

MS08-01 | CAPTURING REACTION INTERMEDIATES OF THE WATER OXIDATION REACTION IN PHOTOSYSTEM II AT X-RAY FREE ELECTRON LASERS

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The water oxidation reaction in nature occurs in Photosystem II (PS II), multi-subunit protein complex, in which the Mn_4CaO_5 cluster catalyzes the reaction. The reaction comprises four (meta)stable intermediates (S_0 , S_1 , S_2 and S_3) and one transient S_4 state, which precedes dioxygen formation occurring in a concerted reaction from two water-derived oxygens bound at the OEC. This reaction is coupled to the two-step reduction and protonation of the mobile plastoquinone Q_B at the acceptor side of PS II.

Using serial femtosecond X-ray crystallography (SFX) and simultaneous X-ray emission spectroscopy (XES) with multi-flash visible laser excitation at room temperature, we studied all (meta)stable states with resolutions of 2.04-2.08 Å. We also collected some timepoint data between the S-states in order to understand the sequence of events. The current status of this research and the mechanistic understanding of the water oxidation reaction based on the X-ray techniques is presented.

[1] J. Kern, et al. Structures of the intermediates of Kok's photosynthetic water oxidation clock, *Nature*, **563**, 421 (2018).