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

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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.