New Opportunities for Structural Biology Research at SSRL and LCLS

Ana Gonzalez, representing the entire SSRL-SMB team.

SSRL, SLAC National Accelerator Laboratory, Menlo Park, California, 94025, USA.

The Structural Molecular Biology (SMB) program at the Stanford Synchrotron Radiation Lightsource (SSRL) provides an integrated suite of macromolecular crystallography (MC) and small angle x-ray scattering (SAXS) beam lines and facilities enabling studies on the most challenging problems in structural biology. These include the undulator station BL12-2 optimized for micro-beam MC experiments, BL9-2, BL7-1 and BL14-1 optimized for high-throughput MC screening and data collection, and BL4-2, a small angle x-ray scattering/diffraction station that provides state-of-the-art experimental facilities for equilibrium and time-resolved structural studies on non-crystalline biological materials in solution. The SMB program also includes x-ray absorption, emission and imaging spectroscopy facilities. A next-generation undulator microfocus beam line, BL12-1, which will provide a preeminent capability for MC research in the US, is under construction. BL12-1 will be outfitted with a broad bandpass capability which will provide exceptional brightness, smaller microbeams and a high number of reflections when rastering on the fly or using crystal injectors. It will be equipped with a high speed EIGER PAD detector and a high speed multi-axis goniometer, enabling new approaches for data collection and phasing. Similarities in instrumentation, existing and new sample delivery systems, and software environments will form the foundation of a synergistic relationship between the SSRL BL12-1 and a new Macromolecular Femtosecond crystallography instrument (MFX) at LCLS, through a Gateway approach.

LCLS-MFX began experiments with the start of the user program on July 1, 2016. Various sample delivery and data acquisition systems are currently being implemented at MFX, which will enable serial crystallography and in-situ spectroscopic monitoring and promise to reveal the structures and dynamics of complex biomolecules. The standard sample environment available to the scientific general user community at MFX is a highly automated goniometer setup for diffraction experiments, developed and supported by the SMB group. The experimental front-end is based on developments at SSRL and LCLS XPP to provide an efficient framework to carry out goniometer-based FX experiments using automated strategies tailored to handle a variety of sample requirements, crystal sizes and experimental goals. These developments coupled with improvements in data processing algorithms make it possible to derive high resolution crystal structures using only 100 to 1000 still diffraction images.