

CPP 28 Biological Systems

Time: Friday 10:30–12:30

Room: ZEU Lich

CPP 28.1 Fri 10:30 ZEU Lich

Can hydrophobically lined channels be gated by water? — ●K. MYRIAM KROLL^{1,2} and ROLAND ROTH^{1,2} — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

Pores of KcsA ion channels possess a hydrophobic region which changes its conformation between a wide pore, when open, to a narrower pore, when closed. Recent studies indicate that a hydrophobic pore can "gate" by capillary evaporation. With this mechanism water is expelled from the permeation pathway and ion flow is thereby stopped although the pore remains wider than the water or ion diameters. We study the connection between geometrical change of a hydrophobic pore and capillary evaporation to estimate the energetics of this gating mechanism in a realistic pore geometry, e.g. the energy it takes to remove the water from the pore and the force exerted by the water on the wall of the pore.

To this end we perform, in a first step, microscopic density functional theory (DFT) calculations, in which we focus on the density profile of water as capillary evaporation takes place. The insight gained from these DFT calculations we transfer and exploit, in a second step, in our mesoscopic morphometric approach. In morphometry the free energy of a liquid confined in a pore is expressed by four terms that describe the geometry of the pore and corresponding thermodynamic coefficients. This separation of geometry and thermodynamics makes calculations very efficient so that effects due to change in geometry can be studied in depth. Both DFT and morphometry have been applied with great success in studies of the physics of confined fluids.

CPP 28.2 Fri 10:45 ZEU Lich

Force-induced desorption and unzipping of semiflexible polymers — ●JAN KIERFELD — Max Planck Institute of Colloids and Interfaces, Science Park Golm, 14424 Potsdam

The thermally assisted force-induced desorption of semiflexible polymers from an adhesive surface or the unzipping of two bound semiflexible polymers by a localized force are investigated. The phase diagram in the force-temperature plane is calculated both analytically and by Monte Carlo simulations. Force-induced desorption and unzipping of semiflexible polymers are first order phase transitions. A characteristic energy barrier for desorption is predicted, which scales with the square root of the polymer bending rigidity and governs the initial separation process before a plateau of constant separation force is reached. This leads to activated desorption and unzipping kinetics accessible in single molecule experiments.

CPP 28.3 Fri 11:00 ZEU Lich

Thin Casein films as prepared by spin-coating: Influence of film thickness and of pH — ●P. MÜLLER-BUSCHBAUM¹, R. GEBHARDT¹, E. MAURER¹, E. BAUER¹, R. GEHRKE², and W. DOSTER¹ — ¹TU München, Physik-Department E13, James-Frank-Str. 1, D-85747 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, D-22603 Hamburg, Germany

Casein films are successfully prepared by spin-coating water based casein solution on base treated glass surfaces. The film structure is investigated in real space by optical microscopy and atomic force microscopy and in reciprocal space by grazing incidence small angle X-ray scattering (GISAXS). Due to the changed electrostatic repulsion, with increasing pH value the size of the casein micelles increases. Dynamic light scattering confirms good agreement of the micelle size in solution and building a bulk like casein film as determined with GISAXS. As long as homogeneous casein films are producible, with decreasing film thickness the micelle size is reduced. At the moderate pressure introduced by spin-coating the micelles rearrange in a more compact size.

CPP 28.4 Fri 11:15 ZEU Lich

Thermodynamic stability of proteins — ●JOHANNES WIEDERSICH¹, SIMONE KÖHLER¹, JOSEF FRIEDRICH¹, and ARNE SKERRA² — ¹Physikdepartment E14, Lehrstuhl für Physik Weihenstephan, TU München, Germany — ²Lehrstuhl für Biologische Chemie, TU München

The folding of proteins shows a complex scenario, the details of which are not yet fully understood. One important aspect concerns the stability of proteins. By means of fluorescence spectroscopy, we study the stability of the anticallin FluA–fluorescein complex, a small protein specifically

tailored to bind the fluorophore fluorescein, as a function of pressure and temperature.

Although it is known that protein folding follows a complex path, the temperature and pressure denaturation of FluA is well described by a simple two-state model. The observed elliptic shape of the p - T phase diagram implies that—despite the complexity of protein folding—the thermodynamic parameters (namely specific heat capacity, compressibility, thermal expansion) are rather well defined and do not significantly depend on pressure and temperature. We discuss the implications of our findings on the understanding of generic features of the protein folding transition, especially on its similarities to the glass transition.

CPP 28.5 Fri 11:30 ZEU Lich

In-situ Studies of Protein Resistance of Oligo(Ethylene Glycol) Self-Assembled Monolayers — ●MAXIMILIAN SKODA^{1,2}, FRANK SCHREIBER¹, JAMES WILLIS², ROBERT JACOBS², REINER DAHINT³, MICHAEL GRUNZE³, and MAXIMILIAN WOLFF⁴ — ¹Universität Tübingen — ²Oxford University — ³Universität Heidelberg — ⁴Institut Laue-Langevin

The structure of the interface between organic matter, such as self-assembled monolayers (SAMs), and water is currently subject of intensive studies due to its importance for the understanding of surface-solvent and surface-surface interactions [1,2]. We report results from Polarisation Modulated (PM) Fourier Transform Infrared Spectroscopy (FTIR) studies that enable us to address the local interaction of water with OEG groups. Our data suggest a rather strong interaction of water molecules with the EG section of the SAM, potentially the penetration of water into the SAM. We will also discuss the potential of true in-situ investigations (i.e. under a layer of water) using PM-FTIR. In addition, we will discuss neutron reflectivity (NR) measurements on the same system. NR provides insight to the structure of the solid-liquid interface in-situ and without perturbation of the system. The measurements reveal changes in the structure of water and the protein solution in the vicinity of the SAM upon changes in temperature.

[1] F. Schreiber, J. Phys.: Cond. Matter 16 (2004) R881

[2] D. Schwendel et al., Langmuir 19 (2003) 2284

CPP 28.6 Fri 11:45 ZEU Lich

Solvent induced forces on bio-molecules — ●HENDRIK HANSEN-GOOS^{1,2}, ROLAND ROTH^{1,2}, KLAUS MECKE³, and SIEGFRIED DIETRICH^{1,2} — ¹MPI für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart — ²ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart — ³ITP, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Understanding conformations of complex molecules in organisms requires to account for solvent induced forces. The most elementary of these being the depletion force which arises even in absence of internal energy contributions from a system's tendency to maximise entropy. Additionally, solvent-solvent and solvent-molecule interactions can strongly influence the conformation of the solvated molecule. A first step towards the understanding of depletion forces is the Asakura-Oosawa (AO) model which neglects solvent-solvent interactions. More realistic solvent models like the hard-sphere fluid or attractive (water-like) solvents can be realised within the context of morphological thermodynamics recently put forward. The approach is based on the Hadwiger theorem which implies that (under certain assumptions) the change in free energy upon insertion of a molecule into the solvent is a linear function of the molecule's Minkowski measures with interaction specific coefficients. We introduce a self-consistent scaled particle calculation yielding quasi-exact coefficients for the hard-sphere fluid. The morphological approach is applied for different interactions, illustrating that conclusions drawn from the AO model for phenomena such as helix formation are somewhat misleading. Limits of the approach are discussed by comparison with density functional theory calculations.

CPP 28.7 Fri 12:00 ZEU Lich

Experimental and Theoretical Investigation of the Elasticity of Poly(azobenzene-peptides) — ●GREGOR NEUERT^{1,2}, THORSTEN HUGEL^{2,3,4}, ROLAND R. NETZ^{2,3}, and HERMANN E. GAUB^{1,2} — ¹Lehrstuhl für Angewandte Physik — ²Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität, Amalienstrasse 54, 80799 München — ³Physics Department — ⁴Zentralinstitut für Medizintechnik, TU-München, 85748 Garching

Since the mechanical properties of individual polymers have become accessible with single molecule force spectroscopy, detailed insight was gained into the molecular origin of their elasticity. Active, optically switchable polymers were introduced as photonic muscles and used in single molecule motors. Here, we present experimental data and calculations to describe the mechanical properties of poly(azobenzene-peptides) in the complete force regime accessible by AFM. The high force regime is very well described by ab-initio quantum mechanical calculations, while for the low force regime we combine ab-initio calculations with a description of the entropic forces based on the freely rotating chain model. Finally, a one-parameter fit for the different configurations of the poly(azobenzene-peptide) and a quantitative description of the optically induced actuation are given [1-2].

[1]Holland, N. B.; Hugel, T.; Neuert, G.; Cattani-Scholz, A.; Renner, C.; Oesterhelt, D.; Moroder, L.; Seitz, M.; Gaub, H. E. *Macromolecules* 2003, 36, 2015-2023

[2]Neuert, G.; Hugel, T.; Netz, R. R., Gaub, H. E., *Macromolecules* accepted

CPP 28.8 Fri 12:15 ZEU Lich

Nanofriction: Pulling polymers along surfaces — ●ANDREAS SERR^{1,2} and ROLAND R. NETZ¹ — ¹Physik Department, Technische Universität München, James-Franck-Str., D-85748 Garching, Germany — ²serr@ph.tum.de

Over the last decade the method of AFM force spectroscopy has been used to extract single polymer data, e.g. on protein unfolding dynamics, polymer elasticity, covalent bond breaking and adsorption strengths. When pulling on polymers physisorbed to surfaces, a transition from stick to slip has been noted by change of pH, ionic strength or solvent conditions, which is yet not understood. Using a simple, parameterized model for polymer-surface interactions we predict the lateral and vertical forces for both pulling the polymer off from the surface and for pulling laterally alongside the surface [1]. In principle, the friction coefficient can be extracted from such experiments and its dependence on polymer & surface type, pH, etc. could be mapped out. Microscopic models and simulations provide insight into the fundamental dissipation processes for different types of polymer-surface interactions.

[1] A. Serr, R. R. Netz, *Pulling adsorbed polymers from surfaces with the AFM: stick versus slip, peeling versus gliding*, submitted to *Europhys. Lett.*, **2005**.