

Review

Recent Advances in Electrocatalysts for Water Splitting: Fundamental Mechanism, Material Design and Challenges in Performance

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DOI: 10.62896/ijmsi.2.s1.11

Conflict of interest: NIL

Article History

Received: 08/06/2026

Accepted: 16/06/2026

Published: 20/06/2026

Abstract:

Electrochemical water splitting is a viable method for producing hydrogen (H₂) sustainably and a crucial part of clean energy technology. However, the slow kinetics of the hydrogen evolution reaction (HER), especially the oxygen evolution reaction (OER), limit its effectiveness, making the development of effective electrocatalysts necessary to lower overpotential and increase reaction rates.^[9,22] This overview outlines the fundamentals of water splitting, with a focusing on mechanism of HER and OER.. Noble metal catalysts—such as platinum for HER and Iridium or Ruthenium oxides for OER—serve as benchmarks because of their higher activity but are constrained by their high cost and scarcity.^[6,21] As a result, considerable efforts have focused on earth-abundant alternatives that balance performance and cost, such as transition metal oxides, sulfides, carbides, and nitrides. Key design strategies, including defect engineering, heterostructure generation, nanostructuring, and electronic structure manipulation, are emphasised for their role in boosting active site density and optimizing adsorption properties to enhance catalytic efficiency. Advances in computational modelling have enabled rational catalyst design. Despite these advances, challenges such as gas crossover, high overpotentials, catalyst degradation, and scalability remain. To achieve effective and large-scale green hydrogen production, these challenges must be addressed through better materials and system design.

Keywords: Water Splitting, Electrocatalysis, Hydrogen Evolution Reaction, Oxygen Evolution Reaction, Nanomaterials, Green Hydrogen.

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1. INTRODUCTION

Research on alternative energy conversion technologies has increased due to the world's

growing need for sustainable and clean energy. Because of its tremendous energy density and ecologically friendly combustion products,

hydrogen is regarded as the perfect energy carrier. Electrochemical water splitting has become one of the most promising techniques for producing high-purity hydrogen utilizing renewable energy sources.^[5]

The hydrogen evolution reaction (HER) at the cathode and the oxygen evolution reaction (OER) at the anode are the two half-reactions that make up water splitting. The process has substantial kinetic hurdles despite its conceptual simplicity, especially for OER, which entails intricate multi-electron transfer steps. Therefore, effective electrocatalysts are necessary to improve reaction kinetics and decrease overpotential.^[9, 23]

Large-scale uses are limited by the scarcity and high cost of noble metals like iridium and platinum, despite their exceptional catalytic activity. As a result, current studies have concentrated on creating affordable, naturally occurring substitutes^[1,7,8], such as transition-metal oxides, sulfides, phosphides, and nanostructured materials^[6,22].

With a focus on design tactics, catalytic mechanisms, and present difficulties, this article attempts to give a thorough summary of recent developments in electrocatalysts for water splitting.

2. OBJECTIVES OF REVIEW:

- To critically analyze the fundamental mechanisms of HER and OER, with emphasis on reaction pathways, kinetic limitations, and the role of key intermediates in determining catalytic performance.
- To evaluate the design principles of electrocatalysts, focusing on structure–activity relationships, including adsorption energetics, electronic structure, and surface properties that govern catalytic efficiency.
- To compare the performance of noble metal catalysts and earth-abundant alternatives, highlighting their advantages, limitations, and potential for large-scale hydrogen production.
- To assess advanced material engineering strategies, such as defect engineering, heterostructure formation, doping, and nanostructuring, in enhancing catalytic activity, stability, and conductivity.
- To identify current challenges and future directions in electrocatalysis, including issues

related to overpotential, durability, scalability, and the integration of computational and data-driven approaches for catalyst development.

3. METHODS

In order to examine the electrochemical parameters and current developments in electrocatalysts for water splitting, the current work used a methodical literature review technique. The approach is predicated on a critical assessment of published theoretical and experimental research on the evolution reactions of hydrogen (HER) and oxygen (OER).

Standard electrochemical methods such as linear sweep voltammetry (LSV), cyclic voltammetry (CV), chronoamperometry, and electrochemical impedance spectroscopy (EIS) have been published in the literature to evaluate electrocatalytic performance^[17,22]. These methods are frequently used to assess the long-term stability, charge transfer kinetics, and catalytic activity of electrocatalysts. Overpotential (η), Tafel slope, exchange current density (j_0), turnover frequency (TOF), electrochemical surface area (ECSA), and Faradaic efficiency are important evaluation metrics that together shed light on catalytic efficiency and reaction kinetics.^[17, 22]

To understand the electrochemical behavior of water splitting, thermodynamic and kinetic analyses are used. The Gibbs free energy change ($\Delta G^\circ = 237.2 \text{ kJ mol}^{-1}$) and a standard electrode voltage of 1.23 V under ambient conditions control the process.^[5] HER at the cathode and OER at the anode are the two half-reactions that the reaction goes through. To comprehend the adsorption–desorption behavior of hydrogen intermediates, mechanistic paths for HER, such as the Volmer, Heyrovsky, and Tafel stages, are examined. In a similar vein, the multi-step electron transfer process is explained by OER processes such as the electrochemical oxide pathway, Lattice Oxygen mechanism (LOM), and adsorbate evolution mechanism (AEM).^[8, 9, 23]

The methodology further emphasizes structure–activity relationships by correlating catalytic performance with parameters such as Hydrogen adsorption free energy (ΔG_{H^*}) and binding energies of reaction intermediates. Comparative analysis of catalyst classes including

noble metals, transition metal oxides, hydroxides, and emerging nanostructured materials is performed to evaluate their efficiency, cost-effectiveness, and stability.

4. REVIEW OF LITERATURE:

Electrochemical water splitting is widely recognized as a sustainable approach for Hydrogen production, addressing global energy and environmental concerns. Hydrogen, with a high energy density ($\sim 120 \text{ MJ kg}^{-1}$), is an attractive clean fuel that produces only water as a by-product^[5].

Because of their high catalytic activity and low overpotential, noble metal catalysts like Pt for HER and $\text{RuO}_2/\text{IrO}_2$ for OER were the focus of early study^[6,22]. However, the focus has switched to earth-abundant transition metal catalysts (Fe, Co, Ni), which exhibit promise performance, especially in alkaline media, due to their high cost and unavailability. The Volmer–Heyrovsky–Tafel mechanism provides a good description of HER dynamics, and one important descriptor is the hydrogen adsorption free energy (ΔG_{H^*}). Volcano plot relationships show that optimal catalytic activity occurs when $\Delta G_{\text{H}^*} = 0$ ^[8,23]. OER, on the other hand, is the rate-limiting phase because it is kinetically slow and involves a four-electron transfer process with intermediates ($^*\text{OH}$, $^*\text{O}$, $^*\text{OOH}$) ^[9,23]. OER pathways are frequently described by mechanistic models like the Lattice Oxygen

Mechanism (LOM) and Adsorbate Evolution Mechanism (AEM).

Overpotential is a critical parameter representing the excess potential beyond the thermodynamic requirement (1.23 V), with practical systems operating at 1.6–2.0 V due to kinetic and resistive losses. Contributions include activation, ohmic, concentration, and bubble effects. Kinetic parameters such as Tafel slope and exchange current density are essential for evaluating catalytic efficiency.

Recent developments emphasize nanostructured materials, two-dimensional systems, and hybrid composites, which provide higher surface area, improved conductivity, and tunable electronic properties. Additionally, optimization of electrolytes and cell design has been explored to enhance efficiency and reduce losses.

This study employs a systematic literature review approach, analyzing experimental and theoretical works using electrochemical techniques such as LSV, CV, chronoamperometry, and EIS. Key performance metrics include overpotential, Tafel slope, exchange current density, turnover frequency (TOF), and Faradaic efficiency. Overall, the literature highlights a transition toward cost-effective, high-performance catalysts, supported by theoretical modeling and advanced material design strategies.



Fig.1. Design, Strategies and challenges in Developing water splitting.

The current study examines recent developments in electrocatalysis for electrochemical water splitting using a methodical, theory-driven literature approach. To clarify the mechanisms of the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), it combines density functional theory (DFT), computational modeling, and experimental electrochemical investigations. Reaction energetics, adsorption behavior, and electronic structure are assessed using DFT-based analyses that are backed by models like the computational hydrogen electrode (CHE) and free energy diagrams (FEDs).^[4, 8] Catalytic activity and stability are predicted using key characteristics such as hydrogen adsorption free energy (ΔG_{H}), binding energies of intermediates (*OH, *O, *OOH), and electronic density of states.

Noble metal catalysts like Pt, RuO₂, and IrO₂ have good intrinsic performance, according to the literature, but their scarcity and high cost restrict their practical use. As a result, research has turned to earth-abundant substitutes such as heterostructures, sulfides, phosphides, transition metal oxides, and doped carbon materials. According to mechanistic research, OER develops by intricate multi-step electron-transfer reactions, while HER follows the Volmer–Heyrovsky–Tafel pathways. The significance of structure–activity connections, volcano plots, scaling relations, defect engineering, heteroatom doping, and nanostructuring has also been highlighted in recent work^[23], and catalyst screening has been expedited by machine learning. In general, the rational design of effective, stable, and affordable electrocatalysts for sustainable hydrogen production has advanced through the integration of theoretical modeling and experimental validation.^[12, 13, 25]

5. FUNDAMENTALS OF WATER SPLITTING:

A crucial step in the synthesis of sustainable hydrogen is electrochemical water splitting, which

entails two linked half-reactions at the electrodes. The Oxygen Evolution Reaction (OER) oxidizes water to produce oxygen gas at the anode, whereas the Hydrogen Evolution Reaction (HER) uses proton reduction at the cathode to create molecular hydrogen.

These reactions can be represented as:

- HER (Cathode): $2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2$
- OER (Anode): $2\text{H}_2\text{O} \rightarrow \text{O}_2 + 4\text{H}^+ + 4\text{e}^-$

Although both reactions are essential for overall water splitting, their kinetic behaviors differ significantly. The HER is generally a two-electron transfer process and follows relatively simpler reaction pathways, typically described by the Volmer–Heyrovsky or Volmer–Tafel mechanisms. As a result, HER usually exhibits faster kinetics, particularly on efficient catalysts such as platinum.

In contrast, the OER is inherently more complex, involving a four-electron transfer process coupled with the formation and transformation of multiple oxygen-containing intermediates (e.g., *OH, *O, *OOH). This multistep mechanism requires the sequential breaking and formation of O–H and O–O bonds, which leads to higher activation energy barriers. Consequently, OER suffers from sluggish reaction kinetics and requires significantly higher overpotential to proceed at practical rates.^[8,10]

Due to these intrinsic kinetic limitations, OER is widely recognized as the rate-determining step in overall water electrolysis.^[9] Its slow kinetics not only reduce the overall efficiency of the process but also increase energy consumption. Therefore, considerable research efforts are focused on developing highly active and stable electrocatalysts to accelerate OER and minimize energy losses in water splitting systems.^[9,23]

Table 1: Comparison of Different Types of Electrocatalysts for Water Splitting

Category	Representative Materials	Key Features	Advantages	Limitations	Typical Applications
Noble Metal Catalysts	Pt (HER), RuO ₂ , IrO ₂ (OER)	High intrinsic activity; optimal adsorption energies;	Very low overpotential; fast kinetics;	High cost; scarcity; limited large-scale	Benchmark catalysts; fundamental studies; high-

		excellent conductivity	high efficiency	applicability; stability issues (especially RuO ₂)	performance electrolysis systems
Transition Metal-Based Catalysts	Oxides (NiO, Co ₃ O ₄), Sulfides (MoS ₂), Phosphides (Ni ₂ P)	Earth-abundant; tunable electronic structure; moderate conductivity	Low cost; good catalytic activity; scalable; chemically versatile	Lower intrinsic activity compared to noble metals; may require modification (doping, defects)	Practical water splitting systems; alkaline electrolysis; industrial-scale applications
Nanostructured Catalysts	Nanoparticles, nanosheets, nanowires, core-shell structures	High surface area; abundant active sites; enhanced charge transfer; morphology control	Improved catalytic efficiency; better utilization of active material; tunable properties	Complex synthesis; possible aggregation; stability concerns at long-term operation	Advanced catalyst design; hybrid systems; high-efficiency and next-generation electrolysis

5.2 KEY DESIGN STRATEGIES FOR ELECTROCATALYSTS:

The rational design of efficient electrocatalysts for water splitting relies on tailoring their structural, electronic, and surface properties to enhance catalytic activity and durability. Several key strategies have been developed to achieve these objectives.

5.2.1 Defect Engineering

Defect engineering involves the intentional introduction of vacancies, such as oxygen, sulfur, or metal vacancies, into the catalyst lattice. These defects can significantly modify the local electronic environment, leading to enhanced electrical conductivity and the creation of additional active sites. Consequently, defect-rich materials often exhibit improved catalytic performance due to increased adsorption and activation of reaction intermediates.^[14,25]

5.2.2 Heterostructure Formation

Heterostructure design involves integrating two or more distinct materials to form interfaces with synergistic properties. Such interfaces facilitate efficient charge transfer and separation, thereby

enhancing reaction kinetics. The coupling of different phases or compositions can also optimize adsorption energies and improve overall catalytic efficiency.^[12,15]

5.2.3 Doping Strategy:

The process of adding foreign atoms to a host material in order to alter its electronic structure is known as doping. By changing variables like the d-band center, charge density, and conductivity, this method can adjust how the catalyst surface and reaction intermediates interact. Doping is therefore frequently used to increase both HER and OER activity.^[7,23]

5.2.4 Surface Engineering

Surface engineering focuses on modifying the catalyst surface through functionalization or coating strategies to increase the accessibility of active sites. These modifications can improve adsorption characteristics, enhance catalytic selectivity, and facilitate faster reaction kinetics by optimizing the surface chemical environment.

5.2.5 Morphology Control

Enhancing performance requires controlling the morphology of electrocatalysts, such as creating

three-dimensional (3D) hierarchical structures or two-dimensional (2D) nanosheets. These structures improve electron transfer channels, increase surface area, and facilitate effective mass transport of reactants and products.^[12,25]

5.2.6 Performance Parameters for Electrocatalyst Evaluation

The efficiency of electrocatalysts is evaluated using several key electrochemical parameters:

- **Overpotential (η):** The excess potential required beyond the thermodynamic value to drive the reaction; lower values indicate better catalytic activity^[22].
- **Tafel Slope:** Provides clear idea about reaction kinetics and the rate-determining step; smaller slopes correspond to faster reaction rates.
- **Exchange Current Density (j_0)^[22]:** Represents the intrinsic catalytic activity at equilibrium; higher values indicate superior performance.
- **Stability:** Assessed through long-term cycling and durability tests, reflecting the catalyst's ability to maintain performance under operational conditions.

The performance of electrocatalysts for water-splitting reactions, including HER and OER, is

evaluated using key electrochemical parameters such as Tafel slope, overpotential (η), exchange current density (j_0), and stability. Overpotential is the excess potential required beyond the thermodynamic value (1.23 V) to drive the reaction, where lower η indicates higher catalytic efficiency. The Tafel slope gives an idea about reaction kinetics and the rate-determining step, with smaller values reflecting faster electron-transfer processes. Exchange current density (j_0), obtained from Tafel extrapolation, represents the intrinsic catalytic activity at equilibrium, and higher values indicate superior performance. Stability is a crucial parameter that determines the practical applicability of a catalyst under prolonged operation.

It is typically evaluated using cyclic voltammetry, chronoamperometry, and chronopotentiometry techniques^[22,17]. Minimal changes in overpotential and current density after long-term testing indicate good durability. These parameters collectively reflect thermodynamic efficiency, kinetic behavior, and intrinsic activity. They provide a comprehensive basis for comparing different electrocatalysts. Overall, such evaluation criteria are essential for the rational design of durable and efficient catalysts for water splitting.

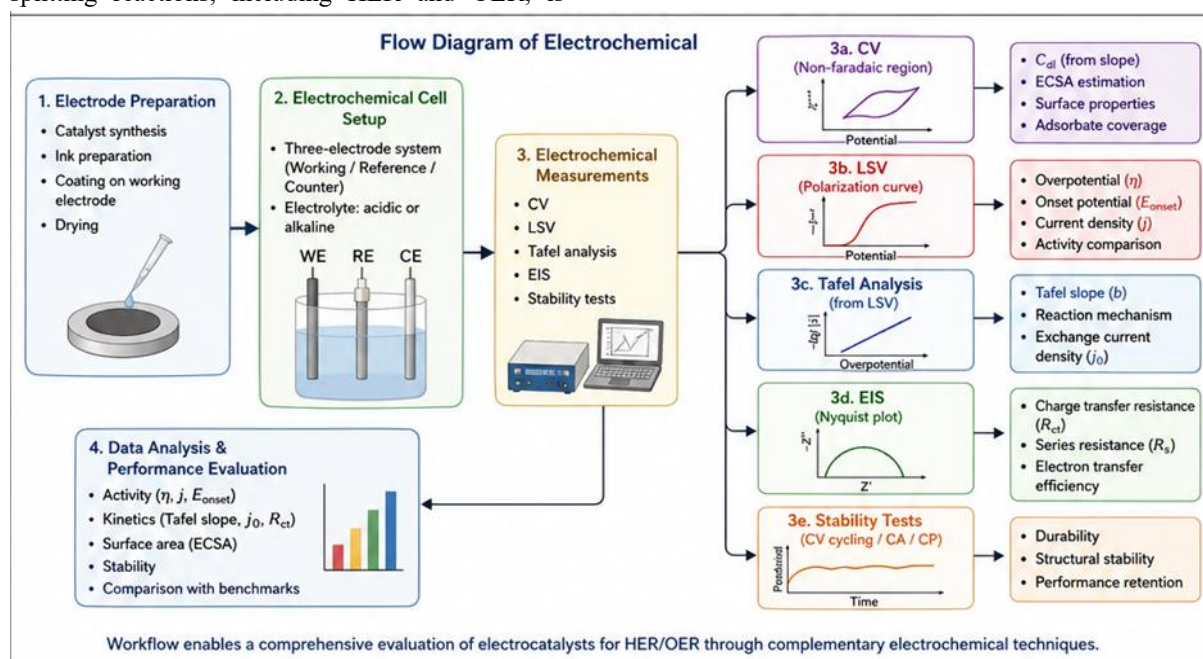


Fig.2 : Flow diagram of Electrochemical sensing

Category	Parameter	Symbol / Expression	Experimental Technique(s)	How it is Extracted / Interpreted
Thermodynamic	Hydrogen adsorption free energy	ΔG_{H^*}	CV (indirect), LSV (correlation)	Not directly measured; inferred from activity trends (overpotential, Tafel slope) and compared with DFT predictions
	OER intermediate energies	$\Delta G_{OH^*}, \Delta G_{O^*}, \Delta G_{OOH^*}$	LSV (indirect)	Correlated with onset potential and overpotential; validated via theoretical models
	Step free energy changes	$\Delta G_1 - \Delta G_4$	LSV (indirect)	Reflected in polarization behavior and kinetic regions
	Potential determining step	PDS	Tafel slope, LSV	Identified from slope regions and rate-determining kinetics
Electrochemical	Overpotential	η	LSV	Determined at a fixed current density (e.g., η @ 10 mA cm ⁻²)
	Onset potential	E_{onset}	LSV	Potential where current sharply increases (reaction begins)
	Current density	j	LSV, CV	Directly obtained from polarization curves
	Exchange current density	j_0	Tafel plot	Extrapolated from Tafel plot at zero overpotential
Kinetic	Tafel slope	b (mV dec ⁻¹)	Tafel analysis (from LSV)	Indicates reaction mechanism (Volmer, Heyrovsky, Tafel step)
	Charge transfer resistance	R_{ct}	EIS	Obtained from Nyquist plot; smaller R_{ct} → faster kinetics
	Reaction kinetics	—	LSV, EIS	Evaluated from slope and impedance behavior
Surface / Interfacial	Double-layer capacitance	C_{dl}	CV	Measured from non-faradaic region; used to estimate ECSA
	Electrochemically active surface area	ECSA	CV	Calculated from C_{dl} values (ECSA $\propto C_{dl}$)
	Adsorbate coverage	θ	CV (qualitative), EIS	Changes in capacitance and surface states indicate coverage
Electronic / Transport	Electron transfer efficiency	—	EIS	Evaluated from semicircle diameter (Nyquist plot)
	Conductivity / resistance	R_s, R_{ct}	EIS	Series resistance (R_s) and charge transfer resistance (R_{ct})
Stability	Catalyst durability	—	CV cycling, Chronoamperometry, Chronopotentiometry	Stability tested via repeated cycles or constant potential/current
	Structural stability	—	CV + LSV (before/after)	Performance retention indicates robustness
Mass Activity / Efficiency	Turnover frequency	TOF	LSV (with active site estimation)	Calculated using current and number of active sites
	Faradaic efficiency	FE (%)	CV / controlled electrolysis	Measured by product quantification (H ₂ /O ₂ evolution)

CV: Cyclic Voltammetry; LSV: Linear Sweep Voltammetry; EIS: Electrochemical Impedance Spectroscopy

Table.2: Correlation of Electrochemical performance parameters with Experimental techniques.

6. DISCUSSION /ANALYSIS:

The present review employs a systematic, theory-driven approach to analyze recent advances in electrocatalysis for electrochemical water splitting. It integrates density functional theory (DFT), computational modeling, and experimental studies to elucidate the mechanisms of Hydrogen evolution (HER) and Oxygen evolution (OER). DFT-based methods^[4,8], including the computational hydrogen electrode (CHE) and free energy diagrams, are used to assess reaction energetics, adsorption characteristics, and electronic structure. Key descriptors such as hydrogen

adsorption free energy (ΔG_{H^*}), intermediate binding energies ($*OH, *O, *OOH$), and electronic density of states are critical for predicting catalytic activity and stability.

While noble metal catalysts (Pt, RuO₂, IrO₂) exhibit superior performance, their high cost limits large-scale application, prompting the development of earth-abundant alternatives such as transition metal compounds and heterostructures.^[6,1] HER proceeds via Volmer–Heyrovsky–Tafel pathways, whereas OER involves complex multi-electron transfer steps. Recent progress emphasizes structure–activity relationships^[23], scaling relations,

defect engineering, heteroatom doping, nanostructuring, and machine learning-assisted screening. Overall, the integration of theoretical insights with experimental validation enables the

rational design of efficient, stable, and cost-effective electrocatalysts for sustainable Hydrogen production.

6.1 Comparison of Electrocatalysts for HER vs OER:

Parameter	HER (Hydrogen Evolution Reaction)	OER (Oxygen Evolution Reaction)
Reaction Type	Reduction reaction	Oxidation reaction
Half-Reaction	$2H^+ + 2e^- \rightarrow H_2$ (acidic)	$2H_2O \rightarrow O_2 + 4H^+ + 4e^-$ (acidic)
Electron Transfer	2-electron process	4-electron process
Kinetics	Fast	Slow (rate-limiting step)
Mechanism	Volmer–Heyrovsky / Volmer–Tafel	Multi-step involving OH*, O*, OOH* intermediates
Overpotential (η)	Low (especially with Pt)	High (even with best catalysts)
Best Catalysts (Benchmark)	Pt-based materials	IrO ₂ , RuO ₂
Cost of Benchmark Catalysts	Very high	Very high
Alternative Catalysts	MoS ₂ , Ni ₂ P, CoP, WS ₂	NiFe ₂ O ₄ , Co ₃ O ₄ , MnO ₂ , perovskites
Catalyst Design Focus	Optimize hydrogen adsorption ($\Delta G_H \approx 0$)	Optimize adsorption of OER intermediates
Key Descriptor	Gibbs free energy of H adsorption (ΔG_H)	Binding energy of OH*, O*, OOH*
Rate-Determining Step	Proton adsorption or hydrogen recombination	O–O bond formation
Tafel Slope (Typical)	30–120 mV/dec	60–120 mV/dec (often higher)
Stability Issues	Generally stable in acidic media	Poor stability, especially in acidic media
Electrolyte Compatibility	Works well in acidic and alkaline media	More stable in alkaline media
Material Challenges	Replacing Pt with cheap alternatives	Achieving both activity + durability
Nanomaterial Role	Increases active sites, conductivity	Enhances surface area and catalytic pathways

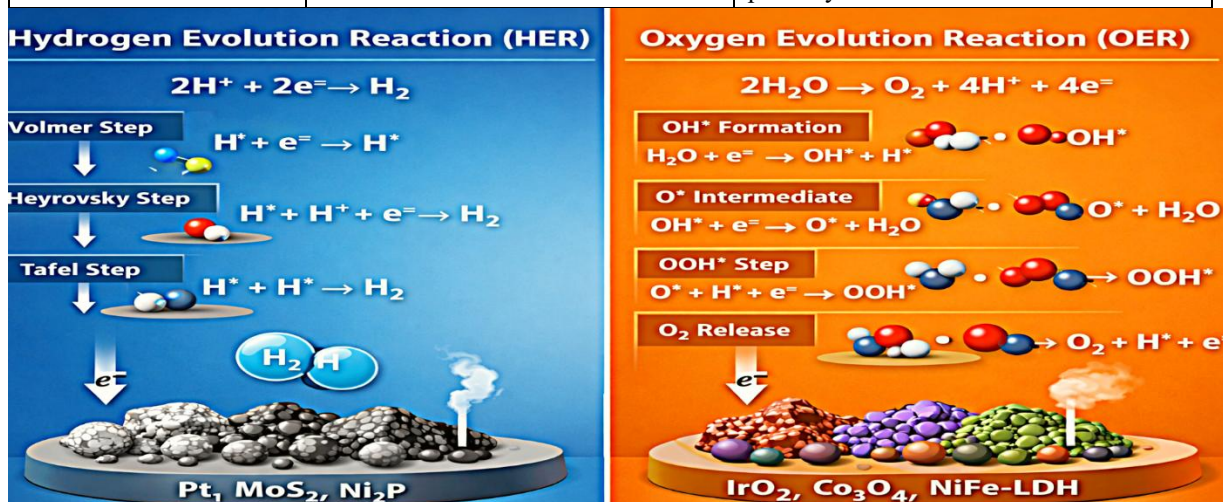


Table.3 : A comparative analysis of HER and OER electrocatalysts^[8,9].

7. CHALLENGES IN ELECTROCATALYTIC WATER SPLITTING:

Despite significant advancements in electrocatalyst design, several critical challenges continue to hinder the practical implementation of electrochemical water splitting technologies.

One of the primary limitations is the requirement of high overpotential in practical systems^[22]. Although the thermodynamic potential for water splitting is 1.23 V, additional energy input is necessary to overcome kinetic barriers associated with the Hydrogen evolution reaction (HER) and particularly the Oxygen evolution reaction (OER). This results in increased energy consumption and reduced overall efficiency of the process.

Another major concern is catalyst poisoning^[14], which arises from the adsorption of impurities or reaction by-products on active sites. These species can block catalytic centers, thereby decreasing the number of available active sites and significantly reducing catalytic activity over time.

Stability under different pH conditions, especially in highly acidic or alkaline media, remains a persistent challenge.^[1,16] Many electrocatalysts undergo structural degradation, dissolution, or surface reconstruction during prolonged operation, leading to performance loss. Ensuring chemical and electrochemical stability in harsh environments is therefore crucial for long-term applications.

Lastly, there are a lot of difficulties with industrial implementation and scale-up. Even while many catalysts function exceptionally well in the lab, problems with material pricing, repeatability, electrode fabrication, and system integration make it challenging to apply these findings to large-scale systems.^[21] Furthermore, sustaining high durability and efficiency under industrial operating circumstances continues to be a major challenge.

8. FUTURE PERSPECTIVES:

The continued advancement of electrochemical water splitting technologies depends on the development of innovative strategies that address current limitations while enhancing efficiency and scalability. One of the primary research directions is the design of non-noble metal electrocatalysts based on earth-abundant elements

such as transition metals.^[1,6] These materials offer a promising pathway toward cost-effective and sustainable hydrogen production, provided that their activity and long-term stability can be further improved through rational design approaches.

Another important direction involves the integration of water electrolysis systems with renewable energy sources, particularly solar energy^[5,20]. Solar-driven electrolysis, including photoelectrochemical and photovoltaic-assisted systems, has the potential to enable green hydrogen production with minimal carbon footprint. Such integrated systems can significantly improve the sustainability and economic feasibility of hydrogen generation.

The application of artificial intelligence (AI) and machine learning (ML) in catalyst design is emerging as a transformative approach^[11,15]. By leveraging large datasets and predictive algorithms, AI-driven methods can accelerate the discovery and optimization of electrocatalysts by identifying structure–property relationships and screening potential materials with high efficiency.

Furthermore, the use of in situ and operando characterization techniques is gaining increasing importance for understanding catalytic mechanisms under realistic working conditions.^[4] These techniques provide real-time insights into structural, electronic, and chemical changes occurring at the catalyst surface during operation, enabling the identification of active sites and degradation pathways.

Overall, the integration of advanced material design, renewable energy coupling, data-driven approaches, and real-time characterization is expected to play a crucial role in the development of high-performance, durable, and scalable electrocatalytic systems for sustainable hydrogen production.

9. CONCLUSION:

One possible method for producing hydrogen sustainably is electrocatalytic water splitting. The development of effective electrocatalysts has evolved significantly thanks to sophisticated design techniques like heterostructure creation and defect engineering. However, issues with cost, scalability, and stability continue to be

major obstacles to commercialization. The logical design of long-lasting, inexpensive catalysts and their incorporation into useful energy systems should be the main topics of future research.

A sustainable hydrogen-based energy economy is mostly dependent on electrochemical water splitting. Although noble metal-based catalysts now set the standard for performance^[6,22], their resource and cost constraints force a shift to earth-abundant substitutes including transition metal oxides, sulfides, and phosphides^[1,7]. Recent breakthroughs in nanostructuring and computational modeling have significantly advanced the design of these materials, enabling enhanced active site exposure and optimized electronic structures through strategies like defect engineering and heterostructure formation.^[12,4]

Despite these technical strides, successfully bridging the gap from laboratory-scale research to industrial application remains contingent on overcoming critical hurdles including long-term material stability, high overpotentials, and the complexities of real-world device integration. Future progress will likely depend on the synergistic integration of artificial intelligence for material discovery, the development of robust bifunctional electrocatalysts, and the adoption of scalable, sustainable manufacturing processes.^[21] By aligning fundamental mechanistic insights with innovative engineering solutions, the field is well-positioned to mitigate environmental impacts and satisfy the escalating global demand for clean energy, ultimately facilitating the commercial viability of green hydrogen production.

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