Han *et al. Chem. Synth.* **2025**, *5*, 54
DOI: 10.20517/cs.2025.47

Chemical Synthesis

Research Highlight

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Accelerating ultrastable catalyst exploration for large-scale water splitting

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How to cite this article: Han, N.; Su, B. L. Accelerating ultrastable catalyst exploration for large-scale water splitting. *Chem. Synth.* **2025**, *5*, 54. https://dx.doi.org/10.20517/cs.2025.47

Received: 31 Mar 2025 **First Decision:** 30 Apr 2025 **Revised:** 2 May 2025 **Accepted:** 9 May 2025 **Published:** 26 May 2025

Academic Editor: Ying Wan **Copy Editor:** Pei-Yun Wang **Production Editor:** Pei-Yun Wang

Keywords: Oxygen evolution reaction, water splitting, PEMWE, electrocatalysis

Electrolytic water splitting can convert renewable electricity from sources such as solar and wind into green hydrogen, which is key for achieving zero carbon emissions[1,2]. The large-scale production of affordable green hydrogen is essential for advancing the industry. Proton exchange membrane water electrolyzers (PEMWEs) are considered the most effective due to their high current density, fast response, and low gas crossover. The oxygen evolution reaction (OER) at the anode is critical for generating the required protons and electrons[3]. Improving OER catalyst activity and stability is vital, with Iridium oxide (IrO_x) as the only suitable catalyst, though its high cost and limited availability present challenges[4].

To minimize iridium use and improve performance, researchers have investigated strategies like alloying[5], compositing[6], and supporting IrO_x nanoparticles (NPs) on metal oxides[7]. While these methods have enhanced catalytic activity, stability continues to be a challenge, with the best voltage degradation rates still falling short of the 2026 target of the U.S. Department of Energy (DOE)[8]. IrO_x NP instability, such as dissolution, re-deposition, detachment, and aggregation, contributes significantly to performance loss. Solutions such as electron donation to prevent excessive oxidation and anchoring iridium sites on supports

show promise. However, current catalysts still fail to meet both activity and stability targets, making further development a priority.

A new strategy proposed by Prof. Bo Zhang's group embeds the catalyst directly into the support by forming Ir NPs on its surface [Figure 1][9]. This method, known as "Ripening-Induced Embedding" (RIE), utilizes polyethylene glycol (PEG) to reduce iridium salts to uniform Ir NPs, which are then loaded onto a metal oxide support through heating in ethylene glycol. The heating induces Ostwald ripening, which helps grow unaged support particles and embeds the NPs within the support. To ensure the success of the RIE process, the support must mature quickly enough to match the fast nucleation rate of Ir NPs. Based on Lifshitz and Slyozov's theory[10], particle growth under diffusion control is proportional to surface energy, meaning supports with higher surface energy grow faster. Stable crystal planes, such as the (111) surface of face-centered cubic metal oxide supports, grow more slowly, which hinders the embedding of rapidly nucleating NPs. In contrast, high-energy crystal planes, such as the (211) surface, grow faster, enabling successful NP embedding. Under PEMWE-OER conditions, these Ir NPs oxidize to IrO_x, and the lattice constant increases. Electron donation from the support, like CeO_x, prevents Ir dissolution, causing the NPs to expand and anchor within the support. To achieve the desired embedded catalyst, the growth of high-energy crystal planes must be both rapid and sustainable, matching the nucleation rate of the Ir NPs.

The authors synthesized sub-10 nm CeO_x particles with rough surfaces, promoting the exposure of high-energy crystal planes. The nucleation of Ir NPs on CeO_x revealed an imbalance in growth kinetics between the support and NPs, preventing successful embedding. Since ultrasound-induced cavitation accelerates nucleation and disrupts growth pathways, stabilizing high-energy crystal planes and promoting surface restructuring, fragmentation, and recrystallization to enhance catalytic surface exposure. To resolve this, ultrasound was reintroduced during the Ir loading process, which accelerated CeO_x maturation and enabled the successful embedding of Ir NPs with a depth of around 1 nm. The embedding process was observed using cryo-electron microscopy and electron tomography, demonstrating the critical role of the support's high surface energy for the effectiveness of the RIE strategy. Additionally, kinetic Monte Carlo simulations revealed that the ultrasound-induced surface erosion of CeO_x facilitated the embedding of Ir NPs by speeding up the maturation process.

The resulting RIE-Ir/CeO_x showed impressive electrochemical activity (1.72 V at 3 A/cm^{-2}) and stability (voltage degradation rate of 1.33 μV/h) with 0.4 mg/cm^{-2} PGM loading, meeting the U.S. DOE targets for PEMWE devices by 2026. RIE-Ir/CeO_x has already reached the DOE's ultimate target for voltage degradation rate (2.0 μV/h), ensuring it will last more than ten years. This catalyst offers superior performance, balancing activity, stability, and cost compared to other Ir-based PEMWE-OER catalysts. Meanwhile, the catalyst's reliability was tested across ten PEMWE devices, demonstrating consistent performance at varying current densities. The RIE strategy enhances the activity and stability of various metal and metal oxide-supported catalysts, regardless of specific elements or compounds. These catalysts were tested in both the OER and hydrogen evolution reaction (HER) within PEMWE, as well as in $NaBH_4$ hydrolysis for hydrogen production. When ZrO_x was used as a support for OER, RIE-Ir/ZrO_x showed improved stability, though its activity was less than RIE-Ir/CeO_x due to ZrO_x's weaker electron donation. This opens up a unique pathway for the design of robust catalyst systems.

In the future, the rapid advancement of materials design and synthesis for large-scale water splitting relies heavily on high-throughput experiments, which allow for the efficient evaluation of a wide range of catalyst candidates and reaction conditions. This work includes extensive parallel repeat experiments, such as those using ten different PEMWE devices. In this context, the large usage of parallel repeat experiments, such as

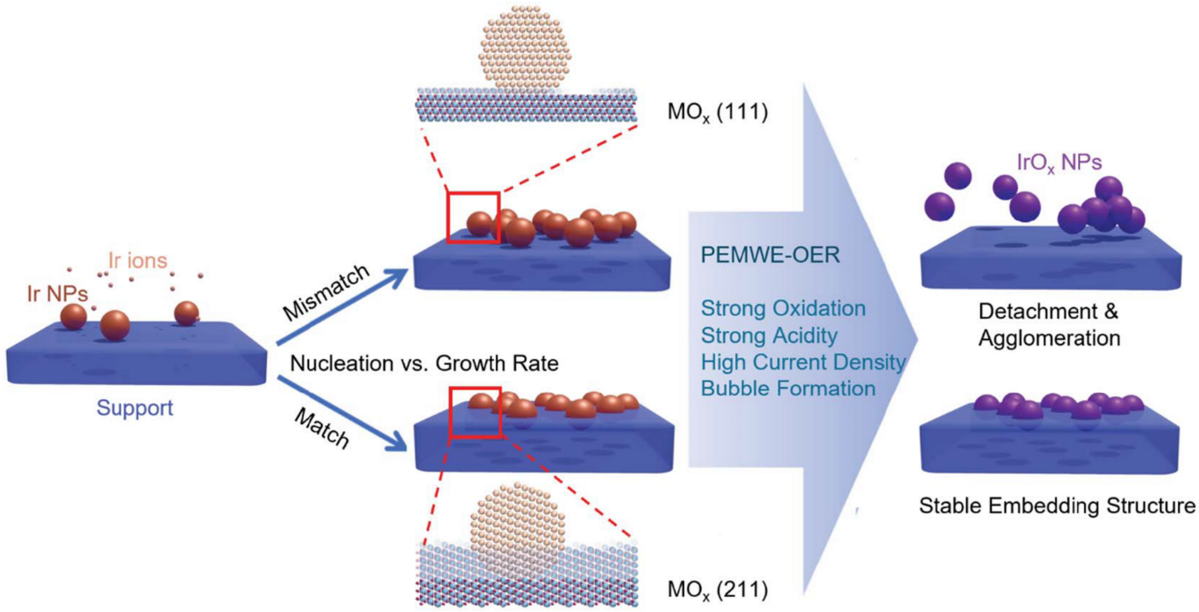

Figure 1. Illustrative overview of the embedding method (This figure is reproduced with permission from Zhang *et al.*[9]).

testing hundreds of catalysts across hundreds of different PEMWE devices at various current densities, will be a crucial approach. This kind of experiment will provide valuable insights into the stability and performance of catalysts under diverse operational conditions, enabling researchers to identify optimal configurations for industrial-scale applications. By conducting this kind of high-throughput experiment, researchers can quickly generate large datasets that inform the design of more efficient and stable catalysts.

In addition, artificial intelligence (AI) plays an increasingly vital role in accelerating the materials discovery process[11]. AI and machine learning algorithms can analyze experimental data at an unprecedented scale, identifying patterns and correlations that might otherwise go unnoticed. This capability allows for the prediction of catalyst performance under different conditions, guiding the selection of materials with high potential before they are synthesized and tested. Furthermore, AI-driven simulations can aid catalyst design by predicting properties and behavior, thereby optimizing the synthesis process and reducing trial and error in laboratory experiments. For example, very recently, a machine learning pipeline trained on 36,000+ oxides predicts Pourbaix decomposition energy from unrelaxed structures (77 meV/atom), enabling rapid screening of 2,070 new metal oxides for acid-stable, iridium-free oxygen evolution catalysts to meet growing green hydrogen demands[12]. The integration of high-throughput experimentation with AI-driven data analysis also has a profound impact on the evolution of PEMWE and membrane electrode assembly (MEA)-based N_2 or CO_2 electrocatalytic reduction systems. As the demand for efficient, scalable hydrogen production grows, and carbon dioxide conversion, these advanced techniques provide a pathway to discover catalysts that exhibit both high activity and long-term stability. By leveraging the synergy between experimental approaches and AI, researchers can accelerate the development of new materials, bringing us closer to achieving cost-effective, sustainable, renewable energy production on a large scale.

DECLARATIONS

Authors' contributions

Made substantial contributions to conception and design of the study and performed data analysis and interpretation: Han, N.; Su, B. L.

Performed data acquisition and provided administrative, technical, and material support: Han, N.; Su, B. L.

Availability of data and materials

Not applicable.

Financial support and sponsorship

This work was supported by the National Natural Science Foundation of China (22293020 and 22293022), the International Science & Technology Cooperation Program (2021YFE0115800), Ministry of Science and Technology of China, the Program of Introducing Talents of Discipline to Universities-Plan 111 (No. B20002) from the Ministry of Science and Technology and the Ministry of Education of China and the Wallonia-Brussels International, Belgium (SUB/2021/IND493971/524448).

Conflicts of interest

Su, B. L. is Editor-in-Chief of the journal *Chemical Synthesis*. Su, B. L. was not involved in any steps of editorial processing, notably including reviewer selection, manuscript handling, or decision-making. Han, N. declares that there are no conflicts of interest.

Ethical approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

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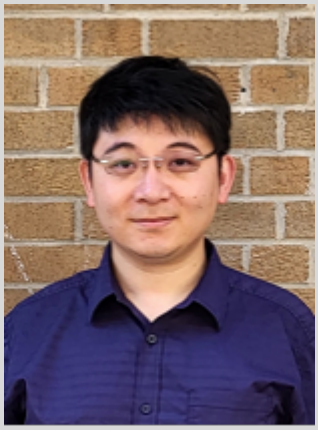

Ning Han

Ning Han earned his Ph.D. from KU Leuven, Belgium, and is currently an A3MD Postdoctoral Research Fellow at the University of Toronto, Canada, working with Professor Edward H. Sargent. He has received several prestigious honors, including the Chinese Government Award for Outstanding Students Abroad (2021), The Electrochemical Society (ECS) Award (2023), recognition as one of the "Stanford Top 2% World Scientists" (2023, 2024), and designation as an Emerging Investigator by *Journal of Materials Chemistry A* (2025). His research focuses on applying artificial intelligence to accelerate the discovery of materials, particularly catalysts for renewable fuel production.

Bao-Lian Su

Bao-Lian Su established the Laboratory of Inorganic Materials Chemistry (CMI) at the University of Namur, Belgium, in 1995. He is a Full Professor, Member of the European Academy of Sciences, Member of the Royal Academy of Belgium, Honorary Fellow of the Chinese Chemical Society, Fellow of the Royal Society of Chemistry (UK), and Life Member of Clare Hall College, University of Cambridge. He also serves as a "Strategy Scientist" at Wuhan University of Technology, China. His research interests include the synthesis, property investigation, and molecular engineering of organized, hierarchically porous materials and bio-organisms for applications in artificial photosynthesis, (photo)catalysis, energy conversion and storage, biotechnology, cell therapy, and biomedical science.