

The present status of DFT studies on water oxidation in photosystem II is described. It is argued that a full understanding of all steps is close. In each S-transition, the manganese that is oxidized and the proton released are strongly implicated, and structures of all intermediates have been determined. For the S<sub>2</sub>-state, recent important experimental findings support key elements of the structure and the mechanism. In this mechanism, the O-O bond is formed between an oxyl radical in the center of the cluster and a Mn-bridging  $\mu$ -oxo ligand, which was suggested already in 2006. The DFT structure of the oxygen evolving complex, suggested in 2008, is very similar to the recent (2011) high-resolution X-ray structure.