research highlights

WATER OXIDATION It takes two Proc. Natl Acad. Sci. USA 115, 2902-2907 (2018)

Splitting water in a photoelectrochemical cell produces hydrogen, which can be used as a fuel, and oxygen, which can be considered a by-product. Efficient water splitting requires optimization of catalysts for the hydrogen evolution reaction as well as the oxygen evolution reaction, which occurs at the anode. Iridium species are known to be effective water oxidation catalysts but, being expensive, it is desirable to minimize the quantity of iridium used. Single-atom catalysts, in which the catalytically active metal is atomically dispersed on the surface of a support, are increasingly explored to maximize the utilization of such precious metals. For some reactions, it may be advantageous to have two active metal atoms next to each other; however, this is synthetically challenging. Now, Gary Brudvig, Victor Batista, Dunwei Wang and colleagues in the United States, Germany and China prepare a wateroxidizing photoanode that possesses two iridium atoms per catalytic site and has 2.6 times higher activity per iridium atom than the corresponding photoanode with only singly dispersed sites.

The researchers use α -Fe₂O₃ as the light absorber on which to disperse the Ir atoms. To place two Ir atoms next to each other, they use a molecular Ir dimer, which is introduced to the surface of the photoanode before the organic ligands of the dimer are removed photochemically. The results imply that a bridged Ir-O-Ir structure forms, bound to specific threefold hollow sites on the surface of α -Fe₂O₃, preventing the active sites from aggregating. Computational studies of the oxygen evolution mechanism suggest that the presence of two nearby Ir atoms is crucial in minimizing the energy requirement of a key reaction step in the catalytic cycle, corroborating the experimentally observed enhanced intrinsic activity of the dinuclear catalyst.

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