Time resolved structural investigation of oxygen evolving complex In Photosystem II

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Photosynthesis is responsible for the accumulation of dioxygen in the earth´s atmosphere. Photosynthetic water oxidation in green plants, algae and cyanobacteria is catalyzed by the Mn_4CaO_5 cluster associated with the Photosystem II core complex (PSIIcc), a multi subunit membrane protein complex. In the last decade, the electronic and geometric structures of this light-driven water splitting catalyst have been extensively investigated. Until now, the dynamic mechanism of the water oxidation reaction at the Mn_4CaO_5 cluster is still elusive. During the last decade, conventional synchrotron X-ray radiation crystallography was used to determine the structure of PSIIcc from cyanobacteria, which always implies radiation damage of the Mn_4CaO_5 cluster to a certain extent (Umena et al, 2011). In contrast, employing femtosecond X-ray diffraction on PSIIcc microcrystals by using a free electron laser provides the possibility for recording the diffraction data at room temperature before the onset of radiation damage (Nature; Kern et al, Science, 2013). In addition, this technique allows to follow the dynamic changes in the structure of the Mn_4CaO_5 cluster at ambient conditions, which is a key to deriving the water oxidation mechanism. In our previous Linac coherent light source (LCLS) experiments, we were able to continuously improve the diffraction pattern of our PSIIcc microcrystals (i.e., < 50 µm) and obtained a crystal structure of an intact dark resting state, S_1 state (Kern et al, 2013, PNAS). We also measured preliminary X-ray diffraction data of the light-induced next state in the catalytic cycle, the S_2 state, and developed snap-shot X-ray emission data collection from the microcrystals and solution samples (Kern et al, Science, 2013; Kern et al, submitted). For these dynamic LCLS experiments, we are continuously improving our seeding protocol in order to produce better PSIIcc microcrystals. The microcrystals obtained using the traditional detergent β-n-dodecyl-maltoside showed a diffraction resolution of 4.5 Å. Very recently, a new detergent, octaethylene glycol monododecyl ether ($C_{12}E_8$) was used for crystallization leading to a structure at 2.44 Å resolution (Hellmich et al, submitted). Work is in progress to obtain $C_{12}E_8$-PSIIcc microcrystals for room temperature femtosecond X-ray diffraction experiments.