

Dethroning electrocatalysts for hydrogen production with inexpensive alternative material

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Iron-based Bimetallic Electrocatalysts May Be Key for Hydrogen Synthesis

Electrochemical water splitting is an efficient way to produce hydrogen (H₂) fuel

- ✓ Clean fuel
- ✓ High energy density

However, the oxygen evolution reaction (OER) requires costly electrocatalysts

Platinum, Ruthenium, Iridium

Could we use iron-based bimetallic catalysts instead?

New promising electrocatalyst for OER found

Orthorhombic CaFe₂O₄

Can be easily synthesized
Needs only calcination of Fe and Ca chemicals in air

Superior specific activity vs other iron-based bimetallic oxides
Also higher than the benchmark, iridium oxide!

2OH
OOH

New mechanism for the OER proposed
Multi-iron sites help form direct O-O bonds

CaFe₂O₄ is

- Highly active
- Easily produced
- Cost-effective

Paves the way to hydrogen societies

Efficient Oxygen Evolution Electrocatalysis on CaFe₂O₄ and its Reaction Mechanism
Sugawara et al. (2021) | ACS Applied Energy Materials | DOI: 10.1021/acsaem.0c02710

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Electrochemical water splitting demands highly active, easily produced, and cost-effective electrocatalysts for the oxygen evolution reaction (OER). An iron (Fe)/calcium (Ca)-based bimetallic oxide, CaFe₂O₄, exhibits outstanding OER activity in alkaline media. CaFe₂O₄ is expected to be a promising OER electrocatalyst for water splitting. Credit: Tokyo Tech

Today, we can say without a shadow of doubt that an alternative to fossil

fuels is needed. Fossil fuels are not only non-renewable sources of energy but also among the leading causes of global warming and air pollution. Thus, many scientists worldwide have their hopes placed on what they regard as the fuel of tomorrow: hydrogen (H_2). Although H_2 is a clean fuel with incredibly high energy density, efficiently generating large amounts of it remains a difficult technical challenge.

Water splitting—the breaking of water molecules—is among the most explored methods to produce H_2 . While there are many ways to go about it, the best-performing water splitting techniques involve electrocatalysts made from expensive metals, such as platinum, ruthenium, and iridium. The problem lies in that known electrocatalysts made from abundant metals are rather ineffective at the oxygen evolution reaction (OER), the most challenging aspect of the water-splitting process.

In a recent study published in *ACS Applied Energy Materials*, a team of scientists at Tokyo Institute of Technology, Japan, found a remarkable [electrocatalyst](#) candidate for cost-effective water splitting: calcium iron oxide ($CaFe_2O_4$). Whereas iron (Fe) oxides are mediocre at the OER, previous studies had noted that combining it with other metals could boost their performance to actually useful levels. However, as Assistant Professor and lead author Dr. Yuuki Sugawara comments, no one had focused on $CaFe_2O_4$ as a potential OER electrocatalyst. "We wanted to unveil the potential of $CaFe_2O_4$ and elucidate, through comparisons with other iron-based bimetallic oxides, crucial factors that promote its OER activity," he explains.

To this end, the team tested six kinds of iron-based oxides, including $CaFe_2O_4$. They soon found that the OER performance of $CaFe_2O_4$ was vastly greater than that of other bimetallic electrocatalysts and even higher than that of iridium oxide, a widely accepted benchmark. Additionally, they tested the durability of this promising material and found that it was remarkably stable; no significant structural nor

compositional changes were seen after measurement cycles, and the performance of the CaFe_2O_4 electrode in the electrochemical cell remained high.

Eager to understand the reason behind the exceptional capabilities of this unexplored electrocatalyst, the scientists carried out calculations using density functional theory and discovered an unconventional catalytic mechanism. It appears that CaFe_2O_4 offers an energetically favorable pathway for the formation of oxygen bonds, which is a limiting step in the OER. Although more theoretical calculations and experiments will be needed to be sure, the results indicate that the close distance between multiple iron sites plays a key role.

The newly discovered OER electrocatalyst could certainly be a game changer, as Dr. Sugawara remarks, " CaFe_2O_4 has many advantages, from its easy and cost-effective synthesis to its environmental friendliness. We expect it will be a promising OER electrocatalyst for [water splitting](#) and that it will open up a new avenue for the development of energy conversion devices." In addition, the new OER boosting mechanism found in CaFe_2O_4 could lead to the engineering of other useful catalysts.

More information: Yuuki Sugawara et al, Efficient Oxygen Evolution Electrocatalysis on CaFe_2O_4 and Its Reaction Mechanism, *ACS Applied Energy Materials* (2021). [DOI: 10.1021/acsaem.0c02710](https://doi.org/10.1021/acsaem.0c02710)

Provided by Tokyo Institute of Technology

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