of an investigation of collagen scaffolding materials and a comparison concerning chondrocyte density will be discussed.

[1] J. Martini, K. Tönsing, M. Dickob, D. Anselmetti: Proc. of SPIE, 5860: 16-21, 2005 [2] J. Martini, K. Tönsing, M. Dickob, R. Schade, K. Liefeith, D. Anselmetti: Proc. of SPIE, 6089: 274-282, 2006 [3] J. Martini, K. Tönsing, D. Anselmetti: BIOspektrum 5, 489-492, 2006

BP 26.14 Thu 17:00 Poster A

Magnetic Relaxation Dispersions of Biomolecules: Effects of Field-Cycling — •Talea Köchling, Konstantin Ivanov, Sergey Korchak, Alexandra Yurkovskaya, and Hans-Martin Vieth — Institute für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

The dynamics of biomolecules is reflected in the spin-lattice relaxation times T1 of individual nuclei. From the change of T1 at variation of the external magnetic field intramolecular mobility can be determined. Combining a field-cycling unit, which shuttles the NMR probe along the bore axis of the spectrometer cyromagnet, with high resolution NMR spectroscopy we are able to measure T1 of individual nuclei between 1 uT and 7 T. Our experiments show that such relaxation dispersion is strongly affected by scalar couplings among the spins. Spins having substantially different T1 at high field relax at low field with a common T1 due to strong coupling. Furthermore peaks or dips are seen at fields corresponding to crossings of spin levels. An adequate theoretical approach to modelling the dispersion curve and extracting motional parameters is presented and experiments on amino acids and peptides (for example, tyrosine and enkephalin) are discussed. It shows that for proper interpretation of relaxation dispersion curves scalar couplings must be taken into account as long as $1/J<T1$.

BP 26.15 Thu 17:00 Poster A

Biological NMR Spectroscopy: Hyperpolarization at Variable Field — •Sergey Korchak, Konstantin Ivanov, Talea Köchling, Alexandra Yurkovskaya, and Hans-Martin Vieth — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

For optimization of nuclear spin hyperpolarization and its transfer to target spins of choice field-cycling schemes have been devised that make use of scalar spin-spin interaction J in the strong coupling regime. A field-cycling unit is described shuttling the NMR probe along the bore axis of the spectrometer cryomagnet and allowing field variation between 1 uT and 7 T combined with high resolution detection. By incrementing spin evolution times an oscillatory exchange of polarization between spins is observable allowing efficient manipulation of polarization flow. We studied coherent transfer of chemically induced dynamic nuclear polarization (CIDNP) in the amino acids histidine, tyrosine and tryptophan and observed well-pronounced quantum beats in their transfer kinetics indicating the coherent nature of the process. In the field dependence of the CIDNP transfer efficiency features such as peaks and dips were found corresponding to anti-crossings of the nuclear spin levels in the molecule. In experiments performed at very low field (about 1 uT) where hetero-nuclei become strongly coupled coherent CIDNP transfer between protons and fluorine atoms was found. An adequate theoretical approach to the phenomena studied was developed. This work was supported by the EU (Bio-DNP grant # 011721 and IFF # 22008) and INTAS (grant # 05-1000008-807).

BP 26.16 Thu 17:00 Poster A

LED illumination for video-enhanced DIC imaging of single — •Volker Bormuth[1], Jonathon Howared[1], and Erik Schäffer[2] — [1]Max Planck Institute for Molecular Cell Biology and Genetics, Pfotenhauerstr.108, 01307 Dresde — [2]Biotechnology Center (BIOTEC), Tatzberg 47-51, 01307 Dresden

In many applications high-resolution video-enhanced differential interference contrast microscopy is used to visualize and track the ends of single microtubules. We show that single ultrabright light emitting diodes from Luxeon can be used to replace conventional light sources for these kinds of applications without loss of function. We measured the signal-to-noise ratio of microtubules imaged with three different light emitting diode colours (blue, red, green). The blue light emitting diode performed best, and the signal-to-noise ratios were high enough to automatically track the ends of dynamic microtubules. Light emitting diodes as light sources for video-enhanced differential interference contrast microscopy are high performing, low-cost and easy to align alternatives to existing illumination solutions.

BP 26.17 Thu 17:00 Poster A

Coherent anti-Stokes Raman scattering (CARS) microscopy - a means to visualize molecular distribution in complex, biological samples — •susana chatzipapadopoulos[1], denis akimov[2], michael schmitt[1,2], and jürgen popp[1,2] — [1]Institute of Photonic Technology, Jena, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University of Jena, Germany

Coherent anti-Stokes Raman scattering (CARS) microscopy is a non linear Raman mapping technique which provides vibrational contrast with high chemical selectivity and high 3D sectioning capability. CARS is applied to complex, biological samples in order to visualize the molecular distribution of various types of molecules with high efficiency, high chemical selectivity and low acquisition times without the need of staining. Unfortunately the CARS signal is not background free and also is derived from the bulk media. In order to develop techniques to yield pure molecular contrast we analyze different, non-linear and linear contrast mechanisms contributing to the CARS image.

BP 26.18 Thu 17:00 Poster A

Mechanically actuated silicon microgrippers for micromanipulation of biological matter — •Marius M. Blideran[1], Jochen Sterr[2], Stephan Kleindiek[2], Matthias G. Langer[3,4], Francois Grauvogel[3], Monika Fleischer[1], and Dieter P. Kern[1] — [1]University of Tübingen, Institute of Applied Physics, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Kleindiek Nanotechnik GmbH, Aspenhaustrasse 25, 72770 Reutlingen, Germany — [3]Department of Applied Physiology, University of Ulm, 89081 Ulm, Germany — [4]Carl Zeiss NTS GmbH, 73447 Oberkochen, Germany

Controlled gripping during the manipulation of objects is widely desired in the fields of microbiology and microassembly. Therefore it is important, especially when targeting biological structures to measure or calculate the forces exerted by the end segment of the manipulator. This way one would know exactly when the object under investigation is grabbed and what pressures are applied to it. Moreover, for handling objects only micrometers in size, microgrippers or tweezers with fine end-segments are required. On the other hand the manipulator has to be attached to a motor or actuator, which implies that the gripper has to be millimeters in size at its other end. The mechanical assembly of the gripper and the actuator proves to be a crucial step in realizing the system. This work presents solutions to the two challenges mentioned above: a method for determining the gripping forces combining experimental with simulation results, and a procedure for the secure construction of our micromanipulator. Finally results from tests of the system on micrometer-sized objects will be shown.

BP 26.19 Thu 17:00 Poster A

Carbon Coated Nanomagnets for Biomedical Applications — •A.U.B. Wolter[1], Y. Krupskaya[1], C. Mahn[1], S. Hampel[1], D. Haase[1], A. Leonhardt[1], A. Vyalikh[1], A. Werner[2], A. Taylor[2], K. Krämer[2], B. Büchner[1], and R. Klingeler[1] — [1]Leibniz Institute for Solid State Research, IFW Dresden, 01069 Dresden, Germany — [2]Universitätsklinikum Carl Gustav Carus, 01307 Dresden, Germany

There is a rapidly increasing interest in applying carbon nanotubes (CNT) in biomedicine since they can be filled with tailored material, thereby acting as chemically and mechanically stable nanocontainers. Furthermore, the carbon shells enhance the possibilities for exohedral functionalization, this way targeting e.g. pathological tissue. We report on a systematic approach to exploit the potential of filled CNT to act as magnetic nano-heaters, temperature sensors and contrast agents which allow a diagnostic and therapeutic usage on a cellular level. Here, we present a detailed field and frequency dependent study of different concentrations of Fe-filled CNT suspensions, which imply their potential for magnetic nano-heaters in a hyperthermia cancer treatment. Indeed, there is a substantial temperature increase of Fe-CNT under applied AC magnetic fields. Furthermore, filled CNT can also be used for diagnostic purposes such as contrast agents in MRI or for the simultaneous detection of the resulting temperature increase, since the nanocontainers can be filled with (additional) appropriate sensor materials. An example is their filling with copper or silver halides, which exhibit a strongly temperature dependent NMR signal so that nanoscaled contactless temperature sensors are realised.

BP 26.20 Thu 17:00 Poster A

A robust surface plasmon resonance biosensor with high resolution — •Sebastian Horstmeier, Andy Sischka, Christoph Pelargus, Katja Tönsing, and Dario Anselmetti — Experimentelle Biophysik und Angewandte Nanowissenschaft, Fakultät für

Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld

We present a simple, robust and easy to use surface plasmon resonance (SPR) biosensor with high resolution which is based on a previous study [1] and can be used in biophysical applications as well as for educational purposes, e.g. practical courses. SPR-based biosensors are able to investigate biochemical reactions according to their kinetics without labeling the molecules. Using the Kretschmann-Raether-configuration the SPR-angular shifts are detected by a method based on a quadrant photo diode like in atomic force microscopy (AFM). The goldfilm is divided into two areas, one for reference measurement, the other for analysing the specific binding-reaction. SPR-angular changes due to the bulk solution as well as errors caused by thermal drift, mechanical stress or fluctuations of the laser are eliminated by the reference measurement which is made parallel under the same conditions. Using this method changes of the refractive index in the order 10^{-8} refractive index units (RIU) can be measured. The experimental setup and first results will be presented and discussed.

[1] H.Q. Zhang, S. Boussaad and N.J. Tao: *High-performance differential surface plasmon resonance sensor using quadrant cell photodetector*, Review of Scientific Instruments, **74**(1):150-153, 2002

BP 26.21 Thu 17:00 Poster A

Magnetic Properties of Iron Nanowires Encapsulated in Carbon Nanotubes — •K. Lipert[1], M. Lutz[1], T. Mühl[1], K. Krämer[2], A. Taylor[2], R. Klingeler[1], and B. Büchner[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, PF 270116, D-01171 Dresden, Germany — [2]Universitätsklinikum der Technischen Universität Dresden, Fetscherstraße 74, D-01307 Dresden, Germany

Introducing nanomagnets into carbon shells provides a promising route to synthesize novel magnetic nanoparticles with well defined geometrical dimensions. Carbon shells provide wear resistance and oxidation protection, can stabilize novel magnetic molecules and enhance possibilities for exohedral functionalisation. Here, we report on a systematic approach to study magnetic nanoparticles encapsulated in carbon nanotubes and nanospheres which are exploited for an application in biomedicine, i.e. as contrast agents or for hyperthermia cancer treatment. We present thorough magnetic and structural studies on ensembles and on individual particles. The ensemble studies are done both inside and outside biological systems. XRD patterns and TEM pictures are shown along with hysteresis loops measured at carbon nanotubes inside cancer cells as well as grown on silicon oxide substrates. Magnetic studies of individual Fe filled CNTs performed by means of the MFM technique and the micro hall magnetometry setup based on a GaAs nanoscaled Hall-cross are presented which provide an insight into the magnetisation reversal.

BP 26.22 Thu 17:00 Poster A

Two-focus fluorescence correlation spectroscopy with an EM-CCD detector — •Markus Burkhardt, Jonas Ries, and Petra Schwille — Biophysics/ BIOTEC/ TU Dresden, Tatzberg 47-51, 01307 Dresden, Germany

Fluorescence Correlation Spectroscopy (FCS) extracts thermodynamic and kinetic parameters from time dependent fluorescence intensity fluctuations of labeled biomolecules in solution. In a standard FCS setup, the fluorescence signal is collected from one specific focus position and detected by a single photon sensitive point detector. Two-focus FCS is based on the information from two spatially fixed laser foci. It enhances the precision of diffusion coefficient determination by evaluating the spatial cross-correlation.

Spatially resolved detection, employing an electron multiplying CCD (EMCCD) camera, is a versatile method perfectly suited for two-focus FCS measurements. The distances between the two laterally shifted focal volumes can be changed easily and they can be determined accurately by imaging a microscopic ruling.

We demonstrate two-focus FCS measurements for different fluorescent molecules and under various measurement conditions.

BP 26.23 Thu 17:00 Poster A

Searching the proper Model for F_1-ATPase rotation — •Florian Werz[1], Alexander Kovalev[1], Nawid Zarrabi[1], Carsten Tietz[1], Michael Börsch[1], Dirk Bald[2], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, Germany — [2]Department of Structural Biology, Vrije Universiteit Amsterdam, Netherlands

The F-type ATP-Synthase is a composed rotary motor enzyme in the plasmamembrane of prokaryotes and in the inner membrane of mitochondria of eukaryotes, respectively, producing the universal fuel ATP, which is used to sustain nearly every chemical reaction in cells. The F_1-part of the enzyme can work in reverse hydrolyzing ATP and rotating backwards showing 120° steps resulting from the threefold symmetry of its $\alpha_3\beta_3$-stator-complex. We recorded trajectories up to half an hour with high time resolution (down to $\Delta = 1$ms) of Polystyrol beads attached to the rotating γ-subunit of single F_1-ATPase using wide field microscopy. We recorded the same molecule for different concentrations of ATP and ADP and therefore different rotational speeds. Analyzing data by hidden Markov models (HMM) we found to reproduce dwell time histograms a model with three or more consecutive states per visible state was required. Introduction of an additional state corresponding to the ADP-inhibited state, which stops rotation of F_1-ATPase for relative long times (up to minutes), significantly improved the fit.

BP 26.24 Thu 17:00 Poster A

Interferometric detection of nanosize diamond particles — •Thomas Wolf, Steffen Steinert, Carsten Tietz, Fedor Jelezko, and Jörg Wrachtrup — 3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

In recent years nanodiamonds have become available with well defined size distributions. It is possible to functionalize these diamonds with many different chemical groups to achieve biocompatibility and use them as markers. Aim of this work is to show the sensitivity of detecting scattering of these diamonds. We use a confocal setup combined with an interferometric detection scheme. The backscattered light of the sample passes the pinhole and is then recombined with the reference beam on our detector, thus yielding an interference pattern. As detector we use a splitted Si-diode to measure the difference signal. In this way it is possible to detect shifts in this interference pattern due to the light scattering of the diamonds. Using such a setup allows the detection of 50nm polystyrene or 10nm gold beads. The high refractive index of diamond should render it possible to detect diamonds down to a size of 10nm. Detecting this size would mean a step towards using nanodiamonds as non-toxic, non-bleaching biological markers.

BP 26.25 Thu 17:00 Poster A

Dynamic Force Spectroscopy studies of native and synthetic point mutated transcription regulators — •Andre Körnig[1], Katrin Wollschläger[2], Norbert Sewald[2], Dario Anselmetti[1], and Robert Ros[1] — [1]Experimental Biophysics and Applied Nanoscience, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld — [2]Bioorganic Chemistry, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld

For many aspects of cellular regulation the specific interaction between proteins and DNA is fundamental. Especially the recognition of specific DNA target sequences by transcription regulators is a central issue for the regulation of gene expression. We are using atomic force microscope (AFM) based force spectroscopy to investigate the molecular mechanism of the interaction of the transcription regulator PhoB with DNA target sequences on a single molecule level. In order to investigate the contribution of single amino acids to the specificity and strength of the binding as well as the role of the protein environment we compare the wild type protein with point mutants and peptides representing the PhoB recognition helix. This allows a quantitative analysis of the dissociation rates of those complexes and gives insights into the energy landscape of the respective interaction.

BP 26.26 Thu 17:00 Poster A

Quantitative Optical Tweezers for Single Molecule Manipulations in 3D — •Andy Sischka, Christoph Kleimann, Katja Tönsing, and Dario Anselmetti — Experimentelle Biophysik & Angewandte Nanowissenschaft, Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielelfeld

We introduce a novel way of measuring minute forces and manipulate single molecules like DNA by means of a quantitative optical tweezers system that is operated in reflection mode using a single laser beam [1].

Our optical setup is based on a compact, stable optical tweezers configuration (2D) that is compatible with an inverted optical microscope (Zeiss Axiovert) [2] and was modified in order to allow quantitative analysis and molecular manipulation in three dimensions (3D) with remarkably high precision.

The optical setup was tested by manipulating individual λ-DNA molecules in the vicinity of a nanopore similar to a previous study [3], and allowed quantitative single molecule experiments with mini-

mal optical interference, and insights into the threading dynamics of DNA into a nanopore.

[1] A. Sischka et al., Rev. Sci. Instrum., submitted, 2008.
[2] A. Sischka et al., Rev. Sci. Instrum. 74, 4827, 2003.
[3] U.F. Keyser et al. Nature Phys 2, 473, 2006.

BP 26.27 Thu 17:00 Poster A

Single-molecule Spectroscopy on Phytochromes — •Jana B Nieder, Marc Brecht, and Robert Bittl — Fachbereich Physik, Freie Universität Berlin, Arnimalle 14, 14195 Berlin, Germany

Phytochromes are red light sensitive photoreceptors controlling flowering, shade avoidance and germination in plants. Their cofactor biliverdin is a linear tetrapyrroles whos conformation is strongly affected by the protein environment. The tight binding by the protein surrounding is the basis for the metastable PR and PFR conformational states. The switching between these isomeric states is reversibly triggered by Red and Far Red light.

Physical properties of the interaction between the pigment and its protein surrounding are accessible by single-molecule spectroscopy at low temperatures . Under low temperature conditions major protein rearrangements are inhibited and the phytochromes are trapped in the dark stable state (here PR). The fluorescence emission of single Agp1 molecules (phytochrome from Agrobacterium tumefaciens) shows marked time dependence. The pigment-protein interaction causes intensity and spectral changes. This spectral fine-tuning is observed by comparison of signals from different molecules and within time-dependent spectra of individual Agp1 molecules. For some of the analysed Agp1 molecules narrow lines in the vibronic energy range could be resolved. The spectral fine-tuning affects all vibrational lines simultaneously. For these molecules the vibrational energies can directly be extracted. In this work detection of vibrational information of single chromophores in their natural protein environment is achieved.

BP 26.28 Thu 17:00 Poster A

Cantilever Based Apertureless Scanning Near-Field Optical Microscopy in Aqueous Solution — •Jan Paskarbeit, Heinrich Frey, Christoph Pelargus, Robert Ros, and Dario Anselmetti — Experimental Biophysics & Applied Nanosciences, Department of Physics, Bielefeld University, Germany

Scanning near-field optical microscopy strives for the highest optical resolution, far beyond the classical diffraction limit of Abbé, and simultaneously provides topographical information. In conventional fluorescence SNOM a metallised glass fibre with an aperture of about 50nm is used to illuminate the sample locally. The main drawbacks are, dependent on the size of the aperture, either reduced light throuput or low optical resolution. We presented already a cantilever based setup, in which the tip of an aluminium or silver coated full body glass tip is used as illumination in air and which could be operated at an optical resolution of 15nm on individual fluorescent dye molecules [1]. Especially for applications in life sciences the operation in aqueous solution is essential. In addition to our recent numerical simulations, we present results of gold, silver and aluminium coated glass tips for SNOM operations in liquids with respect of SNOM performance and stability.

[1] Frey, H. G., C. Bolwien, A. Brandenburg, R. Ros und D. Anselmetti: Optimized apertureless optical near-field probes with 15 nm optical resolution. Nanotechnology, 17(13):3105*3110, 2006.

BP 26.29 Thu 17:00 Poster A

Scanning FCS applied to precise measurement of diffusion coefficients — •Susan Derenko, Zdeněk Petrášek, and Petra Schwille — Biophysics Group, Biotechnologisches Zentrum, TU Dresden, Germany

Although fluorescence correlation spectroscopy (FCS) is a useful technique to obtain diffusion coefficients of fluorescent molecules in solution, the precision of the measurement is limited due to difficulties in the determination of the fixed volume size in standard FCS. In order to avoid the reference to the inaccurate volume size, the beam is scanned in a circle with either two galvanometer scanners or a 2-axis piezo scanner. The diffusion coefficent is then related to the scan radius R and the scanning freqency using the spatial cross-correlated signal. The radius needs to be calibrated carefully and is therefore the most important value for the calculation of the diffusion coefficient D.

To test the applicability of the new approach, several dyes were tested under two-photon excitation, and the important parameters, mainly radius and frequency, were optimized. The method is being extended to one-photon excitation, where triplet-effects of the fluorescent molecules have to be considered. Further, operation under non-ideal conditions and in biological samples will be investigated.

BP 26.30 Thu 17:00 Poster A

Single molecule microscopy using total internal reflection — •Andreas Veenendaal, Jan Peter Siebrasse, Constanze Husche, and Ulrich Kubitscheck — Institute of Physical and Theoretical Chemistry, Bonn, Germany

In single molecule fluorescence microscopy one often wants to reduce the fluorescence background emitted by fluorophores not located in the plane of interest. With total internal reflection fluorescence (TIRF) microscopy this is achieved by reflecting the light at the coverslip/probe interface (coverslip (glass) n = 1.51; sample (e.g. cell) n = 1.33), and thus generating an evanescent wave illuminating the sample. The intensity of the evanescent wave decays exponentially with a penetration depth of roughly half the wavelength of the incident light. We realised objective type TIRF using an NA 1.45 objective from Zeiss. Using this technique we characterized several red fluorescent dyes attached to the surface by a PEG-biotin-streptavidin system at the single molecule level. As a first biological application we studied the transport dynamics of single nuclear pore complexes.

BP 26.31 Thu 17:00 Poster A

Coated particles as enhanced probes for optical tweezers — •Anita Jannasch[1], Volker Bormuth[1], Jonathon Howard[1], and Erik Schäffer[2] — [1]MPI of Molecular Cell Biology and Genetics Dresden — [2]BIOTEC Dresden

In an optical trap, micron-sized dielectric particles in aqueous solutions can be held by a tightly focused laser beam. The optical force on the particle is composed of an attractive gradient force in the direction of highest light intensity, and a scattering force in the light propagation direction, that pushes the particle away from the focus and thereby weakens the trap. To optimize the trapping potential, we reduce the scattering force by using coated microspheres. The shell of the particle is designed such that it acts as an anti-reflection coating. We characterized such particles and found in comparison with the same-sized uniform microspheres a more than two-fold strengthening of the trap. By improving the trapping potential higher overall forces can be achieved with the same laser power, or vice versa the same force can be reached by using less laser power. A higher maximal force increases the range of possible experiments, and a reduced laser intensity leads to less photo-toxic interactions relevant for biological applications, like in vivo cell measurements.

BP 26.32 Thu 17:00 Poster A

Live imaging of signalling complexes using pulsed dual-colour microscopy — •Steffen Steinert[1], Felix Neugart[1], Andrea Zappe[1], Lutz Graeve[2], Carsten Tietz[1], and Jörg Wrachtrup[1] — [1]University Stuttgart — [2]University Hohenheim

Communication between cells is mediated via messenger molecules which bind to a receptor that eventually induces oligomerisation with other molecules and transduce a certain signal. The CNTF receptor is a GPI-anchored protein involved in many signalling pathways which control apoptosis, differentiation and other key cellular functions. In order to gain information about the characteristics of the CNTF receptor at the membrane as well as its internal trafficking, colocalisation analysis with other distinct markers is required. For that purpose we set up a widefield and confocal microscope with pulsed dual-colour excitation which enables us to track two different proteins without crosstalk between the fluorophores. The high sensitivity and adjustable temporal resolution in ms-range of the widefield system facilitates a rapid image acquisition even on single-molecule level. Due to the simultaneous detection of the emission of both fluorophores, FRET signals are detected automatically. FCCS is used to study potential interactions at almost native protein concentrations. It was shown that gp130, an important glycoprotein which is known to associate with CNTF-receptor upon stimulation, and CNTF receptor have comparable diffusion constants in the range of 10-9cm*/s. However, FCCS revealed that both proteins are not pre-associated in the membrane, but both become part of the signalling complex after stimulation.

BP 26.33 Thu 17:00 Poster A

1D diffusion model for inter-site communication by Type III restriction enzymes — •Subramanian Ramanathan[1], Kara van Aelst[2], Mark D. Szczelkun[2], and Ralf Seidel[1] — [1]Biotechnology Center, Dresden University of Technology, Germany — [2]Department of Biochemistry, University of Bristol, UK

Type III restriction enzymes use ATP hydrolysis to communicate between distant target sites on DNA, which subsequently triggers DNA cleavage. Due to amino acid sequence similarities these enzymes belong to the superfamily 2 of helicases. They are therefore generally believed to be molecular motors that directionally translocate DNA in order to communicate between their target sites. However, the low ATPase activity of these enzymes does not support DNA translocation and alternative models involving passive diffusive looping have been suggested. In order to gain insight into the communication mechanism of type III restriction enzymes we used magnetic tweezers to investigate DNA cleavage of multiple single molecules in parallel. This allowed us to measure the cleavage kinetics while keeping the DNA stretched. We observed rapid DNA cleavage even at the highest stretching forces, where DNA looping is completely abolished. Furthermore, the cleavage rates did not change over a large range of forces. These results provide direct evidence for a communication mechanism between the target sites in 1D, i.e. enzyme movement along the DNA contour, rather than in 3D by diffusive DNA looping. Therefore, given the low ATP consumption, we suggest diffusion rather than active translocation as being the mechanism by which the enzymes move along DNA.

BP 26.34 Thu 17:00 Poster A

Single Molecule FRET studies of RNA Polymerese II — •Joanna Andrecka[1], Robert Lewis[1], Florian Brueckner[2], Patrick Cramer[2], and Jens Michaelis[1] — [1]Department of Chemistry and Biochemistry, Ludwig-Maximilians-Universität München, Butenandtstr.11, 81377 Munich, Germany — [2]Gene Center Munich and Department of Chemistry and Biochemistry, Feodor-Lynen-Strasse 25, Ludwig-Maximilians-Universität München, 81377 Munich, Germany

Single-pair Fluorescence Resonance Energy Transfer (FRET) was used to track RNA exiting from RNA Polymerase (Pol II) in elongation complexes [1]. Measuring the distance between the RNA 5'-end and three known locations within the elongation complex allowed us to determine its position by means of triangulation. RNA leaves the polymerase active center cleft via the previously proposed exit tunnel, and then disengages from the enzyme surface. When the RNA reaches lengths of 26 and 29 nucleotides, its 5'-end associates with Pol II at the base of the dock domain. Since the initiation factor TFIIB binds to the dock domain and exit tunnel, exiting RNA may contribute to TFIIB displacement during the initiation to elongation transition and may prevent TFIIB re-association during elongation.

[1] J. Andrecka, R. Lewis, F. Brueckner, E. Lehmann, P. Cramer, J. Michaelis: Single-molecule tracking of mRNA exiting from RNA polymerase II, PNAS (accepted)

BP 26.35 Thu 17:00 Poster A

A Bayesian Approach to 3D Position Determination on the Nanometer Scale by Single-Pair FRET Experiments — •Adam Muschielok[1], Joanna Andrecka[1], Patrick Cramer[1,2], and Jens Michaelis[1] — [1]Department Chemie und Biochemie, Ludwig-Maximilians-Universität München — [2]Gene Center, Ludwig-Maximilians-Universität München

It is often desired to infer the relative position of a domain of a protein/nucleic acid complex that can't be localized by crystallographic means due to its high flexibility. Measurements of distances between two fluorescent dyes based on Fluorescence Resonant Energy Transfer (FRET) can yield this information if one dye molecule (target) is attached to the domain of interest and distance measurements to at least three other dye molecules (anchors) sitting in different but well known positions are carried out. Since the domain of interest is highly flexible, single-molecule measurements are necessary in order to understand the underlying dynamics. We present a new, Bayesian approach to analyze such experiments that is capable of inferring the target dye position and its uncertainty. Based on our measurements, we calculate the probability density distribution of the target dye position and display confidence volumes in the context of crystallographic structure. In contrast to ordinary trilateration this method is able to manage an arbitrarily large number of measurements and accounts for uncertainties in the anchor dye positions, the corresponding Förster radii and the FRET efficiency measurements itself. We apply this method to study yeast RNA polymerase II elongation complexes.

BP 26.36 Thu 17:00 Poster A

Untersuchung supramolekularer Kapseln mittels Dynamischer Einzelmolekül-Kraftspektroskopie — •Tobias Schröder[1], Björn Schnatwinkel[2], Dario Anselmetti[1] und Jochen Mattay[2] — [1]Experimentelle Biophysik, Fakultät für Physik, Universität Bielefeld, Bielefeld — [2]Organische Chemie 1, Fakultät für Chemie, Universität Bielefeld, Bielefeld

Eckel et al. zeigten erstmalig, dass die Einzelmolekül-Kraftspektroskopie zur Charakterisierung der Bindung in (photoschaltbaren) supramolekularen Wirt-Gast-Systemen genutzt werden kann.[1,2] Basierend auf diesen Experimenten werden erste Resultate der Kraftspektroskopie an supramolekularen Kapseln präsentiert und diskutiert. Durch Immobilisierung der Kapselbausteine am Cantilever und einem geeigneten Substrat können supramolekulare Kapseln mittels Dynamischer Einzelmolekül-Kraftspektroskopie untersucht werden.

[1] R. Eckel, R. Ros, B. Decker, J. Mattay, D. Anselmetti, Angew. Chem. 2005, 117, 489*492; Angew. Chem. Int. Ed. 2005, 44, 484*488. [2] C. Schäfer, R. Eckel, R. Ros, J. Mattay, D. Anselmetti, J. Am. Chem. Soc. 2007, 129, 1488*1489.

BP 26.37 Thu 17:00 Poster A

Computational studies of the visual pigment rhodopsin — •Minoru Sugihara[1,2], Peter Entel[1], and Volker Buss[2] — [1]Theoretical Low-Temperature Physics, University of Duisburg-Essen — [2]Theoretical Chemistry, University of Duisburg-Essen

Rhodopsin, the visual pigment in the vertebrate eye, is one of the prototypical G-protein-coupled receptors (GPCRs), which are responsible for signal transduction in mammalian cells. Like all membrane proteins, GPCRs are difficult to crystalize and no high-resolution structure of any GPCRs was known until 2000. There are now five structures of the rhodopsin dark state deposited with the Protein Data Bank and the resolution was extended to 2.2 angstrom [1], however it is still insufficient to unequivocally define the functionally important parts like the chromophore. In this work we address the chromophore geometries in rhodopsin and the first photo-intermediate, bathorhodopsin, by applying quantum mechanical / molecular mechanical (QM/MM) methodolgy based on the X-ray crystal structures [1,2,3]. Based on the calculated chromophore geometries, the spectral tuning mechanisms of the chromophore is discussed [2,4].

[1] Okada, T.; Sugihara, M.; Bondar, A.-N.; Elstner, M.; Entel, P.; Buss, V. J. Mol. Biol. 2004, 342, 571. [2] Schreiber, M.; Sugihara, M.; Okada, T.; Buss, V. Angew. Chem. 2006, 45, 4274. [3] Sugihara, M.; Hufen, J.; Buss, V. Biochemistry 2006, 45, 801. [4] Sekharan, S.; Sugihara, M.; Buss, V. Angew. Chem. Int. Ed. 2007, 46, 269.

BP 26.38 Thu 17:00 Poster A

Emergent vascular network inhomogeneities and resulting blood flow patterns in a growing tumor — •Michael Welter and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

We present and analyze a theoretical model for tumors growing in a host tissue that is vascularized with an arterio-venous blood vessel network. The tumor grows by coopting a massive vascular plexus which is progressively created by angiogenic sprouting. In the center, drastic vessel regression is apparent, accompanied by necrosis in unperfused regions. Few vessels survive, threading the tumor, cuffed by viable tumor cells (TCs). Via Monte-Carlo simulation, we analyze our hybrid cellular-automaton model where this behavior is realized by stochastical processes like sprouting, vessel removal, TC proliferation or TC death. Further we show current simulation results of the time-dependent distribution of drug injected into the blood stream.

BP 26.39 Thu 17:00 Poster A

Formation of Compartment Boundaries in Growing Tissues — •Jonas Ranft[1], Katharina Landsberg[2], Thomas Bittig[1], Reza Farhadi Far[1], Amani Said[2], Christian Dahmann[2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Pfotenhauerstraße 108, 01307 Dresden, Germany

During the development of living organisms, tissues grow due to cell division. As the tissues grow, sharp boundaries between different cell populations within the tissue can emerge. The position of such compartment boundaries plays an important role in the patterning of the tissue. However, the mechanisms of the formation of these boundaries remain still unclear. We developed a stochastic model to describe epithelial tissue growth. The dynamics is described by balancing potential forces with friction forces that account for tissue viscosity. The potential forces describe adhesive forces as well as elastic forces.

Our simulations show that a reduced attraction between cells of different types (which corresponds to a reduced cell-cell adhesion) can lead to the dynamic formation of a straight boundary during the growth process. This is a possible explanation of the presence of a straight interface between two cell populations with similar bulk mechanical properties.

BP 26.40 Thu 17:00 Poster A

Effect of fluctuations for the formation of spatial patterns of gene expression — •Thorsten Erdmann and Pieter Rein ten Wolde — FOM Institute for Atomic and Molecular Physics (AMOLF), Kruislaan 407, 1098 SJ Amsterdam, The Netherlands

During development of a drosophila embryo, the segmented structure of the adult body is determined by a sequentially refined pattern of gene expression domains along the anterior-posterior axis. The first zygotic genes to be expressed are the gap-genes. These are activated by the morphogen molecule bicoid and interact with each other by mutual repression or activation. The anterior-to-posterior gradient of morphogen concentration induces a stripe-pattern of domains in which one gene is predominantly expressed and the relative concentration of the corresponding protein is high. This pattern is very precise and robust against variations, e.g., in embryo length or morphogen concentration. Moreover, the domain boundaries are rather sharp although the small number of molecules makes fluctuations of protein concentration important and although small fluctuations in morphogen concentration close to the activation threshold strongly alter the expression level of a gene. We use a stochastic model for gene expression, protein diffusion and decay to investigate how domains of gene expression are positioned in space and how fluctuations affect the sharpness of their boundaries. Besides looking at a single target gene activated by the morphogen gradient we also investigate how a single morphogen gradient can control expression patterns of several, interacting genes.

BP 26.41 Thu 17:00 Poster A

A physical model for Bicoid controlled enhancers in *Drosophila* — •Wolfram Möbius[1,2] and Ulrich Gerland[2] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), LMU München — [2]Institute for Theoretical Physics, Universität zu Köln

Transcription activity of genes in eukaryotes is regulated by regions called cis-regulatory modules (CRM), in some cases located several thousands of base pairs up- or downstream of the gene of interest. While function of these CRMs, also called enhancers, has been qualitatively understood in terms of activating and repressing proteins binding to the DNA, a quantitative mapping from DNA sequence to transcription activity is still missing. In early Drosophila development, the protein Bicoid forms a concentration gradient along the embryo axis and controls various target genes which are expressed in different regions. We use this experimentally known mapping of Bicoid concentration to gene activation in vivo as well as Bicoid binding data to study correlations between Bicoid assembly at CRMs and transcription activity of the target genes.

BP 26.42 Thu 17:00 Poster A

Signal integration and stochastic decision making phosphorelay signal transduction — •Ilka Bischofs[1,2], Josh Hug[1], Aiwen Liu[1], David Lee[1], Denise Wolf[2], and Adam Arkin[1,2] — [1]University of Berkeley, USA — [2]Lawrence Berkeley Lab, Berkeley, USA

Phosphorelays are common architectures for integrating multiple signals in prokaryotic signal transduction. In B. *subtilis* a phosphorelay controls stress response induction in response to adverse environmental conditions. We investigate mechanisms of signal integration and stochastic decision making by time lapse microscopy of fluorescent reporter strains to quantify the dynamics of population heterogeneity. Through theoretical modelling we furthermore demonstrate that the complex feedback architecture found in the spo-relay confers robust signal amplification and robust integration of starvation and quorum signals.

BP 26.43 Thu 17:00 Poster A

On schemes of sequential transcription logic — •Georg Fritz[1,2] and Ulrich Gerland[1] — [1]Institute for Theoretical Physics, Universität zu Köln — [2]Department of Physics, LMU München

Many regulatory processes in molecular biology do not merely transform a set of simultaneous input conditions into an output signal, but instead yield a response that depends also on signals received in the past. For instance, such "sequential"regulatory logic is well documented in the development of multicellular organisms, where individual cells condition their phenotypic response not only on the present input signals, but also on the history of signals at the specific location in the tissue. In digital logic circuits, sequential logic elements are typically implemented by arrays of NAND-gates connected by feedback loops and comprise latches, flip-flops, and registers. Here, we explore the design characteristics of sequential regulatory logic in biology, starting with bacterial systems, where the basic molecular mechanisms for regulation are well understood. We previously showed that a specific "data-latch"may be readily implemented by cells through the use of protein heterodimerization [1]. We now use an unbiased *in silico* evolution approach to study the more general design principles of sequential transcription logic based on existing protein-protein interactions and simple transcriptional regulation.

[1] G. Fritz, N. Buchler, T. Hwa, and U. Gerland, Systems and Synthetic Biology **1**, 89-98 (2007)

BP 26.44 Thu 17:00 Poster A

Metabolic Synchronization of Yeast Cells — •Christian Warnke, Marcus J. B. Hauser, and Thomas Mair — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung Biophysik, Magdeburg, Germany

Yeast cells exhibit synchronization of their glycolytic activity when exposed to sugar. This behaviour is manifested as the appearance of oscillations in all intermediates of the glycolytiy pathway. The synchronization process is mediated via the extracellular exchange of the signalling molecule acetaldehyde, an intermediate of the glycolytic pathway. We have investigated the synchronization of yeast cells at varying extracellular acetaldehyde concentrations and at different metabolic states of the cells. We found a pronounced difference in the synchronization behaviour in response to acetaldehyde for the yeast strains Saccharomyces cerevisiae and Saccharomyces carlsbergensis. Our data indicate that these different behaviours can be explained by the different fermentative capacity of the two strains.

BP 26.45 Thu 17:00 Poster A

Simulation of protein kinase C alpha (PKCα) membrane translocation processes — •Martin Peglow and Heiko Rieger — Theoretische Physik, Universität des Saarlandes, PF 151150, D-66041 Saarbrücken

PKCα is a versatile key for decoding the cellular calcium toolkit. During their measurements of PKCα membrane translocations, which are activated through intracellular Ca^{2+} release, Reither and Lipp [1] found two populations of so called Local Translocation Events (LTEs). One population whose life times correspond to the duration of the underlaying Ca^{2+}-signals and a second population the so called long lasting LTEs ($T > 4s$). The source or appearance of the long lasting LTEs can't be explained for sure. Theoretical assumptions for possible mechanisms shall be verified by our simulations. An efficient Monte Carlo algorithm for simulations of reaction-diffusion kinetics in single cells, the "Next Subvolume Method" [2], is presented here.

[1] Dr. Gregor Reither, EMBL Heidelberg and Prof. Peter Lipp, Institut für Molekulare Zellbiologie Universität des Saarlandes, JCB, 174, 521, (2006)
[2] J. Elf, A. Doncic, M. Ehrenberg, Proceeding of SPIE, 5110, (2003)

BP 26.46 Thu 17:00 Poster A

Designing Biomolecule-Nanoparticle Interfaces for the Regulation of Cell Fate — •Lisa Maus[1], Roberto Fiammengo[1], Oliver Dick[2], Malte Wittmann[2], Hilmar Bading[2], and Joachim P. Spatz[1] — [1]Max-Planck-Institute for Metals Research, Dept. of New Materials & Biosystems & University of Heidelberg, Dept. of Biophysical Chemistry, Heisenbergstr. 3, D - 70569 Stuttgart — [2]University of Heidelberg, Interdisciplinary Center for Neurosciences, Dept. of Neurobiology, Im Neuenheimer Feld 364, D - 69120 Heidelberg

We are aiming at designing stable nanoparticles functionalized with biomolecules to study cell death pathways in primary hippocampal neurons. Due to their unique properties metal nanoparticles show great promise as drug delivery systems and intracellular contrast agents. Especially gold nanoparticles have been studied intensely, due to their high biocompatibility and well known thiol chemistry. The synthesized particles are passivated with PEG thiol derivatives to prevent aggregation in high ionic strength solutions. They are further functionalized with a peptide that is known to specifically block NMDA receptors

(N-methyl-D-aspartate) crucial for calcium influx in postsynaptic neurons. Elevated intracellular calcium levels triggered by calcium entry through synaptic NMDA receptors promote cell survival. In contrast, calcium entry through extrasynaptic NMDA receptors seems to initiate cell death cascades. This concept of differential signalling by synaptic and extrasynaptic NMDA receptors is important for the understanding of neuronal diseases such as stroke in which brain damage may be caused by activation of extrasynaptic NMDA receptors.

BP 26.47 Thu 17:00 Poster A

Glycolytic oscillations in a layer of interacting cells — •Jana Schütze and Jana Wolf — AG Theoretische Biophysik, Humboldt-Universität zu Berlin

Synchronisation of glycolytic oscillations in populations of yeast cells has been intensively analysed experimentally as well as theoretically. There is evidence that the individual cells communicate by exchanging products of glycolysis as acetaldehyde, for which the plasma membrane is permeable. Whereas previous models considered well stirred cell suspensions we here analyse the dynamics in a layer of cells. We aim to understand the conditions for wave initiation as observed in experiments where glucose was added to starved cells in a limited region of a cell layer.

For the generation of oscillations in the individual cells a two-component model containing an autocatalytic step is used. Cells are embedded in an extracellular medium in which the added glucose and the extracellular product can diffuse. Intercellular coupling takes place via the exchange of the end product. For single cells and a small number of interacting cells, the oscillations can be studied by using bifurcation analysis. In two-dimensional spatial arrangements of cells where glucose injection is continuously confined to a limited number of cells, waves of glycolytic oscillations can be observed. The strength of the product coupling as well as the stationary glucose distribution effect the existence and the range of waves, the propagation velocity and the period of the oscillations.

BP 26.48 Thu 17:00 Poster A

Formation of Domains in Bacterial Flagella — •Reinhard Vogel and Holger Stark — Institute for Theoretical Physics, TU Berlin, Germany

Many types of bacteria swim by rotating a bundle of helical filaments also called flagella. Each filament is driven by a rotatory motor. When its sense of rotation is reversed, the flagellum leaves the bundle and undergoes a sequence of configurations characterised by their pitch, radius and helicity (polymorphism). Finally the flagellum assumes its original form and returns into the bundle.

In general, the helical shape of the bacterial flagellum can assume 11 different configurations depending e.g. on mechanical loading, temperature and chemical composition of the solution. In recent optical tweezer experiments, Darnton and Berg [1] pulled at the flagellum and induced transformations between different helical configurations but they also observed the simultaneous occurrence of two configurations separated by a transition region. We investigate this domain formation based on the helical Kirchoff-rod model and the Calladine model [2] for the bacterial flagellum and present first results of our theoretical study.

[1] N.C.Darnton H.C. Berg, Biophys. J. 92, 2230-2236 (2007)
[2] C.R. Calladine,Nature (London) 255, 121 (1997)

BP 26.49 Thu 17:00 Poster A

Which Network Connectivities generate a given Dynamics? II: Network Reconstruction — •Frank van Bussel[1,2], Lishma Anand[1,2], Raoul-Martin Memmesheimer[1,2], and Marc Timme[1,2] — [1]Network Dynamics Group, MPI f. Dynamics & Self-Organization — [2]Bernstein Center for Computational Neuroscience, Göttingen

We present two alternative perspectives towards understanding relations between structure and dynamics in neural networks. In the first contribution, we present a design method [1], that enables us to find all networks as well as the structurally optimal network that generate a given neural spiking dynamics.

In this second part, we present a method to reconstruct the connectivity of a given network from its response dynamics to external driving signals. For a given driving signal, measuring how the collective state changes, reveals information about how the units are interconnected [2]. Sufficiently many repetitions for different driving conditions yield the entire network connectivity from measuring the response dynamics only [3]. We discuss possible applications to dimensionally reduced time series from coupled high-dimensional systems.

[1] R.-M. Memmesheimer and M. Timme,
Phys. Rev. Lett. 97:188101 (2006); Physica D 224:182 (2006).
[2] M. Timme, Europhys. Lett. 76:367 (2006).
[3] M. Timme, Phys. Rev. Lett. 98:224101 (2007).

BP 26.50 Thu 17:00 Poster A

Which Network Connectivities generate a given Dynamics? I: Optimal Network Design — •Raoul-Martin Memmesheimer[1,2], Lishma Anand[1,2], Frank van Bussel[1,2], and Marc Timme[1,2] — [1]Network Dynamics Group, MPI f. Dynamics & Self-Organization — [2]Bernstein Center for Computational Neuroscience, Göttingen

We present alternative perspectives towards understanding relations between structure and dynamics in neural networks.

First, can we design a network, e.g. by modifying the features of units or interactions, such that it exhibits a desired dynamics? Here we positively answer this question analytically for a class of networks of spiking neural oscillators [1, 2], by finding the set of all networks that exhibit a given arbitrary periodic spike pattern as an invariant dynamics. We illustrate the applicability of the method by designing networks that exhibit a predefined dynamics and simultaneously minimize the networks' wiring costs, i.e. are structurally optimal.

In a second contribution "Network Reconstruction" we present a method to infer the connectivity of a given network from its response dynamics to external driving signals [3,4].

[1] R.-M. Memmesheimer and M. Timme,
Phys. Rev. Lett. 97:188101 (2006).
[2] R.-M. Memmesheimer and M. Timme, Physica D 224:182 (2006).
[3] M. Timme, Europhys. Lett. 76:367 (2006).
[4] M. Timme, Phys. Rev. Lett. 98:224101 (2007).

BP 26.51 Thu 17:00 Poster A

Spectral measures of different integrate-and-fire neurons and how stimulus-induced synchrony varies among them — •Rafael Vilela and Benjamin Lindner — Max Planck Institute for the Physics of Complex Systems - Dresden

Integrate-and-fire (IF) neurons have found wide-spread applications in computational neuroscience, in particular, in stochastic versions of these models. Here we present results on the white-noise driven perfect, leaky, and quadratic integrate-and-fire models and focus on the spectral statistics (power spectra, cross spectra, and coherence functions) in different dynamical regimes (noise-induced and deterministic firing regimes with low or moderate noise). We make the models comparable by tuning parameters such that the mean value and the coefficient of variation of the interspike interval agree for all of them. We find that under these conditions, the power spectrum under white-noise stimulation is very similar while the response characteristics (characterized by the cross spectrum between a fraction of the input noise and the output spike train) differs in part drastically. We also investigate how two neurons of the same kind (e.g. two leaky integrate-and-fire neurons) synchronize if they share a common noisy input. We show that depending on the dynamical regime either two quadratic IF models or two LIFs are best synchronized. Our results suggest that for network simulations when choosing among simple integrate-and-fire models, the details of the model have a strong effect on synchronization behavior and regularity of the output.

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Poisson-Nernst-Planck description of nonequilibrium membrane potentials — •David Hofmann and Joachim Dzubiella — Physics Department, TU-Munich

The time-dependent Nernst-Planck and Poisson equations are solved numerically for a model cell membrane between aqueous reservoirs containing several ionic species. The steady state situation is analyzed and compared to the Goldman-Hodgkin-Katz equation, the analytical description of a cell membrane resting potential. Furthermore the full non-equilibrium situation is analyzed in order to describe the dynamic evolution of an action potential. The results are compared to the Hodgkin-Huxley model and available experimental data.

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A Paradigm for Phenotype Decision: Non-linear Dynamics Coupled to Low Number Stochastic Effects — •Jan-Timm Kuhr[1,3], Madeleine Leisner[2,3], Joachim Rädler[3], Berenike Maier[2,3], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, Germany — [2]Institut für Allgemeine Zoolo-

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Many organisms show a variety of phenotypes, even in populations consisting of genetically identical individuals. An example is the bacterium *B. subtilis*: Upon overpopulation a fraction cells switches to the "competent" phenotype, developing the trait of taking up genetic material from the surrounding medium and integrating it into their own genome, thereby speeding up evolution of the species. The bulk population, reproducing asexual, holds up a status quo while competent cells increase genetic variability by switching to quasi-sexual reproduction.

Here we present a scheme describing this extraordinary process by non-linear dynamics coupled to low-number stochastic effects of the involved molecular components. A two-component system is derived, explaining different phenotypes by bifurcation analysis and switching by intrinsic fluctuations intensified by auto-feedback. All parameters where chosen in accordance with previous experiments. The model quantitatively reproduces our experimental findings and explains the fractional onset of competence development on the single cell level.

BP 26.54 Thu 17:00 Poster A

influence of mass–dependent metabolic rates on food web stability — •Boris Kartascheff and Barbara Drossel — TU Darmstadt, Institute of Condensed Matter Physics, Hochschulstr. 6, D-64289 Darmstadt

Most basic approaches to modeling food web dynamics lead to a negative relation between the complexity and the stability of networks, if complexity is measured in terms of connectance or species number. This is in contrast to empirical data, which suggest that complex food webs are at least as likely to persist in time as simpler predator–prey systems.

In this study, we investigate the effect of allometric scaling, i.e. of metabolic rates that decrease as an inverse power of the body mass (which in turn depends on the trophic level), on food web stability. We randomly initiate networks and evaluate how many species survive until population dynamics reaches a stationary state. We investigate the effect of allometric scaling on the stability of networks with different structure (random, layered, niche models) and with different population dynamics (without and with adaptive foraging).

In this way, we are able to reveal the generic mechanisms that allow certain food web models to show remarkably increased stability when allometric scaling is included. Besides computer simulations, we also apply analytical methods to obtain answers to the question whether the existence of different sized species in ecosystems is crucial to their stability.

BP 26.55 Thu 17:00 Poster A

Dynamics of RNA evolution on realistic fitness landscapes — •Klaus Blindert — University of Cologne, Germany

The folding and function of RNA molecules strongly constrains the evolution of their sequences, by producing complex epistatic interactions between individual sequence positions. For instance, the deleterious effect of a mutation can often be compensated by a different mutation, which either directly or indirectly restores the folded basepairing pattern. To analyye the evolutionary dynamics of such compensatory effects, we use realistic models for RNA folding and fitness functions derived from existing structural alignments. We study the relative importance of direct (that is restoring a Watson-Crick base pair) and indirect compensation (e.g. lowering the free energy of the motif at an unrelated site) using simple RNA structural motifs such as hairpins. Our evolutionary model is based on the well-established Wright-Fisher model. To explore a wide range of parameters in our simulations, we apply a new technique, which approximates the evolutionary dynamics of multiple alleles under mutation, genetic drift and weak selection.