BP 5: Protein structure and dynamics I

Time: Monday 15:00–17:00 Location: ZEU 250

BP 5.1 Mon 15:00 ZEU 250

Rapid force spectroscopy — •Jakob Tómas Bullerjahn, Sebastian Sturm, and Klaus Kroy — Universität Leipzig, Institut für theoretische Physik, 04103 Leipzig, Germany

Dynamic force spectroscopy, the examination of intermolecular binding affinities and kinetics through single-molecule manipulation techniques, is a valuable complement to more traditional means of structural investigation. In contrast to scattering techniques or classical microscopy, it allows the experimentalist to gauge the dynamic and plastic behavior of a given material by directly probing the underlying free energy landscape, on a molecular scale. However, in spite of the strong forces required to do so, established theories of force spectroscopy still build on Kramers' quasistatic theory. Originally devised for the usually slow process of spontaneous unbinding, it is set to break down at high loading rates. We extend these theories to fast loading rates by explicitly resolving the nonequilibrium internal bond dynamics. Our analytical results turn out to hold almost universally, for fast and slow loading alike, breaking down only within a narrow parameter range close to a well-defined critical loading rate. Their large range of applicability moreover renders them an ideal companion to Bayesian methods of data analysis. Yielding highly competitive results, even without precise *a priori* knowledge of the underlying energy landscape, our generic analytical theory suggests itself as a unified framework for analyzing and comparing force spectroscopy data from a wide range of experiments and simulations.

BP 5.2 Mon 15:15 ZEU 250

Influence of Antifreeze Proteins on Local Water Structure Dynamics in Presence of Osmolytes — •Anand Narayanan Krishnamoorthy[1] and Jens Smiatek[2] — [1]Institute of Computational Physics, Stuttgart, Germany — [2]Institute of Computational Physics, Stuttgart, Germany

Antifreeze proteins are synthesized by various organisms to enable their cells to survive low temperature environments like in the polar regions. These proteins produce a difference between the melting and freezing points of the solutions termed as thermal hysteresis. The main objective of this study is to examine the dynamics of water molecules and hydrogen bonds at the protein-water interface of antifreeze protein using atomistic molecular dynamics simulations. For this work a prototype of AFP (antifreeze protein) from antarctic notothenioids (Ala-Ala-Thr repeats) and a mutant which is not antifreeze active were generated and compared. The hydration dynamics results reveal that the retarded water dynamics in the AFP compared to its mutant could be a possible reason for the antifreeze activity. A considerable change of the hydration dynamics was additionally observed for the AFP in presence of osmolytes. The mechanism of the interaction was investigated by analyzing the preferential binding parameter derived from Kirkwood-Buff integrals.

BP 5.3 Mon 15:30 ZEU 250

Electrochromic shift calculations exhibit the light-activation mechanism of BLUF photoreceptors — •Florimond Collette, Marcel Schmidt am Busch, and Thomas Renger — Institut für Theoretische Physik, Johannes Kepler Universität Linz, Altenberger Strasse 69, 4040 Linz, Austria

The photoreceptor family named BLUF, short for 'sensors of blue-light using flavin adenine dinucleotide (FAD)', is involved in a variety of important physiological reactions like phototaxis, photosynthetic gene regulation and virulence. Upon illumination with blue light, the photoreceptor switches into a light-adapted signaling state, with a measurable 10 to 15 nm redshift of the absorption maximum. The spectroscopic shift is explained by an alteration in the hydrogen-bonding pattern surrounding the chromophore [1]. Two opposite molecular models exist. One model is supported by the majority of crystallographic studies [2], whereas the second is favored by most spectroscopical works [3]. Within the framework of a quantum chemical/electrostatic calculation scheme, we estimated absorption shifts of the flavin chromophore for a series of site-directed mutants and different BLUF proteins. Our calculations accurately reproduce a series of spectroscopic data and provide compelling evidence for the model supported by the majority of crystallographic studies [4].

[1] S. Masuda, *Plant Cell Physiol.* **54**, 171 (2013).
[2] S. Anderson *et al.*, *Biochemistry* **44**, 7998 (2005).
[3] A. Jung *et al.*, *Proc. Natl. Acad. Sci. USA* **102**, 12350 (2005).
[4] F. Collette *et al.*, submitted.

BP 5.4 Mon 15:45 ZEU 250

Observation of the size and shape of the initial crystallites involved in crystallisation of the model protein lysozyme — •Raimund J. Heigl[1], Andreas Ostermann[2], Jörg Stellbrink[3], Aurel Radulescu[1], Dieter Richter[3], and Tobias E. Schrader[1] — [1]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Lichtenbergstr.1, 85747 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Lichtenbergstr.1, 85747 Garching, Germany — [3]Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Lysozyme serves as a model protein for the study of protein crystallisation. Yet, the size and shape of the first crystallites leading to the formation of macroscopic crystals is not known. Especially for the method of neutron protein crystallography large crystals need to be grown. Here, good understanding of the evolution of crystal growth would be advantageous. We have found crystallisation conditions of hen egg white lysozyme in D_2O which lead to the growth of a fair number of crystals. Preliminary data has been recorded on the small angle neutron scattering (SANS) instrument KWS-2 at the MLZ. It shows a decrease at an intermediate q-range between 0.01 $Å^{-1}$ and 0.02 $Å^{-1}$ and an increase at smaller q-values indicating the growth of small crystallites. Dynamic light scattering measurements point to a size distribution of three different hydrodynamic radii. One around 5 nm does not change much with time whereas the middle sized radius rapidly increases.

BP 5.5 Mon 16:00 ZEU 250

Correlation between Supercoiling and Conformational Motions of the Bacterial Flagellar Filament — •Andreas Stadler[1], Tobias Unruh[2], Keiichi Namba[3], Fadel Samatey[4], and Giuseppe Zaccai[5] — [1]FZ Jülich, ICS-1 & JCNS-1, 52428 Jülich — [2]Univ. Erlangen-Nürnberg — [3]Osaka University, Osaka, Japan — [4]Institute of Science and Technology, Okinawa, Japan — [5]Institut Laue-Langevin, Grenoble, France

The bacterial flagellar filament is a very large macromolecular assembly of a single protein flagellin. Various supercoiled states of the filament exist, which are formed by two structurally different conformations of flagellin in different ratios.

We investigated the correlation between supercoiling of the protofilaments and molecular dynamics in the flagellar filament using quasielastic and elastic incoherent neutron scattering in the picosecond and nanosecond time scales. Thermal fluctuations in the straight left- and right-handed (L- and R-type) filaments were measured and compared to the wild-type filament. Amplitudes of motion in the picosecond time scale were found to be similar in the different conformational states. Mean square displacements and protein resilience in the 0.1 nanosecond time scale demonstrate that the L-type state is more flexible and less resilient than the R-type, while the wild-type state lies in between. Our results provide strong support that supercoiling of the protofilaments in the flagellar filament is determined by the strength of molecular forces in and between the flagellin subunits.

BP 5.6 Mon 16:15 ZEU 250

Revealing Rad51 and 53BP1 distribution in HeLa cell nuclei after low and high LET irradiation — •Judith Reindl[1], Guido A. Drexler[2], Stefanie Girst[1], Christoph Greubel[1], Christian Siebenwirth[1], Sophie Drexler[2], Anna A. Friedl[2], and Günther Dollinger[1] — [1]Universität der Bundeswehr, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany — [2]Ludwig-Maximilians-Universität München, 80336 München, Germany

53BP1 and Rad51 are prominent representatives for two DNA damage repair compartments, the flanking chromatin and the single-stranded DNA (ssDNA) compartment. The correlation between these two repair proteins is revealed by super high resolution STED microscopy with respect to the damage distribution inside a cell nucleus. Ionizing radiation creates double-strand breaks (DSB) of high local density and different complexity with respect to its LET (Linear Energy Transfer).

Therefore low LET proton and high LET carbon ion irradiation at the irradiation facility SNAKE are used to generate different damage distributions inside cell nuclei. It is possible to image and analyse the ionizing radiation induced foci (IRIF) in their fine structure and visualize the mutual exclusion of the two damage repair compartments in one cell nucleus by analysing the correlation of Rad51 and 53BP1. Therefore a newly designed analysis program is used, which examines the local correlation of two signalling channels. The presented experimental findings clearly support the two compartment model which could be demonstrated for the first time in one cell for Rad51 and 53BP1.

Topical Talk BP 5.7 Mon 16:30 ZEU 250

Particle-based stochastic computer simulations of biological systems — •Ulrich Schwarz — Heidelberg University, Heidelberg, Germany

Evolution is a tinkerer and biological systems have evolved because they work, not because they are beautiful or optimal. Although some biological systems show striking examples of pattern formation, self-assembly or control circuits that occur in a similar manner in physical or engineered systems, very often these aspects are strongly intertwined in biological systems. From the modelling point of view, particle-based stochastic computer simulations are a very fruitful approach to investigate these different aspects of biological systems in one unifying framework. We will first discuss this point for the Min-proteins, which have been shown to develop beautiful spatio-temporal oscillations patterns in reconstitution assays, but which are also related to bacterial regulation. We will then discuss self-assembly of viral capsids, which in some cases might be regulated by event-driven switches in capsomere reactivity. In both cases, particle-based stochastic computer simulations have been successfully used to investigate the detailed dynamics leading to the final state.