Lipid-mediated protein interactions in lipid bilayers — •Beate West and Friederike Schmid — Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

Lipid-mediated interactions play a central role for the interactions between proteins in a lipid bilayer. The lipid bilayer as well as the proteins are simulated using a coarse-grained model.

We study how proteins influence the structure of the lipid bilayer at different temperatures, and, on the other hand, how the lipids influence the interactions of the proteins. To this end, we calculate the effective pair potential between the proteins with the method of umbrella-sampling.

BP 16.6 Tue 17:00 Poster D

Fluctuation-dissipation relation for colloidal particles in shear flow — •Thomas Speck and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

In equilibrium, the well-known fluctuation-dissipation theorem (FDT) connects the response of an observable with its auto-correlation function. For driven systems, breaking of detailed balance leads to dissipation and to the breakdown of the FDT. We have shown recently how to quantify this violation in terms of velocity correlations and how to restore then the original form of the FDT [1]. We investigate the violation function in the case of two interacting colloidal particles driven by shear flow and illustrate our results with numerical calculations.

[1] T. Speck and U. Seifert, Europhys. Lett. **74**, 391 (2006).

BP 16.7 Tue 17:00 Poster D

Cell shape-dependent forces at focal adhesions — •Sebastian Schmidt[1], Ilka Bischofs[2], and Ulrich Schwarz[1] — [1]University of Heidelberg, Im Neuenheimer Feld 293, D-69120 Heidelberg, Germany — [2]University of California at Berkeley, Department of Bioengineering, 717 Potter Street, Berkeley CA 94720, USA

Adhesion-dependent cells probe the mechanical properties of their environment by internally generated forces transmitted to the extracellular environment at sites of focal adhesions, with dramatic consequences for different physiological processes, including cell division and lineage specification. We introduce a mechanical model which allows to relate cellular forces applied to focal adhesions with their shape. Our model predicts that forces at focal adhesions are mainly determined by the line tension present in the cell contour. Both surface tension in the cell envelope and extracellular stiffness have an indirect effect by changing the geometrical arrangement through which the line tension acts. We also discuss the effect of tension-mediated reinforcement of the cell contour.

BP 16.8 Tue 17:00 Poster D

Energy transfer processes in a bisporphyrinic switch — •Jedrzej Szmytkowski[1,3], Robert Hauschild[1], Manfred Scholdt[1], Teodor Silviu Balaban[2,3], and Heinz Kalt[1,3] — [1]Univesität Karlsruhe (TH), Karlsruhe, Germany — [2]Forschungszentrum Karlsruhe, Institute for Nanotechnology, Karlsruhe, Germany — [3]Center for Functional Nanostructures (CFN), Karlsruhe, Germany

Energy transfer processes are the first step in light-harvesting and have been optimized in photosynthetic organisms. Artificial mimics are essential in understanding and controlling the efficiency with which after photon capture an energetic trap can be accessed. We have studied various bis-porphyrinic constructs, covalently attached to spacers such as a rigid steroidal skeleton or a terpyridine capable of undergoing a conformational switch from an extended "W" conformation into a more compact "U" form. The switching can be performed by addition of coordinating metals or of ditopic ligands. Singlet-singlet energy transfer was put into evidence by time-resolved fluorescence and the data have been analyzed using decay associated spectra (DAS). While in the steroidal systems a Förster-type energy transfer occurs, the rate and efficiency of the energy transfer can be influenced by the added ligand in the terpyridinc constructs.

BP 16.9 Tue 17:00 Poster D

Accuracy check of detection algorithms for fluorescent colloidal spheres by simulation — •Markus Gyger — Institute for Soft Matter Physics, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

In the discussion about like-charge attraction of colloidal spheres confined between parallel glass-plates there have been indications that the observed attraction is an artifact due to diffraction effects in optical video microscopy. We present a simulation technique which checks the accuracy of the detection algorithms for confined fluorescent colloidal particles and allows for determination of the difference between real and detected particle position in dependance on the interparticle separation. To that aim, images of interacting particles, whose positions were detected by different particle detection algorithms, were computer generated, simulating the image-taking process of digital video microscopy. Re-detecting the particle positions from the simulated images and comparing them with the originally detected positions provides some insight into the detection accuracy and systematic errors of the detection algorithms.

BP 16.10 Tue 17:00 Poster D

Brownian dynamics simulations of protein cluster assembly — •Jakob Schluttig and Ulrich Schwarz — University of Heidelberg, Im Neuenheimer Feld 293, D-69120 Heidelberg

Most proteins in the cell are active in complexes with two to several hundreds of components. Because only very small assemblies can be studied in an all-atom framework, coarse-grained approaches are required to model the association and dissociation dynamics of larger protein assemblies. We model proteins as spherical particles covered with few binding sites. Their motion is simulated with Brownian dynamics and binding is allowed to occur if two binding sites approach each other to a prescribed encounter length. The diffusion of clusters is treated using bead models for the hydrodynamics in the viscous regime. Using computer simulations, we measure the mean first passage times for the formation of clusters of different sizes.

BP 16.11 Tue 17:00 Poster D

Evolutionary emergence of complexity in model food webs — •Christian Guill and Barbara Drossel — Institut für Festkörperphysik, Technische Universität Darmstadt, Deutschland

Explaining the amazing diversity of ecological communities remains one of the greatest challenges in theoretical ecology. We investigate various mechanisms that promote the emergence of large and complex food webs in an evolutionary model that also includes population dynamics. Networks are created by starting from one species and external resources, followed by an iterated process of adding new species that are obtained by modifying existing species. Species are ordered on a one-dimensional niche axis, and links between them that represent feeding relationships are assigned according to the rules of the niche model (R.J. Williams, N.D. Martinez, 2000, Nature 404, 180-183). The average body size (or mass) of the species is assumed to increase with their position on the niche axis. The tested hypotheses for the promotion of complexity are the influence of different functional responses, adaptive behaviour, and body size effects that relate the metabolic rate of a species to its position on the niche axis. Adaptive foraging behaviour is found to be the key mechanism for the emergence of complex networks, while body size effects only determine the degree of complexity.

BP 16.12 Tue 17:00 Poster D

Nanotomography of Human Bone Based on Scanning Probe Microscopy — •Stephanie Röper[1], Christian Dietz[1], Sabine Scherdel[1], Anke Bernstein[2], Nicolaus Rehse[1], and Robert Magerle[1] — [1]Chemische Physik, TU Chemnitz, D-09107 Chemnitz — [2]Experimentelle Orthopädie, Martin-Luther-Universität Halle-Wittenberg, D-06097 Halle/Saale

Natural materials such as bone and teeth are nanocomposites of proteins and minerals, which exhibit a complex hierarchical structure ranging from macroscopic to molecular length scales. Scanning probe microscopy (SPM) based Nanotomography is a novel approach to image these materials. We focus on human bone which is first embedded in a methacrylate resin and then and then sectioned with the use of a microtome. For SPM based Nanotomography the specimen is ablated layer-by-layer by wet chemical etching and imaged with tapping mode scanning force microscopy after each etching step. From the resulting series of images the three-dimensional structure is reconstructed. The etching and imaging is done in-situ in a liquid cell of an SPM connected to reservoirs of etchants and water for flushing after each etching step. The flow of the different liquids is controlled with computer controlled valves which allow for an automated etching and measuring protocol. We will present first results of volume images of human bone and discuss our concepts for adjusting the imaging parameters to maintain a good imaging quality.