

Time-resolved mixing-jet X-ray Free Electron Laser crystallography experiments

Dominik Oberthuer¹, Juraj Knoška¹, Max Oliver Wiedorn¹, Saša Bajt², Henry N Chapman¹

¹Center For Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany, ²Photon Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
E-mail: dominik.oberthuer@desy.de

Serial Femtosecond Crystallography (SFX) at X-ray Free Electron Laser (XFEL) sources enables structure determination from sub-micron sized crystals of biological macromolecules. Because of their size and thus possible short diffusion times of substrates or ligands into them, those crystals can be used for mix-and-diffuse serial crystallography experiments to unravel structural dynamics and/or enzymatic reaction pathways at atomic spatial- and μ s to ms time resolution. The ultimate goal would be to produce molecular movies from such experiments and complementary techniques (e.g. spectroscopy, ultra-microscopy) to understand biological systems on length-scales from atoms to cells and organisms. Here we present results from first successful mix-and-diffuse SFX experiments at the XFEL LCLS [1, 2], the on-going development of novel injection devices for improved and efficient sample delivery [3] and latest progress on the way towards optimized mixing-jets for time resolved experiments.

[1] Stagno, J. R. et al. (2017). Nature 541, 242-246.

[2] Kupitz, C. et al. (2017). Structural Dynamics 4, 044003.

[3] Oberthuer, D. et al. (2017). Sci.Rep. (accepted manuscript)

Keywords: [Time resolved crystallography](#), [SFX](#), [XFEL](#)