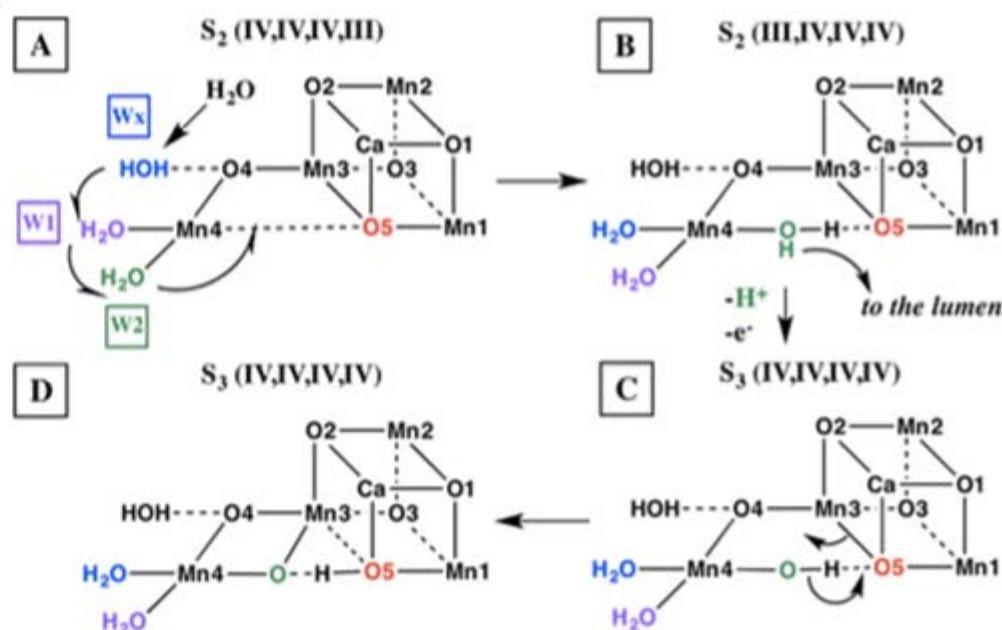
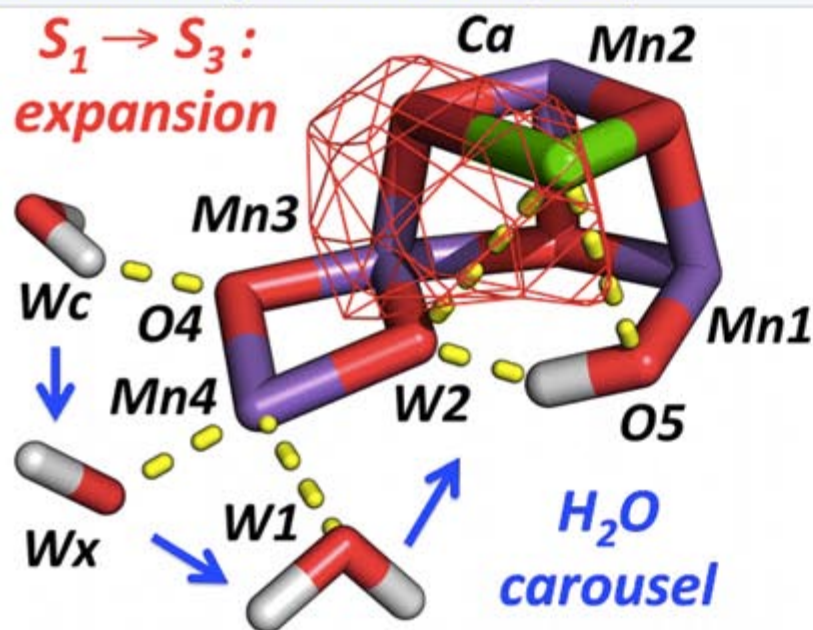


S_3 State of the O_2 -Evolving Complex of Photosystem II: Insights from QM/MM, EXAFS, and Femtosecond X-ray Diffraction

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Calculated S_3 -minus- S_1 difference Fourier maps based on the QM/MM S_3 and S_1 models and observed S_3 -minus- S_1 electron-density difference maps for monomer "A" using data from Fromme et al [Nature 513, 261-265 (2014)] show negative difference densities leading to the proposed mechanism for S_3 -state formation.