Energy conversion in photosynthesis¹
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Photosystem II (PSII) uses light energy to split water into protons, electrons and O₂ [1]. In this reaction, Nature has solved the difficult chemical problem of efficient four-electron oxidation of water to yield O₂ without significant side reactions. In order to use Nature’s solution for the design of materials that split water for solar fuel production, it is important to understand the mechanism of the reaction. The X-ray crystal structures of cyanobacterial PSII provide information on the structure of the Mn and Ca ions, the redox-active tyrosine called YZ, and the surrounding amino acids that comprise the O₂ evolving complex (OEC) [2,3]. We have used computational studies used to refine the structure of the OEC to obtain a complete structural model of the OEC that is in agreement with spectroscopic data [4,5]. The structure of the OEC and the mechanism of water oxidation by PSII will be discussed in the light of biophysical and computational studies, inorganic chemistry and X-ray crystallographic information.

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