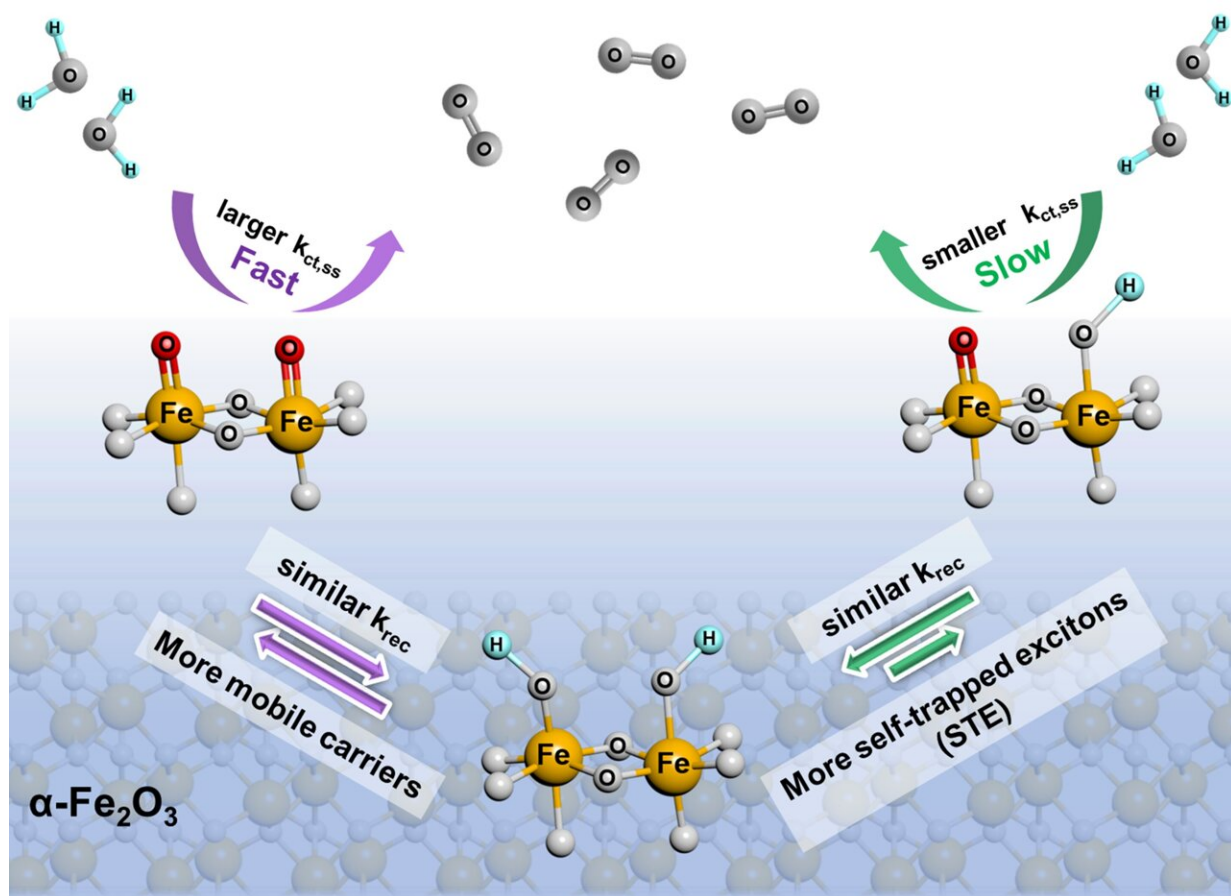


Boosting multi-hole water oxidation catalysis on hematite photoanodes under low bias

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The UV irradiation reduces the formation probability of self-trapped excitons and significantly promotes the multi-hole accumulation process, thereby achieving the efficient water oxidation reaction even under low bias. Credit: Science China Press

Photoelectrochemical (PEC) water oxidation reaction has attracted considerable attention in recent years because of its importance in solar energy conversion. For such a sluggish four-hole and four-proton transfer reaction in a long timescale of ms–s, more and more studies have shown that the accumulation of multiple surface-trapped holes (e.g., high-valent iron oxo on hematite surfaces) or "oxidizing equivalents" is a prerequisite for efficient PEC water oxidation process. Previous PEC water oxidation studies commonly apply high potentials ($>1.2 V_{\text{RHE}}$) to achieve this key. But how to complete multi-hole transfer under low bias (near the onset potential) remains unknown.

A study, published in the journal *Science China Chemistry* and led by Prof. Yuchao Zhang (Key Laboratory of Photochemistry, Chinese Academy of Sciences), sought to address this topic.

Zhang's research group studied the important role of [excitation](#) energy in the multi-hole accumulation process. PEC characterizations and rate law analysis showed that the UV excitation could significantly boost the accumulation of multiple surface-trapped holes, thereby cathodically shifting the onset potential by 220 mV and improving the PEC water [oxidation](#) activity by one order of magnitude.

Subsequent bulk transport dynamics and surface charge-transfer kinetics demonstrated that compared with the visible-light excitation, the UV excitation reduced the formation probability of self-trapped excitons and resulted in ~3 to 5-fold increase of surface holes, which accounted for the promoted multi-hole accumulation process.

These advantages enable the UV excitation to contribute about 40% to the total photocurrent under 1 solar illumination, even though its energy only occupies 6% of the [incident light](#). This mechanism was also applicable to boost other multi-hole catalysis (such as the oxidation of thioether and nitrite) under low bias.

More information: Lei Wu et al, Boosting multi-hole water oxidation catalysis on hematite photoanodes under low bias, *Science China Chemistry* (2023). [DOI: 10.1007/s11426-022-1527-9](https://doi.org/10.1007/s11426-022-1527-9)

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