# AKB 45 Single Molecule Biophysics

Zeit: Montag 14:30–16:00 Raum: TU H2013

**Hauptvortrag** AKB 45.1 Mo 14:30 TU H2013

**Coupled dynamics of DNA-breathing and binding of proteins that selectively bind to single-stranded DNA** — •Ralf Metzler and Tobias Ambjörnsson — NORDITA, Blegdamsvej 17, DK-2100 Copenhagen OE

Under physiological conditions, the double-helix is the thermodynamically stable configuration of DNA. A long-standing puzzle had been why the presence of selectively single-stranded DNA binding proteins (SSBs) does not lead to full DNA-denaturation, as SSB binding is thermodynamically favorable. By detailed single-molecule studies, it was corroborated quantitatively that for the gp32-SSB there exists a kinetic block for SSB-binding: below the melting temperature of DNA, that is, the lifetime of a bubble is shorter than the typical binding time of an SSB, counteracting the expected helix-destabilization through the SSBs. We derived a dynamical model to quantify the coupled dynamics between a fluctuating DNA-bubble and SSBs that attempt to bind to it. Depending on the system parameters (temperature, external force, SSB binding rate and strength, SSB size), the presence of SSBs leads to enhanced bubble lifetime. Effectively, the bubble free energy is lowered, or even full denaturation caused by SSBs.

AKB 45.2 Mo 15:00 TU H2013

**Kinetics of driven RNA translocation through nanopores** — •Ulrich Gerland[1] and Ralf Bundschuh[2] — [1]Department Physik and CENS, LMU München, Germany — [2]Department of Physics, The Ohio State University, Columbus, Ohio

Motivated by recent experiments, we study the translocation of structured RNA molecules through narrow pores that allow single but not double strands to pass. The translocation dynamics is coupled to the base pairing dynamics of the RNA molecules, which we incorporate explicitly in kinetic Monte Carlo simulations. For a number of exemplary molecules as well as for random sequences, we characterize the translocation dynamics as a function of the driving force. For strongly driven translocation, we find a narrow distribution of translocation times with a mean that scales linearly with the RNA length. In contrast, for weakly driven translocation we observe a pronounced sequence-dependence in the distribution of translocation times. Simple physical arguments can explain these two limiting regimes. Furthermore, we identify the sequence-specific properties of RNA molecules that are reflected in the translocation times.

AKB 45.3 Mo 15:15 TU H2013

**Dynamcis of Force-Induced DNA Slippage** — •Richard Neher and Ulrich Gerland — Department für Physik, LMU München

In double-stranded DNA with repetitive sequences, one strand may locally slip with respect to the other, leading to the creation, annihilation, or diffusion of bulge loops. We study the physics of periodic DNA theoretically, focusing on the dynamics under a shear force, which can be probed experimentally with single molecule devices [1]. Using an explicit model, we find a rich dynamical behavior with clear signatures in experimental observables. In particular, at a lower critical force $f_c$ the system displays reptation-like dynamics with a mean rupture time that scales with the sequence length as $\langle\tau\rangle \sim N^3$. In an intermediate regime $f_c < f < f^*$, the distribution of rupture times is well described by drift-diffusion theory, up to an upper critical force $f^*$, where a *dynamical* transition to an unraveling mode of strand separation occurs [2]. We predict that periodic DNA sequences display a viscoelastic behavior with time and force scales that can be *programmed* into the sequence.

[1] T. Strunz *et al.*, PNAS **96**, 11277 (1999).
[2] R. A. Neher and U. Gerland, PRL **93**, 198102 (2004)

AKB 45.4 Mo 15:30 TU H2013

**Molecular Details of Specific Protein-DNA Interaction** — •Frank Wilco Bartels[1], Birgit Baumgarth[2], Christelle Bahlawane[2], Christoph Metzendorf[2], Anke Becker[2], Dario Anselmetti[1], and Robert Ros[1] — [1]Experimental Biophysics, Faculty of Physics, Bielefeld University — [2]Genetics, Faculty of Biology, Bielefeld University

Specific protein-DNA interaction is fundamental for all aspects of gene expression. A regulatory model system is the biosynthesis of exopolysaccharides (EPS) in the nitrogen-fixating bacterium *Sinorhizobium meliloti* 2011. These sugar polymers promote the bacterium's symbiosis with alfalfa plants, a process of agricultural importance.

The EPS biosynthesis is controlled by a complex interplay of several proteins, most prominently the transcriptional activator ExpG. In a combination of standard biochemical and single molecule experiments, we demonstrated that the protein ExpG binds to three different DNA target sequences in a sequence specific manner, albeit with distinct differences in the energy landscape.[1] Dynamic force spectroscopy based on the atomic force microscope (AFM) proved to be sensitive even to small variations of the binding motif. Experiments with DNA mutants lead to a deeper understanding of the binding mechanism.[2]

The method is now applied to other proteins from the same regulatory system.

[1] F.W. Bartels et al., J Struct Biol 143 (2003) 145-152
[2] B. Baumgarth et al., Microbiol (2004), in press

AKB 45.5 Mo 15:45 TU H2013

**Tail Induced Interactions of Nucleosome Core Particles** — •Christian Holm, Frank Mülbacher, and Helmut Schiessel — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz

We present a MD simulation study of the interactions between nucleosome core particles (NCPs). Each NCP consists of a core of eight histone proteins and a strand of DNA, which is wrapped around about two times. Special emphasis was placed on the role of the histone tails. We model the histone core and the wrapped DNA by a charged sphere, while the histone tails are represented by oppositely charged polyelectrolyte chains grafted onto the sphere's surface, interacting via a Debye-Hückel potential. We find that the effect of tail bridging between the spheres does indeed account for the observed attraction, thus reproducing the qualitative features of the experimental results. We further modify our model to use either only one interacting tail, or charge patches instead of the tails in order to isolate the quantitative features of the tail interactions. The reduction of the charge fraction of the tails, that corresponds to the process of acetylation, leads to a reduction or even the disappearance of the attraction, which subsequently can lead to the unfolding of the chromatin fiber, thereby activating genes.