L-24 **Friday, 17.06., 9^{00} - 9^{40}**

High Brilliance SAXS on synchrotrons

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The brilliance of the X-ray beam is the important quality parameter of X-ray sources. Brilliance sums up the beam parameters such as beam intensity, opening angle of the beam, size of the beam and the proportion of monochromaticity of the X-ray radiation. With existing modern X-ray optics many of these beam parameter can be altered, however beam focusing and the opening angle dependent strongly on the source. Because of the special arrangements of the beamline components SAXS relies on the high brilliance of the X-ray beam delivered by modern synchrotrons. At such state-of-the-art high brilliance beamlines high quality SAXS data are collected within several milliseconds on very small sample volumes. On the other hand, high brilliance X-rays are causing radiation damage especially to biological samples, which has to be treated by counteractions.

New developed, advanced sample environments based on microfluidic devices allows handling sample volumes of several pico-liters. Such devices are used for SAXS high throughput screening of hundreds of different sample conditions. If such a screening campaign includes as well automated data analysis procedures up to final model building, SAXS will be the method of choice for e.g. ligand screening in pharmaceutical industries.

Since microfluidic devices can operate on low flow rates on small channels, effects of low Reynolds numbers provide different types of SAXS experiments. For instance fast mixing of liquids is used for time resolved scattering experiments. Further applications are online sample preparation by applying mechanical and physical stress to the sample. While such techniques allow analyzing the kinetics of chemical or biochemical reactions, need investigations on the dynamics of a system a more sophisticated approach.

At high brilliance X-ray sources classical pump-probe experiments facilitates the analysis of reaction dynamics. For these investigations, for instance an ultra-short laser pulse is triggering the reaction in the sample. The high flux synchrotron beam is used for investigated the structural response of the system. Such experiments need, beside the brilliance of a synchrotron beam suitable fast detector system for recording the data in short time frames.

This lecture introduces the brilliance parameter and describe modern X-ray optics. The fields of applications are discussed and some experimental highlights shown. Possible strategies for handling radiation damage will be presented and future directions of SAXS introduced.

L-25 **Friday, 17.06., 9^{40} - 10^{20}**

Integration of SAXS with Complementary Techniques for Structural Characterization of Large Biomolecular Complexes

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Keywords: Integrative Structural Biology, SAXS, NMR, EM

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Structural analysis of multi-domain protein complexes is a key challenge in current biology and a prerequisite for understanding the molecular basis of essential cellular processes. The use of solution techniques is important for characterizing the quaternary arrangements and dynamics of domains and subunits of these complexes. As experimental data for large protein complexes are sparse, it is advantageous to combine these data with additional information from other solution techniques.

In my presentation I will show our recent achievements in integrating Small-Angle X-ray Scattering (SAXS) data with complementary data from Nuclear Magnetic Resonance Spectroscopy, X-ray crystallography, electron microscopy, and mass spectrometry to study structure and dynamics of large disease-related proteins and protein complexes [1-9]. By using our integrated approach we were able to provide a comprehensive and accurate description of protein complex structure and dynamics in a native-like environment. This underscores the central role of SAXS for structure determination of protein complexes and ensures its unique role and contributions in integrated structural biology approaches in the future.

Acknowledgments: This work was supported by the Bavarian Ministry of Sciences, Research and the Arts (Bavarian Molecular Biosystems Research Network), the German Research Foundation (Emmy Noether program MA 5703/1-1), the Center for Integrated Protein Science Munich (CIPSM), and the Austrian Science Fund (FWF: P28854).

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[1] M. Gersch, K. Famulla, M. Dahmen, C. Gobl, I. Malik, K. Richter, V. S. Korotkov, P. Sass, H. Rubsamen-Schaeff, T. Madl, H. Brotz-Oesterhelt, S. A. Sieber, *Nat. Comm.* **6** (2015) 6320.

[2] C. Gobl, T. Madl, B. Simon, M. Sattler, *Prog Nucl Magn Reson Spectrosc* **80** (2014) 26.

[3] V. Haslbeck, J. M. Eckl, A. Drazic, D. A. Rutz, O. R. Lorenz, K. Zimmermann, T. Kriehuber, C. Lindemann, T. Madl, K. Richter, *Sci Rep* **5** (2015) 17058.