

عنوان مقاله:

Progress on Homogeneous Ruthenium Complexes for Water Oxidation Catalysis: Experimental and Computational Insights

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خلاصه مقاله:

This work presents a concise review on the homogeneous ruthenium single-, two, and three-center complexes employed in water oxidation catalysis. The design of efficient and robust water oxidation catalysts has much to benefit from an improved understanding of the mechanism. A strong perspective is established on the progress made so far on the water oxidation catalysis through experimental and complementary computational efforts to understand the water oxidation reaction. The general mechanisms postulated so far are including the acid-base mechanism, the water nucleophilic attack and the direct coupling mechanistic approaches. These proposals are briefly discussed and reports featuring each instance are captured. From experimental perspectives, considerable efforts have been made in optimizing catalyst figures of merit (overpotentials, turnover numbers, and operating conditions) in single-center Ru systems, their efficiencies in most cases are not realistic enough to be adopted in commercial scale. While homogeneous multinuclear ruthenium complexes exist in the literature, few studies have been devoted towards understanding their mechanisms. Further studies in this respect are crucial as they may serve as the golden gate towards understanding (probably) the mechanisms involved in the nature's photosystem II which is the upper-bound catalyst for water oxidation. The present experimental and computational progress made in single- and two-center homogeneous catalytic systems provide a useful blueprint to build on higher homologous series for efficient water oxidation catalysis

كلمات كليدى:

Water oxidation, Catalysis, Water splitting, Ruthenium complexes, Hydrogen fuels, Homogeneous catalysis

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