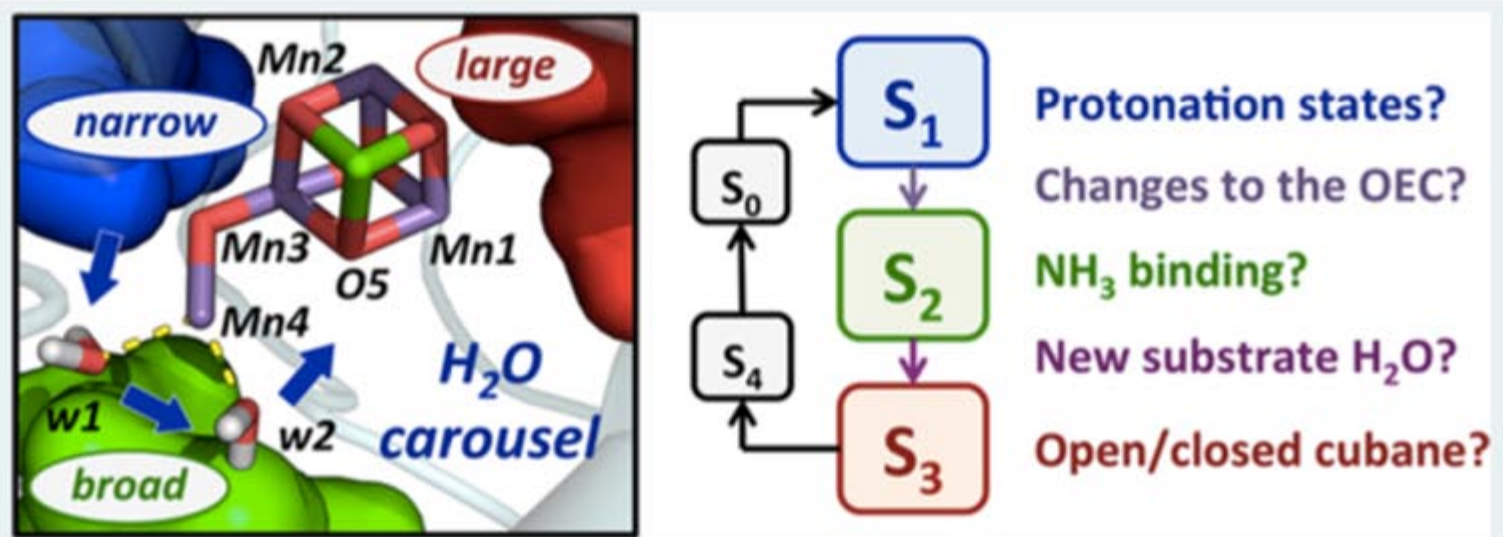


The O₂-Evolving Complex of Photosystem II: Recent Insights from Quantum Mechanics/Molecular Mechanics (QM/MM), extended X-ray Absorption Fine Structure (EXAFS), and Femtosecond X-ray Crystallography Data

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Femtosecond XFEL diffraction experiments in conjunction with QM/MM calculations, mutagenesis experiments, high resolution EXAFS and IR spectroscopy have provided valuable insights into the structure and function of the OEC and the underlying transitions along the catalytic cycle, including changes in protonation/redox states and the mechanism of substrate water binding.