Capturing Reaction Intermediates of the Water Oxidation Reaction In Photosystem II

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The water oxidation reaction in nature occurs in Photosystem II (PS II), multi-subunit protein complex, in which the Mn4CaO5 cluster catalyzes the reaction. The reaction comprises four (meta)stable intermediates (S0, S1, S2 and S3) and one transient S4 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 QB 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 have investigated all (meta)stable states. 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.