

Challenges and Progresses in Modeling Water Oxidation Reactions

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Water splitting driven by light is a promising technology for supplying clean and sustainable fuel by production of hydrogen. The oxidation of water by releasing four protons and four electrons is thermodynamically unfavorable with a relatively large energy demand ($E_0=1.23$ V vs SHE at pH=0), and is therefore quite challenging to accomplish. During the last few decades, considerable progress has been achieved in the development of homogeneous water oxidation catalysts (WOCs) using transition metals.^[1] Quantum chemical calculations^[2] have been used to elucidate the mechanism of water oxidation promoted by a number of catalysts incorporating Ru,^[3] Ir,^[4] Fe,^[5] Mn,^[6] and Cu.^[7] In this talk, some of the challenges in the modeling are discussed.

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