

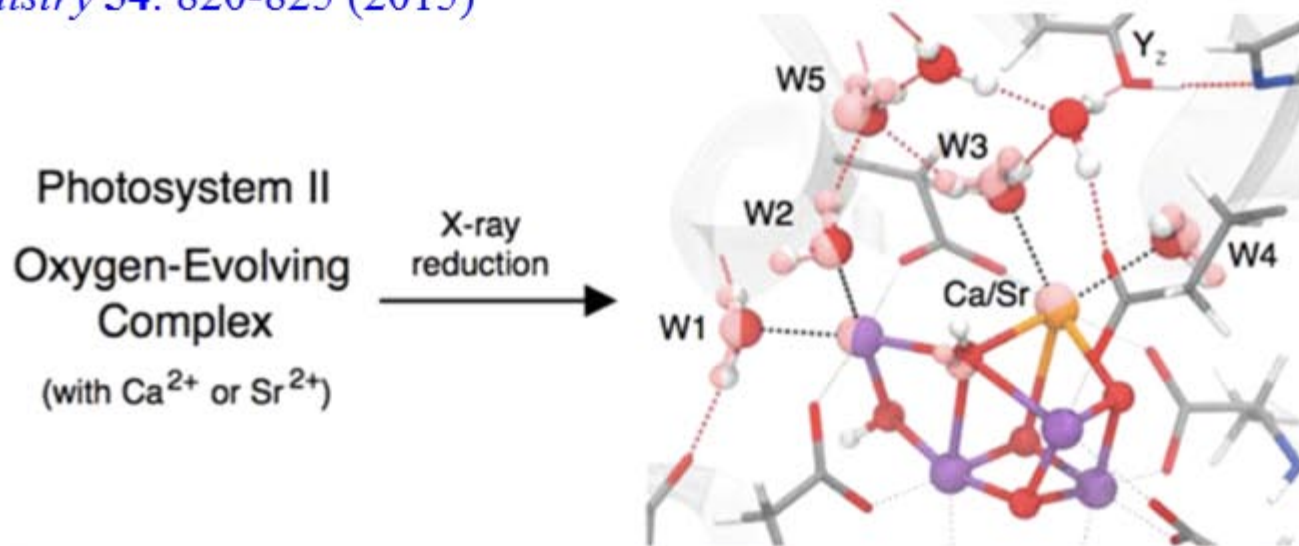
Computational Insights on Crystal Structures of the Oxygen-Evolving Complex of Photosystem II with Either Ca^{2+} or Ca^{2+} Substituted by Sr^{2+}

Leslie Vogt,^{*,†} Mehmed Z. Ertem,^{†,‡} Rhitankar Pal,[†] Gary W. Brudvig,[†] and Victor S. Batista^{*,†}

[†]Department of Chemistry, Yale University, New Haven, Connecticut 06511, United States

[‡]Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973, United States

Biochemistry **54**: 820-825 (2015)



QM/MM-optimized structure of the Ca^{2+} -OEC in the S_2 state with both O4 and O5 protonated. Displacement of W5 as a result of Sr^{2+} substitution in all of the S states studied herein leads us to propose that this water may play an important role in the mechanism of water oxidation.