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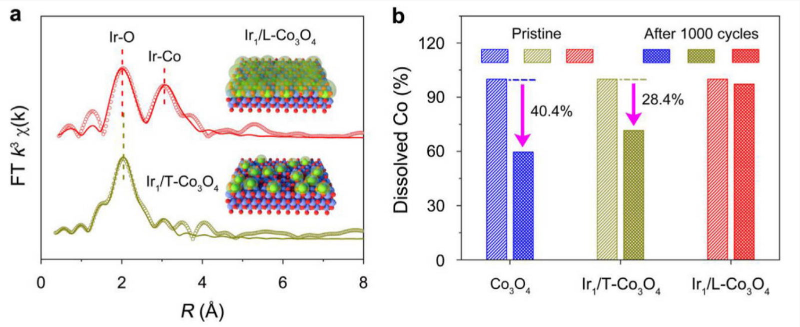
Atomic-precision engineering delivers excellent stability for acidic water oxidation

GA, UNITED STATES, December 22, 2025 /EINPresswire.com/ -- Developing durable oxygen evolution reaction (OER) catalysts for acidic media is vital for advancing proton exchange membrane water electrolyzers (PEMWE). This study reveals that the stability of spinel oxide Co_3O_4 is profoundly dictated by the anchoring sites of iridium single atoms. By directly comparing iridium atoms at surface three-fold hollow sites versus lattice sites, the researchers found that lattice-embedded iridium dramatically suppresses cobalt and oxygen migration, enhances metal–oxygen covalency, and preserves structural integrity under harsh acidic conditions. These findings highlight a site-specific stabilization mechanism and provide an effective atom-level strategy for designing durable and low precious-metal OER catalysts.



Site-specific stabilizing effect of single atoms on spinel oxides for acidic oxygen evolution.

Acidic oxygen evolution reaction (OER) catalysts must withstand severe challenges such as dissolution, lattice distortion, and oxygen migration, which often degrade non-precious spinel oxides such as Co_3O_4. While incorporating precious-metal heteroatoms has improved stability, not all single-atom configurations perform equally well. However, the stabilizing effect of single atoms anchored at different sites on spinel oxides is still poorly understood. Without a mechanistic understanding of how specific atomic positions influence degradation, the rational design of durable, scalable OER catalysts for green hydrogen production remains limited. Due to these challenges, deeper investigations into the site-dependent stabilization mechanisms of single atoms are urgently needed.

A research team from the University of Science and Technology of China and partner institutions reported (DOI: 10.1016/j.esci.2025.100402) on November 2025, in eScience, a new study uncovering how iridium single atoms anchored at different positions within spinel Co_3O_4 govern its stability during acidic oxygen evolution. The team demonstrated that embedding iridium within lattice sites, rather than at surface hollow sites, significantly boosts resistance to dissolution and structural degradation. Their findings establish a powerful design principle for developing robust electrocatalysts suitable in proton exchange membrane water electrolysis.

The team engineered two catalyst configurations: Ir atoms anchored at surface three-fold hollow sites (Ir_1/T-Co_3O_4) and Ir atoms incorporated into octahedral lattice sites (Ir_1/L-Co_3O_4). Structural analyses—including transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray absorption near edge structure (XANES), extended X-ray absorption fine structure (EXAFS), and Raman spectroscopy—confirmed distinct electronic structures for each configuration, with lattice-anchored Ir inducing lattice expansion and forming stronger Ir–O interactions.

Electrochemical durability tests revealed striking performance contrasts. After 1000 cycles in 0.1 M $HClO_4$, Co_3O_4 suffered a cobalt dissolution of 40.4%, while Ir_1/T-Co_3O_4 lost 28.4%. In contrast, Ir_1/L-Co_3O_4 exhibited only 2.8% dissolution with nearly unchanged current density. Long-term tests further showed that Ir_1/L-Co_3O_4 remained stable for 200 hours at a current density of 10 mA cm^{-2} and for 60 hours at a current density 1 A cm^{-2} in PEMWE device, rivaling leading acidic OER catalysts.

In situ XAFS and Raman spectra confirmed that only lattice-embedded Ir maintained Co–O and Co–Co coordination structure under applied potentials. Density functional theory calculations offered mechanistic insight: lattice Ir raised the migration energy barriers of cobalt (3.31 eV) and oxygen (3.26 eV), as well as increased oxygen-vacancy formation energy, drastically reducing structural degradation. Concurrently, the enhanced Co-O and Ir-O covalency further stabilized the Co3O4 support.

“The precise position of a single atom can completely transform catalyst durability,” the study’s co-author explained. “By embedding iridium directly into the lattice, we substantially strengthened the metal–oxygen network and suppressed both cobalt and oxygen migration—the primary causes of acidic OER degradation. This atom-level strategy demonstrates that stability can be engineered with precision, enabling high performance with far lower noble-metal usage. It provides a clear and rational pathway for designing the next generation of robust acidic OER catalysts.”

This discovery provides a powerful framework for designing highly stable OER catalysts with reduced reliance on precious metals. The demonstrated durability of lattice-anchored Ir in PEMWE testing shows strong potential for industrial hydrogen production systems that demand long operational lifetimes under acidic conditions. The site-specific strategy can be extended to other spinel, perovskite, or mixed-metal oxides, enabling tailored covalency and migration resistance across catalyst families. By identifying the atomic-level features that dictate long-term stability, this work moves the field closer to practical, low-cost electrolyzers for large-scale green hydrogen technologies.

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