BP 5: Proteins

Time: Monday 14:30–17:00 Location: ZEU 260

BP 5.1 Mon 14:30 ZEU 260

Self-assembly of peripheral membrane proteins to higher-order structures — •Gernot Guigas and Matthias Weiss — Cellular Biophysics Group, Deutsches Krebsforschungszentrum, Bioquant Center, Im Neuenheimer Feld 267, 69120 Heidelberg

Membrane proteins take part in a plethora of processes that are of vital importance for cells, e.g. signaling, vesicle formation, or protein translocation. In these processes not only transmembrane proteins are of major importance but also peripheral membrane proteins (which are embedded only in one leaflet of the lipid biayer) are involved. Using dissipative particle dynamics (DPD), we have studied generic properties of peripheral membrane proteins. Owing to the local deformation of the leaflets of the bilayer we observed a transient oligomerization of the proteins embedded in the same and/or opposing leaflets. Moreover, the diffusive mobility of these inclusions was slightly increased as compared to transmembrane proteins. Our results may explain the transient formation of gramicidin channels and the eole/function of peripheral membrane proteins in budding events.

BP 5.2 Mon 14:45 ZEU 260

The Kinetics and Structure of Protein Energy Landscapes — Michael Prentiss[1], •David Wales[2], and Peter Wolynes[1] — [1]University of California, San Diego USA — [2]Cambridge University, UK

The complexity of the physical interactions that guides the folding of biomolecules presents a significant challenge for atomistic modeling. Minimal representation protein structure prediction potentials have previously been used to predict protein structure from sequence. The resulting landscapes suggests the actual protein energy landscapes are funneled as predicted from theory. We show how basin-hopping global optimisation can identify low-lying minima for the corresponding mildly frustrated energy landscapes. Further more we calculate several disconnectivity graphs for the folding reaction a protein using a database of minima and transition states. Using these databases we calculate the diffusion of the polypeptide change as a function of an native contacts.

BP 5.3 Mon 15:00 ZEU 260

influence of external electrical fields on the protein folding process — •Ojeda May Pedro and Garcia R. Martin E. — Heinrich-Plett- Strasse 39, 34132 Kassel

We show that an external electric field can be used to modify the folding path of the peptide V3-loop, Protein Data Bank ID 1NJ0. We employ a force field which includes explicitly the dipole-dipole interactions as an Ising-term [PRL **96**, 078103, 2006]. The external electric field interacts with the dipoles. The density of states (DOS) employed to calculate the thermodynamical properties, is obtained by means of a re-weighted histogram method. In the absence of the field the dipoles can be oriented in any direction and the total free energy is minimized by a β-sheet. On the other hand, in the presence of the field an easy direction is created and the dipoles tend to be parallel to the field giving rise to a helix structure.

BP 5.4 Mon 15:15 ZEU 260

Sequence-specific size, structure, and stability of tight protein knots — •Joachim Dzubiella — Physik, TU München

Approximately 1% of protein structures display knots in their native fold. Nothing however, is known about their function. By using all-atom computer simulations we show that tightened protein knots (TPKs) exhibit a bulky size in quantitative agreement with recent atomic force microscopy (AFM) pulling and a complex stability behavior. TPKs are thus capable of blocking peptide transport through narrow (˜ 2 nm) biological pores in a sequence-dependent way. Hydrophobic side chains shield the knot core from the polar solvent, leading to an exceptionally strong H-bonding and water trapping capability of TPKs. This kinetically arrests knot diffusion along the peptide, and is controllable by the tightening force in special cases. Intriguingly, macroscopic tight knot structures are reproduced microscopically and can be tuned by sequence. Our findings may explain a function of knots in proteins, challenge previous mathematical and physical studies of macromolecular knots, and are readily verifiable in AFM or optical tweezer experiments.

BP 5.5 Mon 15:30 ZEU 260

Hydration and Temperature dependent far-infrared Investigations on Proteins — Christian U. Stehle, Wasim Abuillan, •Bruno Gompf, and Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Besides the well studied mid-infrared region with sharp absorption bands, little work has been done on proteins in the far-infrared, where they have several broad absorption bands. Extensive investigations on proteins with a high reproducibility and defined temperature/humidity have been made from 65cm-1 to 690cm-1. Several bands in the spectra of different proteins have been found in comparison to the featureless THz studies, where a protein distinction is not possible up to now. We identified the basic absorption frequencies and found at least one band that seems to be common in all proteins, which is not one of the known amide bands. Via the sorption isotherm equation the protein hydration process could be quantified and compared to the spectra, which show just small hydration dependence. This reveals that protein bound water molecules absorb much less and different than liquid water molecules. The temperature dependence shows a strong over all decrease of absorption with rising temperature. An additional frequency dependent effect especially of the low frequency band around 200cm-1 has been found.

15 min. break

BP 5.6 Mon 16:00 ZEU 260

Investigating The Protein Conducting Channel SecYEb from Methanococcus jannaschii Using Molecular Dynamics Simulation — •Andrew Aird and Jörg Wrachtrup — 3rd Physics Institute, Stuttgart University, D-70569 Stuttgart, Germany

Protein translocation, the transport of a protein through a pore is of great importance for all living organisms. It is essential for cells to have membrane channels which are able to transport proteins to different compartments inside the cell where they are needed. An example for such a channel is the protein conducting channel SecYEb from Methanococcus jannaschii. Molecular dynamics simulations are performed to understand the overall mechanism of protein transport across the membrane and address questions concerning the opening mechanism and sealing of the pore region against water and ions. Translocation processes usually take place on timescales (˜ms) not accessible to standard molecular dynamics simulation. By using steered molecular dynamics simulation to accelerate the opening process together with statistical analysis using fluctuation theorems the potential of mean force for removal of the plug is obtained.

BP 5.7 Mon 16:15 ZEU 260

Influence of solvent particles on molecular recognition — •Johannes Taktikos and Hans Behringer — Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld

We present a coarse-grained lattice model to study the influence of water on the recognition process of two rigid proteins. The basic model is formulated in terms of the hydrophobic effect. We then investigate several modifications of our basic model showing that the selectivity of the recognition process can be enhanced by considering the explicit influence of single solvent particles. When the number of cavities at the interface of a protein-protein complex is fixed as an intrinsic geometric constraint, there typically exists a characteristic fraction that should be filled with water molecules such that the selectivity exhibits a maximum. In addition the optimum fraction depends on the hydrophobicity of the interface so that one has to distinguish between dry and wet interfaces.

BP 5.8 Mon 16:30 ZEU 260

High Quality Protein Sequence Alignment combining Structural Profile Prediction and Structural Profile Alignment with SABERTOOTH — Florian Teichert[1], •Jonas Minning[1], Ugo Bastolla[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Centro de Biología Molecular 'Severo Ochoa', CSIC-UAM, Madrid, Spain

To discover evolutionary and functional relationships between proteins by alignment is a major issue in various fields. In many cases, protein

structures are not known and one has to rely on aligning protein sequences. Here, we combine (i) a recently developed ansatz to predict structural profiles from sequence with (ii) our structural alignment algorithm SABERTOOTH which is based on structural profiles [1]. Comparing the performance of the resulting sequence alignment algorithm with established tools, we prove a significantly higher quality of the determined alignments evaluated from a structural point of view.
[1] F. Teichert, U. Bastolla, and M. Porto, BMC Bioinformatics **8**, 425 (2007)

BP 5.9 Mon 16:45 ZEU 260

DNA-protein electrostatic recognition: lessons from the Protein Data Bank analysis of DNA-protein complexes — •Andrey Cherstvy — IFF, Theorie-II, FZ Jülich, 52425 Jülich, Germany

We study the details of charge distributions on DNA-binding domains of some DNA-binding proteins. This is a continuation of our research on facilitated protein diffusion on DNA and the mechanism of DNA-protein charge-charge recognition [AC et al., JPCB, 112 4741 (2008)]. We show that relatively large structural proteins of eukaryotes and prokaryotes, which involve DNA wrapping around protein cores and induce severe bends in DNA structure, do obey the theoretical model we proposed. Namely, positively charged protein residues in close proximity of DNA prefer to track the positions of individual DNA negative phosphate charges [AC, submitted to JPCB]. To show this, we have used the computational algorithm for dealing with atomic coordinates of protein amino acids and DNA phosphates available from the Protein Data Bank files for a variety of crystallized DNA-protein complexes. The specificity of amino acid distribution observed contributes to the sequence-specific DNA-protein electrostatic interactions. For the majority of DNA-protein complexes, the latter are however considered in the literature to be rather nonspecific to DNA bp sequence. For many simple/small DNA-protein complexes involving basic motifs of protein binding to DNA, we could not detect any statistical preference in distributions of positive atoms on Arginine and Lysine in DNA vicinity.