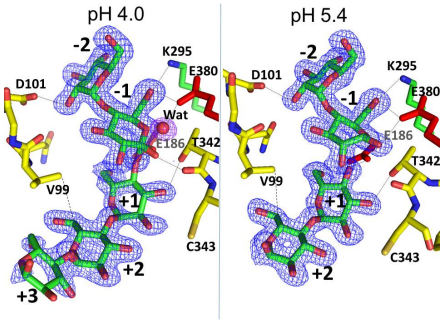

Figure 1. The effect of pH on the binding mode of maltose in the active site of SBA.

Keywords: β-amylase, capillary measurement

MS9-O5 Lipidic cubic phase injector is a viable crystal delivery system for time-resolved serial crystallography

Przemyslaw Nogly[1], Valerie Panneels[1], Garrett Nelson[2], Cornelius Gati[3], Tetsunari Kimura[4], Christopher Milne[5], Despina Milathianaki[6], Minoru Kubo[4], Wenting Wu[1], Chelsie Conrad[7], Jesse Coe[7], Richard Bean[3], Yun Zhao[2], Petra Bath[8], Robert Dods[8], Rajiv Harimoorthy[8], Kenneth Beyerlein[3], Jan Rheinberger[1], Daniel James[2], Daniel DePonte[6], Chufeng Li[2], Leonardo Sala[5], Garth Williams[6], Mark Hunter[6], Jason E. Koglin[6], Peter Berntsen[8], Eriko Nango[9], So Iwata[9], Henry Chapman[3], Petra Fromme[7], Matthias Frank[10], Rafael Abela[5], Sébastien Boutet[6], Anton Barty[3], Thomas A. White[3], Uwe Weierstall[2], John Spence[2], Richard Neutze[8], Gebhard Schertler[1], Jörg Standfuss[1]

1. Laboratory for Biomolecular Research, Paul Scherrer Institute, 5232 Villigen, Switzerland
2. Department of Physics, Arizona State University, 85287 Tempe AZ, USA
3. Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany
4. Biometal Science Laboratory, RIKEN SPring-8 Center, 679-5148 Hyogo, Japan
5. SwissFEL, Paul Scherrer Institute, 5232 Villigen, Switzerland
6. Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, 94025 Menlo Park, USA
7. Department of Chemistry and Biochemistry, and Center for Applied Structural Discovery, Biodesign Institute, Arizona State University, 85287-1604 Tempe, USA
8. Department of Chemistry and Molecular Biology, University of Gothenburg, Gothenburg, Sweden
9. SACLA Science Research Group, RIKEN/SPring-8 Center, 679-5148 Hyogo, Japan
10. Lawrence Livermore National Laboratory, 94550 Livermore, USA

email: przemyslaw.nogly@psi.ch

Serial femtosecond crystallography (SFX) using X-ray free-electron laser (XFEL) sources is a newly developed method with considerable potential for time-resolved pump probe experiments. I will present a lipidic cubic phase SFX structure of the light-driven proton pump bacteriorhodopsin (bR) to 2.3 Å resolution and a method to investigate protein dynamics with modest sample requirement. Time-resolved serial femtosecond crystallography (TR-SFX) with a pump-probe delay of 1 ms yields Fourier difference maps (F_o-F_o) compatible with the dark to M state transition of bR. Importantly the method is sample efficient and reduces sample consumption to a few milligrams of protein per collected time point. Accumulation of M intermediate within the crystal lattice is confirmed by time-resolved visible absorption spectroscopy. The impact of radiation damage free data collection using femtosecond XFEL pulses on the study of structural intermediates is discussed and compared with serial millisecond crystallography (SMX) at a synchrotron source. This study provides an important step towards characterizing the dynamics of complete photocycles of retinal proteins and demonstrates the feasibility of a sample efficient viscous medium jet in TR-SFX.

Nogly, P., Panneels, V., Nelson, G., Gati, C., Kimura, T., Milne C., Milathianaki, D., Kubo, M., Wu, W., Conrad, C., Coe, J. Bean, R., Zhao, Y., Bath, P., Dods, R., Harimoorthy, R., Beyerlein, K.R., Rheinberger, J., James, D., DePonte, D., Li, C., Sala, L., Williams, G., Hunter, M., Koglin, J.E., Berntsen, P., Nango, E., Iwata, So., Chapman, H.N., Fromme, P., Frank, M., Abela, R., Boutet, S., Barty, A., White, T.A., Weierstall, U., Spence, J., Neutze, R., Schertler, G. &Standfuss, J. *Lipidic cubic phase injector is a viable crystal delivery system for time-resolved serial crystallography.* (2016) under revision. Nogly, P., James, D., Wang, D., White, T. A., Zatsepin, N., Shilova, A., Nelson,

G., Liu, H., Johansson, L., Heymann, M., Jaeger, K., Metz, M., Wickstrand, C., Wu, W., Bath, P., Berntsen, P., Oberthuer, D., Panneels, V., Cherezov, V., Chapman, H., Schertler, G., Neutze, R., Spence, J., Moraes, I., Burghammer, M., Standfuss, J. &Weierstall, U. *Lipidic cubic phase serial millisecond crystallography using synchrotron radiation.*(2015) IUCrJ 2.

Keywords: time-resolved crystallography, bacteriorhodopsin, Xray Free Electron Laser

MS10 H-bonding & weak interactions in crystals: neutrons and X-rays

Chairs: Boris Zakharov, Amber Thompson

MS10-O1 Nanoscale hydrogen bound network revealed by neutron scattering

Heloisa N. Bordallo[1]

1. The Niels Bohr Institute - University of Copenhagen - Copenhagen - Denmark

email: bordallo@nbi.ku.dk

Neutron science is the science of everyday life, providing a microscopic view of the materials we rely on for modern life. Neutrons, similarly to X-rays, penetrate matter. However, unlike X-rays, neutrons interact with matter in a different manner, thus allowing the identification of elements with very low molecular weight, including hydrogen. Thus while X-rays is one of the most important characterization methods in solid state chemistry and materials science, neutron diffraction is more commonly used to provide information on proton distribution within the structure. For this reason, both X-rays and neutron diffraction, complemented by neutron spectroscopy, which brings information about hydrogen mobility, can contribute for better understanding of complex structures. In this talk I will discuss on this promising approach by presenting a couple of specific examples. The first is related to a number of differences in the structural and dynamical behavior of D-alanine when compared to L-alanine[1] and the second to the interplay of molecular flexibility and hydrogen bonding manifested in the polymorphs of paracetamol.[2] Finally I will give a brief overview in how this approach can extend to the study of highly intricate pore structures.[3]

[1] E. Belo, P.T.C Freire, J. E. M. Pereira, D. N. Argyriou, T. Seydel, H.N. Bordallo (2016) Manuscript in preparation.

[2] N. Tsapatsaris, B.A. Kolesov, J. Fischer, E.V. Boldyreva, L. Daemen, J. Eckert, and H.N. Bordallo (2014) Polymorphism of Paracetamol: A new understanding of molecular flexibility through local methyl dynamics. Molecular Pharmaceutics **11**, 1032-1041.

[3] A.R. Benetti, J. Jacobsen, B. Lehnhoff, N.C.R. Momsen, D.V. Okhrimenko, M.T.F. Telling, N.Kardjilov, M. Strobl, T. Seydel, I. Manke and H.N. Bordallo (2015) How mobile are protons in the structure of dental glass ionomer cements? Sci. Rep. **5**, 8972 (8 pages)

Keywords: hydrogen bond dynamics, flexibility, conformational change