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"Trans to cis isomerization in a biological macro-molecule observed with ultrafast time-resolved serial femtosecond crystallography"

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April 15, 2016, UWM EMS E237

Abstract:

Serial Femtosecond Crystallography (SFX) is an emerging technique performed at ultra-brilliant and ultra-shortly pulsed X-ray sources. The Linac Coherent Light Source (LCLS) at SLAC in Stanford, Ca is a Free Electron Laser for Hard X-rays (X-ray FEL) which produces ultra-short (~40 fs, 40 x 10^{-15} s) X-ray pulses with 10^{12} X-ray photons in each pulse. The X-ray beam can be focused to spots smaller than 1 micrometer which is exquisitely suited to investigate tiny specimen such as nano- and micro crystals down to the single molecule level. The tiny crystals are injected into the X-ray beam one by one, in a serial fashion, each crystal in random orientation. When a crystal in flight is hit by the intense 40 fs X-ray pulse, it disintegrates. However, before it is destroyed, it scatters and a diffraction pattern with Bragg spots is recorded on a specially designed detector with fast readout times. This is called the diffraction-before-destruction principle and lies at the heart of SFX. From tens of thousands of these diffraction patterns complete crystallographic datasets with accurate intensities can be collected. If a reaction can be initiated in the crystal for example with an ultrashort optical laser pulse a time-delay delta-t before it is probed by the X-ray pulse, the reaction can be structurally investigated. The time-resolution is essentially given by the 40 fs duration of the X-ray pulse. The tiny crystals are intercepted twice in flight, first by the optical pump laser pulse, and then by the probe X-ray pulse. SFX becomes time-resolved (TR-SFX) . Here, TR-SFX results are presented on a time-scale from 100 fs to 1 ms. We show the earliest events of a photo-activated reaction in a protein and gain unprecedented insight into the chemistry and the mechanism of the reaction.