Advanced computational approaches for bio-inspired water splitting

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Solar energy is an inexhaustible source for a sustainable solution to the increasing global energy consumption. The storage of large amounts of light energy can be achieved by conversion into chemical energy saved in biomass. Artificial photosynthesis permits the splitting of water into molecular hydrogen and oxygen and is therefore a very promising strategy to meet the increasing worldwide need for clean energy. This requires the development of high-performance water reduction and water oxidation catalysts where the latter is currently the main bottleneck for efficient photocatalytic water splitting.

Thorough analysis of catalytic processes and factors determining their efficiency is a prerequisite for development of better catalysts. We present our recent research on advanced *ab initio* approaches for the in-depth study of water splitting with focus on bio-inspired water oxidation catalysts closely mimicking nature's photosystem II. Using forefront computational methods [1] and in collaboration with experimental groups [2], we study their structure and dynamics in detail [3]. This paves the way for the derivation of novel guidelines, which are essential for informed design of more efficient catalysts [4].

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