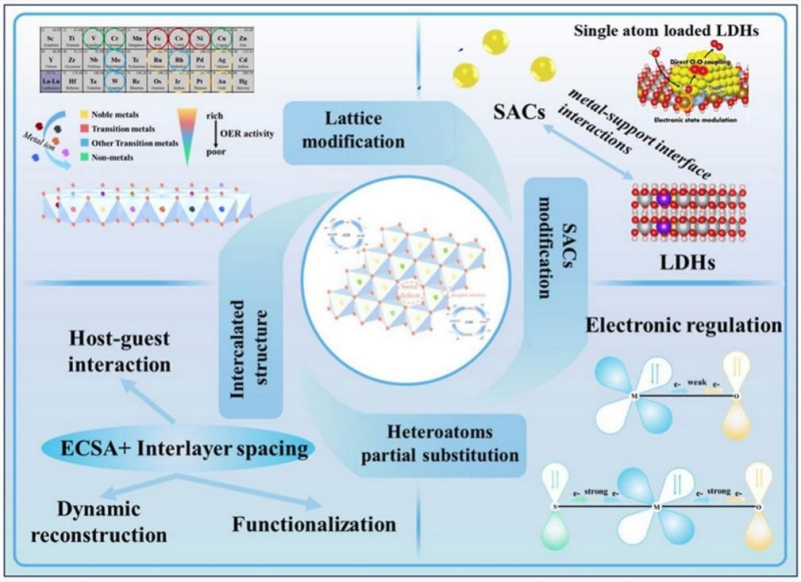
Defect-tuned layered double hydroxides open new path for clean energy catalysts

GA, UNITED STATES, December 22, 2025 /EINPresswire.com/ -- Layered double hydroxides (LDHs) are emerging as promising electrocatalysts for the oxygen evolution reaction (OER), a key barrier in clean hydrogen production. However, their catalytic performance has long been restricted by limited active sites, sluggish electron transfer, and structural instability under operational conditions. A new review summarizes how electronic defect engineering, including vacancy creation, heteroatom doping, single-atom incorporation and lattice modulation, which reconfigures electron distribution, enhances active site exposure, accelerates reaction kinetics, and strengthens catalytic durability. The work highlights strategies that effectively lower OER overpotential and improve stability by tuning LDH atomic coordination environments, providing a unified framework for the design of next-generation high-performance water-splitting catalysts.



Defect Engineering Strategies for Enhancing LDH-Based OER Catalysts.

Efficient catalysts are required to reduce energy consumption in electrocatalytic hydrogen production reactions. Although noble metal oxides such as RuO□ and IrO□ show excellent activity, high cost and instability under high potential hinder scalability. Layered double hydroxides (LDHs) offer a low-cost alternative with tunable metal compositions, flexible 2D structure, and abundant oxygen sites. Still, only metal atoms at edges are catalytically active, layer stacking decreases surface availability, and intrinsic conductivity remains weak. Understanding reaction mechanisms including adsorbate evolution (AEM) and lattice oxygen mechanism (LOM)—is essential to overcome kinetic limits and improve electron transport. Addressing these challenges requires further in-depth research on structural and electronic modulation to advance LDH-based catalysts for the oxygen evolution reaction (OER)..

Researchers from Zhengzhou University and the University of Surrey published (DOI:

10.1016/j.esci.2025.100380) a comprehensive review in eScience (September 2025) summarizing recent advances in electronic defect engineering for LDH-based oxygen evolution catalysts. The paper systematically categorizes defect types, characterizations, and performance-enhancing mechanisms, offering a roadmap for designing highly active and stable LDHs for alkaline water electrolysis. The review highlights metal vacancies, oxygen vacancies, heteroatom doping, single-atom loading, and interlayer modification as core strategies to boost intrinsic activity and unlock LOM pathways.

The review outlines three major electronic defect categories: metal vacancies, oxygen vacancies, and heteroatom incorporation, that explains how each influences electronic structure and reaction kinetics. Metal vacancies create unsaturated metal coordination sites with high-energy dangling bonds, enhancing OH adsorption and accelerating O–O bond formation. Oxygen vacancies modulate electron density near metal sites, lower band gap, and promote faster charge transfer, while also enabling lattice-oxygen-involved mechanisms. Heteroatom doping—including transition metals (Co, V, Cr), rare-earth elements (Ce, Gd, Er), and even noble metals (Ru, Ir, Au) that reshapes electron distribution and stabilizes high-valence catalytic states.

Advanced characterization tools such as HAADF-STEM, XAS/EXAFS, and EPR allow atomic-scale visualization of defects and surface reconstruction during OER. The authors further discuss lattice strain regulation, interlayer anion exchange, and single-atom anchoring, which break traditional scaling relationships and significantly reduce OER overpotential. Combining defect engineering with theoretical simulations (DFT) provides reliable descriptors to guide rational design of catalysts that approach volcano-curve optimization. Overall, the review demonstrates how atomic-level electronic tailoring pushes LDHs beyond conventional performance limits.

“We are entering an era where catalytic performance can be programmed through electrons rather than elements,” the authors note. They emphasize that controlling vacancy distribution and redox states offers more powerful tuning capability than traditional composition optimization. As they suggest, the next breakthroughs will likely emerge from integrating electronic-defect simulations with operando spectroscopy, enabling real-time observation of lattice oxygen behavior and active-site evolution. Such insight is essential for revealing rate-determining steps, balancing AEM–LOM pathways, and achieving industrial-level catalytic stability.

The study provides a blueprint for developing LDH electrocatalysts capable of powering large-scale hydrogen fuel production, metal-air batteries, CO reduction systems, and renewable energy storage devices. By mastering defect chemistry, researchers may construct catalysts that match or surpass noble metals while cutting material costs dramatically. Looking forward, combining defect engineering with machine learning and in-situ monitoring could accelerate catalyst discovery and enable automated structure-performance prediction. This approach lays the foundation for efficient, durable water-splitting technologies that support future clean-energy infrastructure worldwide.

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