Exploring the dynamic of PSII at room temperature by simultaneous femtosecond X-ray spectroscopy and dffraction

Photosystem II (PSII) is a membrane protein that catalyzes photo oxidation of water into dioxygen, one of nature's most fascinating and important reactions. The water-splitting reaction takes place at the oxygen evolving complex (OEC), through five intermediate S-states (S_0 to S_4)[1], where S_1 is the dark-stable state and S_3 is the last semi-stable state before O-O bond formation and O_2 evolution. The structure of PSII in the dark state has been solved by X-ray diffraction and X-ray free electron laser (XFEL) providing information of the structural geometry of the Mn_4CaO_5 cluster in OEC. However, to fully understand the O-O bond formation mechanism, elucidating the structures of the OEC in the different S-states is essential.

In our recently published study, we report high-resolution structures of PSII at room temperature using XFEL coupling with X-ray spectroscopy under different illumination conditions. This enables us to gain new insights about the dynamic changes in the structure of the Mn_4CaO_5 cluster as well as the ligands and the bound water molecules. We further use ammonia as water analogue to investigate the water-binding site(s) and discriminate between mechanisms proposed in literature. We discuss the precise role of the water bound to OEC in electron transfer and the water-splitting reaction.

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