

Insights into the oxygen-evolving mechanism of photosynthesis using XFELs

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X-ray free electron lasers (XFELs) provide a unique opportunity for time resolved, damage-free studies of dynamic systems due to the ability of femtosecond-long laser pulses of extreme intensity to diffract on a much shorter time scale than the onset of radiation damage. We have applied this technique to the study of water oxidation in photosystem II (PSII), the transmembrane protein where water is converted to oxygen in plants and photosynthetic cyanobacteria. A nanoflow liquid jet¹ or acoustic droplet ejection² is used to deliver microcrystals suspended in buffer to the XFEL beam. Placement of visible lasers in the path of the jet or droplets allows timed illumination for selection of any stable or transient state of the catalytic center in the water-splitting cycle. In recent XFEL experiments, we obtained the first high-resolution room-temperature diffraction data for the dark and twice-illuminated (2F) states of PSII, which allowed us to exclude several proposed mechanisms for water oxidation.³

We are currently investigating the structural differences between our room-temperature crystal structures and recent high-resolution cryogenic PSII crystal structures as well as structural differences at the catalytic center in our room temperature datasets in various illuminated states (unpublished work). We are also continuing development of XFEL-specific data processing methods and a graphical user interface for real-time data processing during XFEL experiments.

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Keywords: [photosynthesis](#), [XFEL](#), [time-resolved](#)