CPP 25 Biological systems I

Zeit: Dienstag 14:00–15:00 Raum: TU C230

CPP 25.1 Di 14:00 TU C230

Perspectives for variable-temperature investigations of single-protein dynamics — •Florian Kulzer, Rob Zondervan, Joris Berkhout, and Michel Orrit — Molecular Nano–Optics and Spins (MoNOS), Huygens Laboratory, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands

The conformational dynamics of proteins, a key issue in molecular biology, are characterized by the existence of a complex energy landscape, leading to a potentially huge number of possible folding routes for a given protein. This presents the experimenter with the challenge of following simultaneous rapid transitions between many different conformational states. Optical experiments on individual protein molecules naturally avoid the difficulties associated with unsynchronized ensembles, but their scope is severely limited by photoblinking and photobleaching of the probe chromophores (reversible and irreversible transitions to non-emissive states).

Our contribution will present our efforts to develop a novel approach to overcome some of these inherent limitations of “conventional” single-molecule experiments on biological systems. Our method tries to avoid the problems with photoblinking and photobleaching by relying on rapid thermal cycling of a microscopic sample. This way the long-time conformational evolution of single proteins could be split up in successively frozen structural “snapshots,” which could be subjected to detailed probing at low temperatures. We will present our recent results showing that we have managed to implement the rapid thermal cycling procedure and discuss the perspectives for further investigations.

CPP 25.2 Di 14:15 TU C230

Multivariate Analysis of Single-Molecule Spectra: Surpassing Spectral Diffusion — •Clemens Hofmann[1], Hartmut Michel[2], Marin van Heel[3], and Jürgen Köhler[1] — [1]Experimental Physics IV and BIMF, University of Bayreuth, 95440 Bayreuth, Germany — [2]Department of Molecular Membrane Biology, Max-Planck Institute of Biophysics, Frankfurt, Germany — [3]Department of Biological Sciences, Imperial College London, London SW7 2AY, United Kingdom

The full exploitation of single-molecule spectroscopy in disordered systems is often hampered by spectral diffusion processes of the optical transitions due to structural fluctuations in the local environment of the probe molecule which leads to temporal averaging of the signal. Multivariate statistical pattern recognition techniques, originally developed for single-molecule cryo-electron microscopy, allow us to retrieve detailed information from optical single-molecule spectra. As an example, we present the phonon-side band of the B800 excitations of the LH2 complex from *Rhodospirillum molischianum*, revealing the electron-phonon coupling strength for these transitions. The measured Debye-Waller factors, ranging from 0.4 – 0.8, fall in the regime of weak electron-phonon coupling.

CPP 25.3 Di 14:30 TU C230

Statistical physics of a single DNA chain and its interaction with binding proteins — •Ralf Metzler — NORDITA, Blegdamsvej 17, DK-2100 Copenhagen OE

In my talk I want to illustrate the multiscale nature of the behaviour of DNA and its interaction with binding proteins (transcription factors that regulate gene expression, and repair proteins): starting from the scale of single base-pairs, I will introduce some basic models on how transcription factors guarantee the high stability of gene regulation. A rather new finding is that in fact the largest number of transciption factors appears to be bound non-specifically, posing new questions to the dynamical modelling of gene regulation. On a ‘mesoscopic’ level of dozens of base-pairs, I will move to the interaction of fluctuating DNA-bubbles and single-strand binding proteins, introducing a dynamical modelling of the protein binding that is necessary as binding kinetics and bubble lifetimes are competing. Finally, on the level of the entire DNA, I will discuss the relevance of the DNA topology on physiological processes such as transcription, and the interaction of topological defects (knots, catenanes) with repair proteins.

References: A Bakk and R Metzler, FEBS Lett 563 (2004), A Bakk et al, Biophys J 86 (2004); A Hanke and R Metzler, J Phys A Lett L473 (2003); R Metzler et al, Phys Rev Lett 88 (2002).

CPP 25.4 Di 14:45 TU C230

Local Compressibilities of Proteins Reveal the Coupling Between Protein and Solvent Dynamics — •Christina Scharnagl and Josef Friedrich — TU München, Fakultät für Physik E14, 85350 Freising

We carry out molecular dynamics simulations of cytochrome c (cyt c) in different solvents and under different external pressure. From the volume fluctuations we calculate intrinsic compressibilities. We show that the intrinsic compressibility values capture the collective correlation of local volume fluctuations with volume fluctuations in the surrounding protein-solvent system. Therefore, properties probed by a local sensor reflect also the coupling between protein and solvent dynamics.

In cyt c the heme chromophore is the local probe in optical experiments which report the low compressibility value of 0.05 1/GPa in glycerol/water (3:2 v/v) solvent. The simulations reveal that glycerol as a cosolvent decouples the volume fluctuations of the protein core from the hydration shell, while the application of high pressure reduces the localized volume fluctuations drastically. To both external perturbations, the protein responds with a reduction of its intrinsic compressibility.