EXPLORATIONS OF WATER OXIDATION WITHIN AN EXPLICITLY SOLVATED ENVIRONMENT

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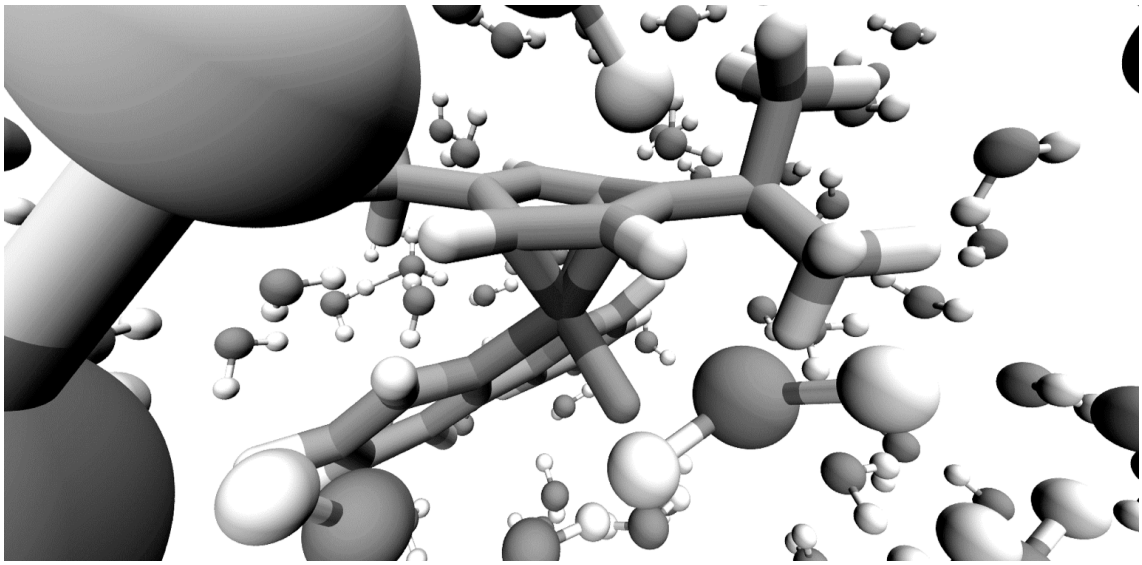

Water oxidation catalysis is a crucial process in any device designed to convert solar energy into storable chemical energy. The search for efficient and stable homogenous water oxidation catalysts remains a scientific challenge, especially when considering those based on abundant transition metals. Computational methods based on quantum chemical calculations do allow for significant insights into the relevant catalytic mechanisms, however it is becoming increasingly clear that explicit solvent molecules are needed to obtain realistic descriptions of these catalytic mechanisms. Here we analyse and evaluate, based on ab-initio molecular dynamics, the effects of a changing solvent environment on the water oxidation mechanism of a mononuclear ruthenium based water oxidation catalyst. Moreover, proton and electron acceptors are included within the simulation box to more closely represent experimental conditions. This allows for a more detailed description of proton-coupled electron transfer processes.

References:
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