BP 9: Biomaterials and Biopolymers I (joint BP/CPP)

Time: Monday 14:30–17:15 Location: EB 202

BP 9.1 Mon 14:30 EB 202

Determination of Conformational Entropy of Fully and Partially Folded Conformations of Holo- and Apomyoglobin — •Andreas Stadler[1], Marek Koza[2], and Jörg Fitter[3,4] — [1]Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Institut Laue-Langevin, CS 20156, 38042 Grenoble, France — [3]Institute of Complex Systems (ICS-5): Molecular Biophysics, Forschungszentrum Jülich GmbH, 52425 Jülich — [4]I. Physikalisches Institut (IA), AG Biophysik, RWTH Aachen, Sommerfeldstrasse 14, 52074 Aachen

Holo- and apomyoglobin can be stabilized in native folded, partially folded molten globules (MGs) and denatured states depending on the solvent composition. In a comparative experimental study we investigated the correlation between protein folding and dynamics on the picosecond time scale using incoherent quasielastic neutron scattering (QENS). The conformational entropy difference ΔSconf between the folded conformations and the acid denatured state could be determined from the measured mean square displacements and was compared to the entropy difference ΔS obtained from thermodynamic parameters. The observed difference between ΔS and ΔSconf was attributed to the entropy difference ΔShydr of dynamically disordered water molecules of the hydration shell. The entropy content of the hydration water is significantly larger in the native folded proteins than in the partially folded MGs. We demonstrate the potential of incoherent neutron scattering for the investigation of the role of conformational dynamics in protein folding.

BP 9.2 Mon 14:45 EB 202

Mechanical rupture of mono- and bivalent coordination compounds — •Manuel Gensler[1], Christian Eidamshaus[2], Arthur Galstyan[2], Ernst-Walter Knapp[2], Hans-Ulrich Reissig[2], and Jürgen P. Rabe[1] — [1]Department of Physics, Humboldt-Universität zu Berlin — [2]Institute of Chemistry and Biochemistry, Freie Universität Berlin

Biomolecular systems are commonly exposed to a manifold of forces, often acting between multivalent ligands. To understand these forces we studied a monovalent and three bivalent pyridine Cu(II) coordination complexes with varying backbone structures. We performed SFM based single-molecule force spectroscopy in aqueous environment and compared results with ab-initio DFT calculations. According to the Kramers-Bell-Evans theory, all interactions show remarkably long rupture lengths of more than 3 Å. We explain this observation by dissociation mechanisms involving hydrogen-bound intermediate states. Additionally we show that most probable rupture forces of the bivalent systems can be larger, but also smaller than those of the monovalent counterpart. In contrast, when our results are extrapolated to forceless conditions, all bivalent systems show lower thermal off-rates. The mechanical stability is not solely determined by binding energy, but also by rupture lengths. Thus both parameters should be considered in the rational design of biomolecular ligands.

BP 9.3 Mon 15:00 EB 202

Opposite translocation of long and short oligomers through a nanopore — •Thomas Töws, Sebastian Getfert, and Peter Reimann — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

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

BP 9.4 Mon 15:15 EB 202

Hydrodynamic Slip on DNA in Nanopore Translocation Experiments — Lukas Galla[1], •Andreas J. Meyer[1], Andre Spiering[1], Andy Sischka[1], Michael Mayer[2], Adam R. Hall[3], Peter Reimann[1], and Dario Anselmetti[1] — [1]University of Bielefeld, Germany — [2]University of Michigan, USA — [3]Wake Forest University School of Medicine, USA

In a recent paper, we reported on the observation of hydrodynamic slip on DNA by optical tweezers-controlled translocation experiments in solid-state and lipid-coated nanopores [1]. After a short introduction to the performed experiments, I will present our theoretical model describing the dominating electrohydrodynamic effects, with particular emphasis on the hydrodynamic slip boundary condition.

By solving the Poisson-Nernst-Planck and Stokes equations using finite element methods it is possible to gain insight into the influence of nanopore geometry and composition on translocation experiments. Furthermore, these continuous models of electrohydrodynamics can serve as an appropriate basis for dynamic DNA simulations.

[1] L. Galla, A. J. Meyer, A. Spiering, A. Sischka, M. Mayer, A. R. Hall, P. Reimann, and D. Anselmetti (2014). Hydrodynamic slip on DNA observed by optical tweezers-controlled translocation experiments with solid-state and lipid-coated nanopores. Nano Letters, 14(7), 4176-4182.

BP 9.5 Mon 15:30 EB 202

How to escape the maze — •Teresa Behl[1], Felix Höfling[2], and Thomas Franosch[3] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität, München — [2]Max Planck Institute for Intelligent Systems, Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart — [3]Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Austria

Recently, novel materials such as carbon nanotubes extended the interest in the diffusion dynamics of semiflexible polymers far beyond classical biophysics. Semiflexible polymers form entangled networks when dispersed in solution by virtue of their lengthy nature. Due to their relative stiffness they exhibit a reptation movement to escape their local surrounding maze of crossing polymers, usually modelled as a tube constraining the polymer sterically.

We have investigated the dynamics of a semiflexible polymer via computer simulations of a 2D bead-rod-algorithm. Point obstacles mimic the cross sections of the surrounding polymers with the plane in which the polymer diffuses. Extensive computer simulations are performed to resolve the slow disentanglement processes. In particular we measure the translational and rotational diffusion for a broad density range. Furthermore, we discuss the intermediate scattering function and the chances and limitations of the performed simulations.

15 min break

BP 9.6 Mon 16:00 EB 202

Theory on linear viscoelasticity of a cytoskeletal network — •Tetsuya Hiraiwa and Roland Netz — Freie Universität Berlin, Germany

Mechanical properties of a cortical cytoskeleton, which is a network consisting of actin filaments and crosslinker proteins located underneath the cell membrane, govern the elastic and viscous resistances of living cells to deformation and are crucial for wide variety of cellular functions. I would like to present a theoretical method to evaluate linear viscoelasticity of a filamentous network like a cortical cytoskeleton based on properties of single segments. Using the method, we can explain a universal power-law in complex moduli, which is also found in several experiments and our numerical simulation.

BP 9.7 Mon 16:15 EB 202

Scaling with persistence length: Expanding the accessible phase space of semi-flexible polymer networks via DNA tubes — •Carsten Schuldt[1,2], Jessica Lorenz[2], Jörg Schnauss[1], Tina Händler[1], Martin Glaser[1], Josef A. Käs[1], and David M. Smith[2] — [1]University of Leipzig, Soft Matter Physics Division, Leipzig, Germany — [2]Fraunhofer Institute for Cell Therapy and Immunology, Leipzig, Germany

Biologically evolved materials are often used as inspiration in both the development of new materials as well as examinations of underlying physical principles governing their general behavior. One prominent

example is actin and its set of accessory proteins. However, a major limitation lies in the molecular toolbox provided by naturally occurring biological systems. The inability to deterministically modulate or "program" basic properties such as stiffness or interaction strengths hinders a meticulous examination of the parameter space, and the subsequent potential for developing new classes of materials.

We overcome these limitations emplyoing model systems assembled from programmable nanomaterials such as DNA. Nanotubes with similar dimensions and mechanical properties as actin filaments can be constructed from small sets of specially designed DNA strands. Properties such as stiffness and inter-filament attraction (i.e. crosslinking) can be controlled through the design of a particular set of DNA strands. Forming networks from these semi-flexible polymers, we test established theories with respect to these parameters for the first time.

BP 9.8 Mon 16:30 EB 202

pH-dependent Ordered Fibrinogen Adsorption on Polyethylene Single Crystals — •Christian Helbing[1], Robert Schulze[1], Dominik Hering[2], and Klaus D. Jandt[1] — [1]Chair of Materials Science (CMS), Otto-Schott-Institute of Materials Research (OSIM), Friedrich Schiller University Jena, Jena, Germany — [2]Clemenshospital Münster, Münster, Germany

The biological performance of materials is mostly determined by protein adsorption at the biomaterials surface. Nanostructured surfaces can influence the assembly and orientation of adsorbed proteins. The aim of the current study was to control the protein adsorption by nanostructured surfaces. For this, we tested the hypothesis that human plasma fibrinogen (HPF) assemblies can be oriented on the (001) surface nanostructures of Polyethylene Single Crystals (PE-SC).

At a physiological pH of 7.4, HPF assemblies consisted of crosslinked HPF molecules, e.g., protofibrils, networks or sponge-like structures in dependence of the protein concentration. However, at an increased pH of 9.2 spherical-shaped and trinodal-shaped single HPF assemblies were observed. The observation of these multi protein assemblies (pH 7.4) and the single HPF assemblies (pH 9.2) can be explained by activated (pH 7,4) and deactivated (pH 9.2) HPFs αC-domains. While the single trinodal-shaped HPF molecules preferred an orientation along crystallographic [100] and [010] directions on the nanostructured PE-SC surface the HPF protofibrils showed no preferential orientation. The current study deepens the understanding of controlled protein assembly and orientation on nanostructured surfaces.

BP 9.9 Mon 16:45 EB 202

Insights into diatom biomineralization with nanoscale silica-peptide hybrid films — •Helmut Lutz[1], Vance Jaeger[2], Jim Pfaendtner[2], Mischa Bonn[1], and Tobias Weidner[1] — [1]Max-Planck-Institute for Polymer Science, Mainz — [2]University of Washington, Chemical Engineering, Seattle

Taking clues from diatom silification we have recently shown that amphiphilic peptides consisting of lysine and leucine (LK peptides) are capable of producing silica wires, spheres and tubes, depending on their secondary structure. Precipitating particles, i.e. mineralization in three dimensions is very different from the two dimensional silification required for the cell walls of diatoms. Hence, we studied mineralization in 2D at the air-water interface. At the interface, slightly different peptides can adopt alpha helical or beta sheet structures depending on the hydrophobic periodicity of amino acids. Upon addition of a silica precursor we were able to obtain peptide-silica hybrid films with a thickness of ~4 nm. By means of surface sensitive techniques, such as sum frequency generation (SFG) and X-ray photoelectron spectroscopy (XPS) we were able to probe the film composition and interactions between peptides and silica at the early stages of biomineralization. Electron and atomic force microscopy show that the fine structure of the film resembles the in-solution silica precipitates of each peptide. We employed molecular dynamics simulation techniques to complement the experimental insights with a computational model. Our results provide insights into the biomineralization of structured films, which might prove useful in materials design and surface engineering.

BP 9.10 Mon 17:00 EB 202

Mapping internal mineral strains in human dentine under tension: X-ray diffraction insights into the contribution of the mineral nano-particles to the load-bearing capacity of tooth tissue. — Jean-Baptiste Forien[1], •Claudia Fleck[2], Peter Fratzl[3], and Paul Zaslansky[1] — [1]Julius Wolff Institut, Berlin, Germany — [2]Technical University, Berlin, Germany — [3]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Teeth are hierarchical strong and stiff structures, consisting of a mineralized protein-based composite (dentine). They function under mechanical load, and the nanometer-sized hydroxyapatite mineral particles in the collagen fiber matrix deform as a response to applied external stress (Deymier-Black,2012). In this study, we report on the mineral response in human dentine to mechanical tensile testing. We track mineral particles following changes in the mineral dimension using X-ray diffraction. It is thus possible to compare the stresses experienced by the mineral particles with the stress applied by the external load. We find that the tissue to mineral strain ratios observed increase until they reach a value of 2, which is three times lower than for bone (Gupta,2006), and suggests that a different load-partitioning mechanism exists in teeth. We also find that the Poisson's ratio decreases with increasing load, suggesting that as load increases, there is some dynamic change in the loads transferred to the crystals, similar to what was found for bovine dentine loaded in compression. With increasing load, more strain-energy is orientated along the tensile axis and less is distributed into particles oriented along other orientations.