MS36.O05

Improving the accuracy for Photosystem II and other XFEL structures

N. Sauter[1], A. Brewster[1], J. Hattne[1], M. Amin[1], J. Kern[1], J. Yano[1], V. Yachandra[1]
[1]*Lawrence Berkeley National Laboratory, Physical Biosciences Division, Berkeley, CA, USA*

Femtosecond-scale XFEL pulses can produce diffraction free from radiation damage, under functional physiological conditions where reaction dynamics can be studied for systems such as photosystem II. However, it has been extremely difficult to derive accurate structure factors from the data since every shot is a still exposure from a distinct specimen. Accuracy can be improved by software methods implemented in the program cctbx.xfel, including optimal indexing and retention of data from multiple lattices, and separate determination of the resolution cutoff for individual lattices. Various techniques can produce well-conforming descriptions of the Bragg spot shape and crystal mosaicity, enabled in part by sub-pixel characterization of the detector geometry. By carefully discriminating between image pixels known to contain diffraction signal and the surrounding pixels containing only background noise, and by extending postrefinement techniques that lead to a better crystal orientation, we derive accurate structure factors with substantially fewer crystal specimen exposures. It is hoped that these developments will make it easier to measure small structure factor differences, such as those from anomalous scattering that will enable the de novo determination of macromolecular structure.

[1] *Hattne, J., et al. (2014) Accurate macromolecular structures using minimal measurements from X-ray free-electron lasers. Nature Methods, advance online publication, 16 March 2014.,* ***[2]*** *Kern, J., et al. (2013) Simultaneous femtosecond X-ray spectroscopy and diffraction of photosystem II at room temperature. Science 340, 491-495.*

Keywords: XFEL, Macromolecular Crystallography, Serial femtosecond crystallography