BP 23: Posters - Protein Structure and Dynamics

Time: Monday 17:30–19:30 Location: Poster C

BP 23.1 Mon 17:30 Poster C

Structural Changes of Human IgG Antibody under High Hydrostatic Pressure — •Nico König[1,2], Julian Schulze[1], Karin Julius[1], Michael Paulus[1], Clara Grüning[2], Philipp Ellinger[2], Matthias Voetz[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund — [2]Bayer Technology Services GmbH, Leverkusen

A new trend in food industry is to pasteurize foodstuff via high pressure. It is therefore of interest if proteins withstand a high hydrostatic pressure treatment conserving their native structure. In the future this question might also be of relevance in the life science industry.

We report on the investigation of the human antibody Immunoglobulin G (IgG) under high hydrostatic pressure. IgG antibodies play a crucial role in the adaptive immune system of vertebrates. The tips of the Y-shaped IgG antibody represent the paratopes which bind their respective epitopes on the antigen (e.g. other proteins or small molecules). The high binding affinity and engineering of antibodies opens a wide range of applications within the life science industry.

Thus, for future applications of high-pressure treatment in the life science industry it is interesting to investigate the behaviour of IgG antibodies under high hydrostatic pressure. We conducted high-pressure small-angle X-ray scattering (SAXS) experiments on IgG to check for structural changes. Additional experiments were performed using circular dichroism spectroscopy (CD) and dynamic light scattering (DLS).

BP 23.2 Mon 17:30 Poster C

Protein folding investigated by SANS/SAXS small angle scattering and neutron spin-echo — •Felix Ameseder[1], Aurel Radulescu[2], Olaf Holderer[2], Andreas Stadler[1], and Dieter Richter[1] — [1]Forschungszentrum Jülich GmbH, Neutron Scattering, JCNS/ICS-1 — [2]Forschungszentrum Jülich GmbH, Neutron Scattering, JCNS-FRMII

The process of protein folding is highly dependent on the amino acid composition as well as on the solution condition, especially on the presence of denaturant. Our approach is to describe the folding by coefficient dimension of polymer scaling laws, and measure the folding as a function of denaturant type and denaturant concentration which has proved to be promising in singlemolecule FRET experiments. Here, we use SANS/SAXS to determine the structure of bovine serum albumin m=66kD in H20/D2O buffer solution and at various concentrations of guanidine hydrochloride and β-mercaptoethanol as additional solvent. The global dynamics of native and unfolded BSA is investigated with dynamic light scattering spectroscopy. The advantage of neutron spin-echo spectroscopy is used to cover a time range up to 140ns with spacial resolution from $q = 0.05A^{-1}$ to $q = 0.17A^{-1}$. SANS and SAXS results of native BSA show agreement with coherent scattering intensities calculated from crystal structure model of a respective monomer. All scattering data of unfolded structures reveal distinct evidence of the lost of internal order. NSE measurements of disordered structures reveal a contribution of internal dynamics to global diffusion.

BP 23.3 Mon 17:30 Poster C

On the α-Helical Coiled Coil to β-Sheet Conversion in Regenerated Hornet Silk — •Andreas Schaper[1], Taiyo Yoshioka[2], Tsunenori Kameda[2], Kohji Tashiro[3], Takashi Nemoto[4], and Tetsuya Ogawa[4] — [1]Philipps University, Marburg, Germany — [2]National Institute of Agrobiological Sciences, Tsukuba, Japan — [3]Toyota Technological Institute, Nagoya, Japan — [4]Kyoto University, Uji, Japan

Alpha-helices, alpha-helical coiled coils and β-sheets are fundamental principles of chain folding in fiber-forming proteins. Evolution has been creating numbers of different structures by varying the intrinsic properties of the amino acid sequences as well as the pathway the fibrillar structures are produced. Studies of protein denaturation as it is initiated by solvents, inappropriate pH level, elevated temperature or other forms of stress, including mechanical deformation and distortion, are key for solving fundamental questions regarding the stability of native α-helix structures and their tendency to undergo amyloid or amyloid-like structure formations under non-physiological conditions.

Resuming our recent studies of the structural details of native silk from the hornet Vespa mandarinia [1], here we report X-ray and electron diffraction observations of regenerated silk under different drawing regimes. We succeeded in evaluating the transformation from a dominant four-strand alpha-helical coiled coil [1,2] to an advanced twisted cross-beta state.

[1] T. Kameda et al., J. Struct. Biol. 185, 303 (2014); [2] R.D.B. Fraser and D.A.D. Parry, J. Struct. Biol. 192, 528 (2015)

BP 23.4 Mon 17:30 Poster C

Dissociation dynamics of the viral protein hemagglutinin and the cellular receptor sialic acid analyzed by single-molecule force spectroscopy — •Valentin Reiter[1], Sumati Bhatia[2], Daniel Lauster[3], Manuel Gensler[1], Luis Cuellar[2], Rainer Haag[2], Andreas Herrmann[3], and Jürgen P. Rabe[1] — [1]Department of Physics + IRIS Adlershof, Humboldt-Universität zu Berlin — [2]Department of Chemistry, Freie Universität Berlin — [3]Department of Biology, Humboldt-Universität zu Berlin

The trimeric transmembrane protein hemagglutinin (HA) comprises over 80% of the envelope proteins present in the influenza virus and it has an essential role in the reproduction of the virus in epithelial cells by binding to sialic acid (SA) containing glycoproteins [1]. Binding of nanoparticles to the HA can hinder cell attachment and inhibit viral infection [2]. For the development of more potent inhibitors, the binding should be understood on the single-molecule level. Scanning force microscope (SFM) based single-virion force spectroscopy has proven to be a valuable tool to directly probe molecular interactions of virion-cell binding and precisely determine pN-ranged forces that govern the receptor ligand dissociation [3]. Using immobilized single proteins and SFM cantilevers functionalized with SA we measured the rupture forces of single HA-SA bonds under dynamic loads and derive a significantly larger dissociation rate and rupture length compared to single virion experiments [3] which will be discussed. [1] G. M. Whitesides et al., Angew. Chem. Int. Ed. 1998, 37, 2754; [2] I. Papp et al., ChemBioChem 2011, 12, 887; [3] C. Sieben et al., PNAS, 2012, 109, 13626.

BP 23.5 Mon 17:30 Poster C

Particle-based computer simulations of protein self-assembly in shear flow — •Fabian B. Fuchs, Nikolas Schnellbächer, and Ulrich S. Schwarz — University of Heidelberg, BioQuant, ITP

Many proteins self-assemble into supramolecular complexes, with examples ranging from small signaling complexes through clathrin coats or viral capsids to large scale cytoskeletal structures like actin networks or the mitotic spindle. Many of them, most prominently the viral capsids, can also be studied outside the cellular context. As an important step towards more complex environments, here we study protein self-assembly in hydrodynamic flow. To include hydrodynamic interactions, we have developed a novel hybrid algorithm embedding proteins in an explicit solvent. The proteins are propagated using molecular dynamics with protein reactions being implemented through reactive patches on their surface. The solvent is realized using Multi Particle Collision Dynamics (MPCD). As paradigmatic examples with anisotropic intermediates, we examine the assembly of rods and rings as a function of concentration, shear flow and binding rate constants.