

# 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 (H<sub>2</sub>) 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 CaFe<sub>2</sub>O<sub>4</sub>**

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

**CaFe<sub>2</sub>O<sub>4</sub> is**

- Highly active
- Easily produced
- Cost-effective

Paves the way to hydrogen societies

Efficient Oxygen Evolution Electrocatalysis on CaFe<sub>2</sub>O<sub>4</sub> and its Reaction Mechanism  
Sugawara et al. (2021) | ACS Applied Energy Materials | DOI: 10.1021/acsaem.0c02710

東京工業大学  
Tokyo Institute of Technology

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, CaFe<sub>2</sub>O<sub>4</sub>, exhibits outstanding OER activity in alkaline media. CaFe<sub>2</sub>O<sub>4</sub> 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  $\text{CaFe}_2\text{O}_4$  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  $\text{CaFe}_2\text{O}_4$  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, " $\text{CaFe}_2\text{O}_4$  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  $\text{CaFe}_2\text{O}_4$  could lead to the engineering of other useful catalysts.

**More information:** Yuuki Sugawara et al, Efficient Oxygen Evolution Electrocatalysis on  $\text{CaFe}_2\text{O}_4$  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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