Researchers reveal performance boost mechanism in single-atom catalyst for oxygen evolution reaction

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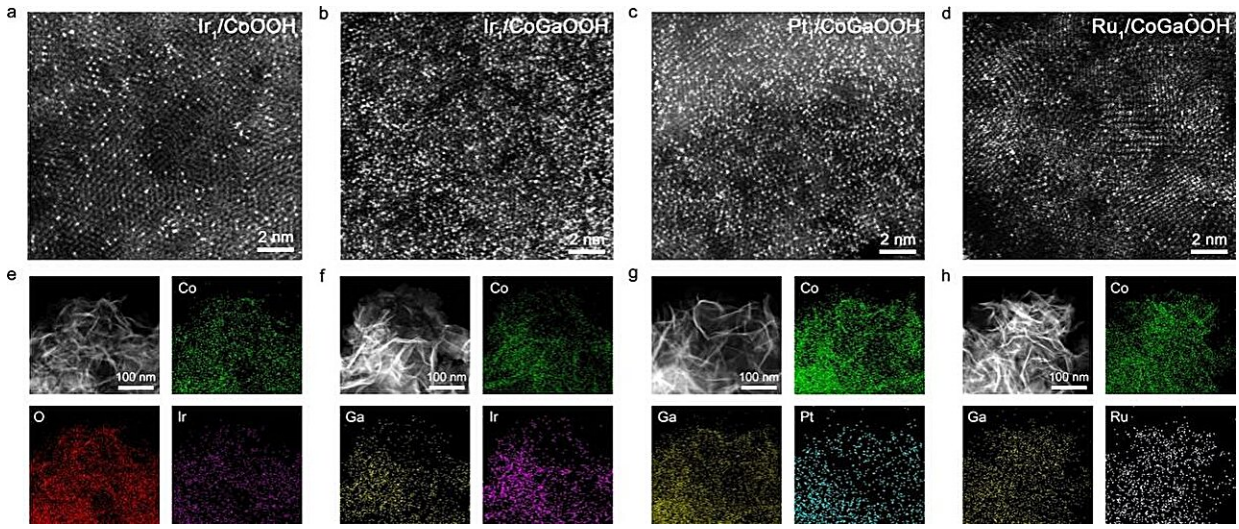


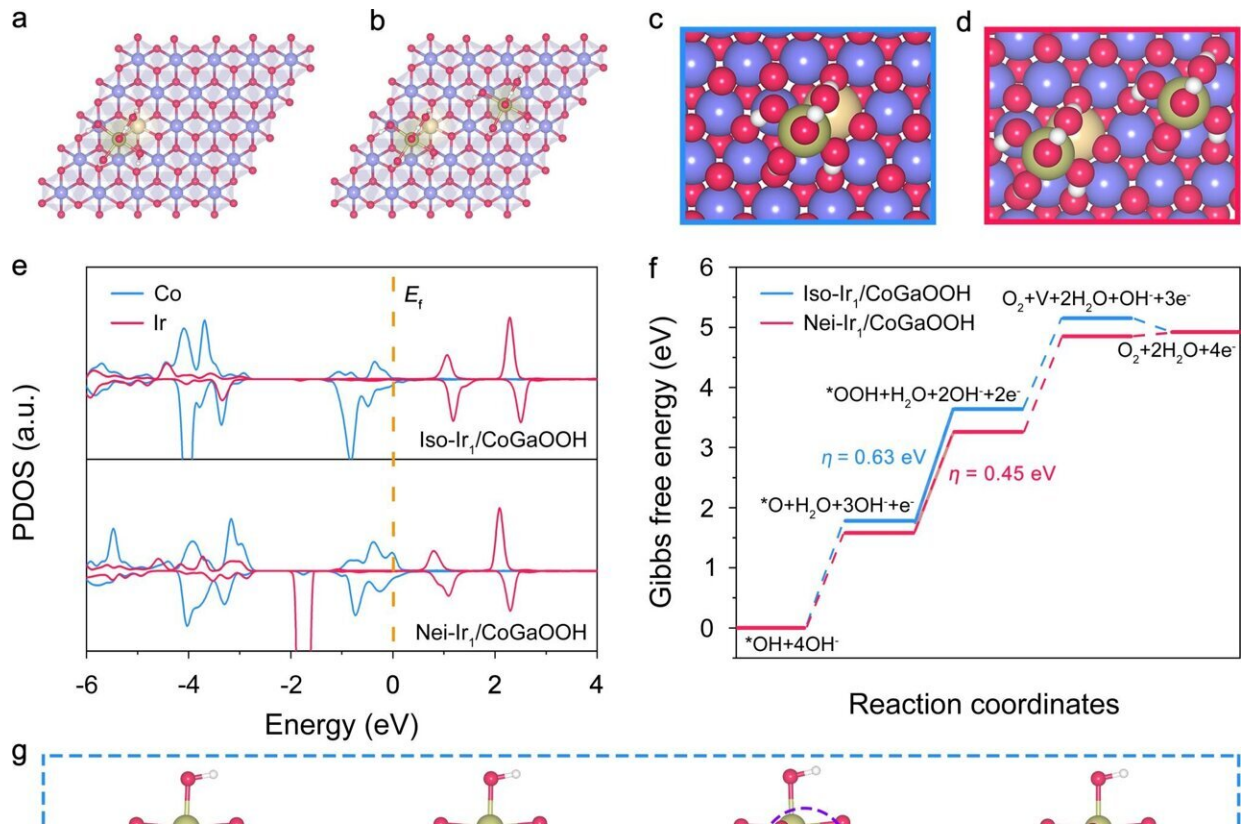
Structural images of high-density single atoms. Credit: Prof. BAO's team

Hydrogen energy, with its green, low-carbon and high-calorific-value properties, is emerging as the new key to solving the energy crisis. Electrochemically, water splitting has garnered much attention as a promising hydrogen production technique. However, the slow kinetics of the oxygen evolution reaction (OER) at the anode limits the overall energy conversion efficiency. Therefore, the development of efficient catalysts for the OER is critically needed.

Recently, a research team led by Prof. Bao Jun from the University of Science and Technology of China (USTC) revealed that the cobalt-based, oxide-supported, high-density Ir single-atom catalyst exhibits excellent performance in electrochemical OER, which is closely related to the neighboring synergetic interactions in neighboring single atoms. The research was published in *Angewandte Chemie*.

The performance of single-atom catalysts (SACs) is closely related to the density of single atoms on the surface. As the density of single atoms increases, the distance between atoms decreases, leading to the emergence of neighboring synergy, which optimizes the adsorption behavior of reaction intermediates and subsequently enhances the overall performance of the catalyst. Therefore, constructing high-density single atoms is an effective strategy to improve the catalyst's performance.

To achieve precise fabrication of high-density single atoms, the team introduced Ga atoms into the cobalt-based oxide lattice, thereby modulating the electronic structure of the single-atom anchoring sites. This approach significantly enhanced the bonding strength between oxygen defect sites and single-atom precursors, successfully constructing a series of high-density SACs.



Mechanism of neighboring synergy of high-density Ir single atoms in regulating OER performance. Credit: Prof. Bao's team

The team evaluated the OER performance of these catalysts to investigate the neighboring synergetic effects of high-density single atoms. The results showed that the high-density Ir single-atom catalyst Nei-Ir_1/CoGaOOH exhibited a low overpotential of 170 mV at a current density of 10 mA cm^{-2}, and a long-durable stability over 2000h. Additionally, the catalyst operated stably at a current density of 1 A cm^{-2} in alkaline electrolyte for over 50h. In situ Raman spectra confirmed that the catalyst maintained structural stability during the OER.

Further mechanism studies revealed that the enhancement in the catalyst's performance does not stem from the optimization of the

electronic structure of the active sites, but rather from the neighboring synergetic interaction of the high-density Ir single atoms. The neighboring synergetic interaction stabilizes the *OOH intermediates through additional hydrogen bonding interactions, thereby reducing the reaction energy barrier and significantly improving the performance of the catalyst.

This research unveils the mechanism underlying the performance enhancement of high-density Ir single-atom catalysts, offering novel insights into the future development of electrochemical OER catalysts.

More information: Peiyu Ma et al, Neighbouring Synergy in High-Density Single Ir Atoms on CoGaOOH for Efficient Alkaline Electrocatalytic Oxygen Evolution, *Angewandte Chemie* (2024). DOI: 10.1002/ange.202404418

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