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ADVANCED TRANSITION METAL OXIDE-BASED HETEROSTRUCTURED ELECTROCATALYSTS FOR EFFICIENT HYDROGEN AND OXYGEN EVOLUTION REACTIONS.

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ABSTRACT

Advanced transition metal oxide-based heterostructure electrocatalysts represent a rapidly evolving and highly promising class of materials that are specifically engineered to improve the efficiency of the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). These two electrochemical processes are fundamental half-reactions involved in overall water splitting, a key technology for sustainable hydrogen production. As the global demand for clean and renewable energy sources increases, the development of efficient, low-cost, and durable electrocatalysts has become a central focus of modern materials science research. In this context, heterostructure transition metal oxides are attracting significant attention due to their unique ability to combine structural versatility, electronic tunability, and synergistic interfacial interactions, all of which contribute to enhanced catalytic performance. In present research, emphasis is placed on optimizing these materials to reduce activation energy barriers, accelerate charge transfer kinetics, and ensure long-term operational stability under rigorous electrochemical conditions

Keywords - Hydrogen evolution reaction HER and Oxygen evolution reaction OER

INTRODUCTION

Transition metal oxides composed of elements such as nickel, cobalt, iron, manganese, and their mixed-metal derivatives are widely explored because of their natural abundance, cost-effectiveness, multiple oxidation states, and adaptable crystal structures. These characteristics make them suitable candidates for catalytic applications. However, despite these advantages, single-phase metal oxides often exhibit inherent limitations, including poor electrical conductivity and relatively low intrinsic catalytic activity, particularly in HER processes. To address these shortcomings, researchers have increasingly adopted heterostructure strategies, where two or more distinct materials or phases are integrated at the nanoscale. This design approach leads to the formation of abundant heterointerfaces, which play a crucial role in modifying the electronic structure of the catalyst. As a result, these interfaces facilitate improved adsorption and desorption behaviour of key reaction intermediates such as H*, OH*, and OOH*, ultimately enhancing catalytic efficiency

In present developments, a wide variety of heterostructure systems are being engineered, including combinations such as metal oxide/metal sulphide, metal oxide/phosphide, metal oxide/nitride, and multi-metal oxide interfaces. These hybrid configurations are particularly effective because they combine the chemical stability of oxides with the superior electrical conductivity of other materials. For example, coupling nickel oxide with cobalt oxide or iron oxide significantly enhances redox activity and supports efficient multi-electron transfer processes, which are essential for OER. Similarly, integrating transition metal oxides with conductive supports such as carbon-based materials (graphene, carbon nanotubes) or metallic substrates improves electron transport pathways, thereby boosting overall catalytic performance

The oxygen evolution reaction is widely recognized as the rate-limiting step in water splitting due to its complex four-electron transfer mechanism. This complexity results in high overpotentials and slow reaction kinetics. Transition metal oxide-based heterostructures address these challenges by effectively tuning the electronic configuration, particularly the d-band structure, of the active metal centres. In present research, it is observed that interfacial charge redistribution between different components leads to optimized adsorption energies for oxygen-containing intermediates. This optimization reduces the energy required for intermediate formation and transformation, thereby lowering the overpotential and accelerating OER kinetics. Furthermore, lattice strain and defect engineering at the heterointerface contribute to the creation of additional active sites, enhancing catalytic activity.

In the case of the hydrogen evolution reaction, achieving an optimal hydrogen adsorption free energy is the key requirement for efficient catalysis. Ideally, the catalyst should bind hydrogen neither too strongly nor too weakly. However, pure metal oxides often fail to achieve this balance. Heterostructure systems overcome this limitation through electronic coupling between different phases, which adjusts the hydrogen adsorption energy toward an optimal value close to thermoneutral. This facilitates rapid hydrogen adsorption and desorption, enabling continuous catalytic turnover. In present experimental studies, such heterostructure catalysts exhibit significantly improved exchange current densities and lower Tafel slopes, indicating faster reaction rates and superior catalytic efficiency compared to single-component systems.

LITERATURE REVIEW

Due to its abundance of catalytically active edge sites and favorable electronic structure, the two-dimensional (2D) atomically thin transition metal dichalcogenide molybdenum diselenide ($MoSe_2$) has emerged as a promising non-noble metal electrocatalyst for the hydrogen evolution reaction (HER). In comparison to conventional noble metal catalysts such as platinum, $MoSe_2$ offers a cost-effective and earth-abundant alternative while still maintaining appreciable catalytic activity. The layered structure of $MoSe_2$, composed of Se–Mo–Se atomic sheets held together by weak van der Waals forces, allows for easy exfoliation into ultrathin nanosheets. These nanosheets expose a large number of active edge sites, which are primarily responsible for HER activity. However, despite these advantages, the intrinsic semiconducting nature of $MoSe_2$ and the relatively inert basal plane significantly limit its electrical conductivity and overall catalytic efficiency. One of the primary challenges associated with $MoSe_2$-based catalysts lies in improving charge transfer kinetics during the HER process.

The basal plane of $MoSe_2$ is thermodynamically stable but catalytically less active, while the edge sites, although active, are limited in number. As a result, enhancing the exposure of active sites while simultaneously improving conductivity becomes essential. In present research, integrating 2D $MoSe_2$ nanosheets with conductive substrates has emerged as an effective strategy to overcome these limitations. In particular, coupling $MoSe_2$ with large-area two-dimensional materials can significantly enhance electron mobility and facilitate rapid interfacial charge transfer, thereby boosting catalytic performance. In this context, titanium carbide MXene (Ti_3C_2), a member of the MXene family of 2D transition metal carbides, has gained considerable attention due to its excellent electrical conductivity, hydrophilic surface, and tunable surface chemistry. The presence of surface terminations such as –O, –OH, and –F groups on Ti_3C_2 MXene provides abundant anchoring sites for the growth of other nanostructures. In the present work, an efficient and scalable synthesis approach is employed to fabricate a 2D/2D heterostructured composite consisting of $MoSe_2$ nanosheets integrated with oxygen-terminated Ti_3C_2 MXene. Through an in situ growth process, layered

$MoSe_2$ nanosheets are uniformly decorated onto the surface of oxygen-functionalized Ti_3C_2 MXene flakes, forming a well-defined heterointerface.[Xiao, Weiping et al., (2021)]

Hydrogen energy has emerged as one of the most promising clean energy carriers due to its high energy density and its environmentally benign nature, producing only water as a by-product upon combustion or electrochemical utilization. As global energy systems shift toward sustainability, the hydrogen evolution reaction (HER), a key half-reaction in water electrolysis, has attracted significant scientific and technological interest. Despite its advantages, the large-scale adoption of hydrogen energy is still constrained by high production costs and the limited availability of efficient, durable, and affordable electrocatalysts. Noble metal catalysts such as platinum exhibit excellent HER activity, but their scarcity and high cost make them impractical for widespread applications. This has led to an increasing focus on alternative catalyst systems based on earth-abundant materials. Among these, mixed metal oxide (MMO) electrocatalysts have gained attention as a highly promising class of materials. Unlike single-phase metal oxides, which often suffer from poor electrical conductivity and suboptimal catalytic activity, MMOs offer unique advantages due to their heterostructured interfaces. These interfaces, formed between different metal oxide components or between metals and metal oxides, create regions of strong electronic interaction that significantly enhance catalytic performance. The presence of multiple metal centers with variable oxidation states allows for improved charge redistribution, facilitating more efficient electron transfer during the HER process. One of the key benefits of MMO electrocatalysts lies in their ability to reduce the activation energy barrier associated with HER. The reaction involves adsorption of hydrogen intermediates (H*) on the catalyst surface, followed by either electrochemical desorption or recombination to form molecular hydrogen. In single-phase oxides, the binding strength of hydrogen is often either too weak or too strong, leading to inefficient catalysis. However, in MMOs, the synergistic interaction between different metal species modifies the electronic structure of active sites, thereby optimizing hydrogen adsorption free energy. This results in enhanced reaction kinetics and improved catalytic efficiency. [Pratama, Dwi Sakti Aldianto et al., (2023)]

AIM AND OBJECTIVE OF THE STUDY

1. To synthesize advanced transition metal oxide-based hetero structured electrocatalysts using cost-effective and scalable chemical methods such as co-precipitation, hydrothermal synthesis, and pyrolysis.

2. To characterize the structural, morphological, optical, and electronic properties of the prepared electrocatalysts using techniques such as XRD, SEM, TEM, XPS, UV-DRS, and BET surface area analysis.

3. To evaluate the electrocatalytic performance of synthesized materials for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) using electrochemical techniques such as LSV, CV, EIS, and chronoamperometry.

4. To investigate the effect of doping, composite formation, and heterostructure engineering on catalytic activity, charge transfer efficiency, and active site enhancement.

5. To analyse the relationship between material structure and electrocatalytic performance in order to identify high-efficiency, stable, and cost-effective catalysts for water splitting applications.

STATUS OF THE STUDY

The need for the study on advanced transition metal oxide-based heterostructured electrocatalysts for efficient hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) will arise primarily from the rapidly increasing global demand for clean, renewable, and sustainable energy sources. In the coming years, the continuous depletion of fossil fuel reserves, along with their harmful environmental impact, will pose serious challenges to energy security and ecological balance. The excessive use of fossil fuels will continue to contribute significantly to greenhouse gas emissions, air pollution, and climate change. Therefore, it will become essential to shift toward alternative energy systems that are both environmentally friendly and economically viable. In this future energy scenario, hydrogen will be expected to emerge as a highly promising energy carrier due to its high energy density and zero carbon emission during utilization. The large-scale production of hydrogen through electrochemical water splitting will become increasingly important, as it offers a clean and sustainable route for energy generation. However, the efficiency of water splitting processes will largely depend on the performance of electrocatalysts used for HER and OER. Existing electrocatalysts, particularly those based on noble metals such as platinum, iridium, and ruthenium, will continue to face limitations due to their high cost, scarcity, and limited long-term stability. These challenges will restrict their widespread industrial application. Therefore, this study will be needed to address the critical limitations associated with current electrocatalytic systems, including high energy consumption, slow reaction kinetics, and poor durability under operational conditions. It will be necessary to develop alternative catalysts that are not only efficient but also cost-effective and composed of earth-abundant materials. In this regard, transition metal oxide-based hetero structured electrocatalysts will be expected to play a vital role in future research and technological advancements. The study will also be important for understanding the fundamental mechanisms that govern catalytic activity in hetero structured systems. The presence of heterointerfaces in these materials will create unique opportunities for enhancing catalytic performance through synergistic effects. These interfaces will enable charge redistribution, optimize electronic structures, and improve the adsorption and desorption behaviours of reaction intermediates. As a result, both HER and OER processes will become more efficient, requiring lower energy input and exhibiting faster reaction kinetics. Furthermore, the study will be required to explore strategies for increasing the number of active catalytic sites and improving electrical conductivity. By tailoring the composition, morphology, and structure of transition metal oxides, researchers will be able to design catalysts with enhanced surface area and improved electrochemical performance. The development of advanced synthesis techniques, such as hydrothermal methods, electrodeposition, and atomic-level engineering, will also be essential to produce well-defined and highly stable hetero structured catalysts. In addition, this study will contribute to improving the scalability and practical applicability of electrocatalysts for industrial use. Long-term stability and resistance to degradation under harsh electrochemical conditions will be critical factors that need to be addressed. The ability to produce catalysts on a large scale without compromising performance will also be a key requirement for commercialization.

PROPOSED METHODOLOGY

The present study on advanced transition metal oxide-based heterostructured electrocatalysts for efficient hydrogen and oxygen evolution reactions will be designed in response to the increasing demand for clean, renewable, and sustainable energy technologies. In the future, the research methodology will be structured to systematically develop, synthesize, characterize, and evaluate high-performance electrocatalytic materials for water splitting applications. The study will primarily focus on overcoming the limitations of precious metal catalysts by employing cost-effective transition metal oxide (TMO)-based heterostructures with enhanced catalytic efficiency, stability, and scalability.

In the future approach, the synthesis of electrocatalysts will be carried out using simple, reproducible, and scalable chemical methods such as co-precipitation, hydrothermal synthesis, and pyrolysis techniques. These methods will be expected to enable controlled growth of nanostructured materials with desired morphology, composition, and surface characteristics. Different transition metal oxides and their hetero structured combinations will be prepared by varying metal precursors, doping concentrations, and reaction conditions to optimize electrocatalytic performance. In addition, composite formation and heterojunction engineering will be employed to improve charge transfer efficiency and catalytic active site exposure.

The synthesized materials will be expected to undergo comprehensive physicochemical characterization to understand their structural, morphological, and electronic properties. Techniques such as X-ray diffraction (XRD) will be used to confirm crystalline phase formation and structural purity. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) will be utilized to analyse surface morphology, particle size, and nanoscale heterointerfaces. X-ray photoelectron spectroscopy (XPS) will be employed to investigate elemental composition, oxidation states, and electronic interactions between components. UV–visible diffuse reflectance spectroscopy (UV-DRS) will be used to evaluate optical properties and band gap variations, while BET surface area analysis will be conducted to determine porosity and surface area. These characterizations will be expected to provide detailed insights into structure–property relationships.

In the future experimental methodology, electrochemical performance evaluation will be carried out using a standard three-electrode system. The prepared electrocatalysts will be tested for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) under different electrolytic conditions. Key electrochemical techniques such as linear sweep voltammetry (LSV), cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and chronoamperometry will be used to assess catalytic activity, charge transfer resistance, reaction kinetics, and long-term stability. Important parameters such as overpotential, Tafel slope, and current density will be analysed to compare the efficiency of different catalysts.

The study will also be expected to include systematic doping and heterostructure engineering strategies to enhance catalytic performance. In future work, controlled doping of transition metals such as cobalt, nickel, or iron into oxide frameworks will be used to tune electronic properties and improve active site density. Formation of heterojunctions between different metal oxides or with carbon-based materials will be expected to enhance charge separation and reduce recombination losses, thereby improving overall catalytic efficiency.

In addition, composite fabrication strategies will be employed to develop multi-component electrocatalysts with synergistic effects. Hybrid systems such as metal oxide–carbon nitride, metal oxide–phosphate, and mixed oxide composites will be synthesized to improve conductivity and stability. These heterostructures will be expected to provide improved adsorption–desorption behaviour for reaction intermediates involved in water splitting.

In future analysis, data obtained from structural, morphological, and electrochemical studies will be systematically correlated to understand the relationship between material design and catalytic performance. Comparative studies will be conducted to identify the most efficient catalyst compositions for HER and OER applications. Statistical tools and graphical analysis will be used to validate reproducibility and reliability of results

EXPECTED OUTCOMES

The expected outcomes of the study on advanced transition metal oxide-based heterostructure electrocatalysts for efficient hydrogen and oxygen evolution reactions will significantly advance future clean energy technologies. In the future, the study will be expected to demonstrate that heterostructure catalysts will show superior electrocatalytic performance compared to conventional single-phase materials. It will be anticipated that improved charge transfer at the interfaces of different metal oxides will enhance reaction kinetics for both hydrogen evolution reaction and oxygen evolution reaction. These catalysts will be expected to exhibit lower overpotentials, higher current densities, and improved energy efficiency during water splitting. The study will further be expected to reveal that nanoscale engineering and defect manipulation will play a crucial role in enhancing catalytic activity. Oxygen vacancies and optimized electronic structures will be anticipated to create more active sites and improve adsorption of reaction intermediates. In addition, the catalysts will be expected to demonstrate long-term stability under harsh electrochemical conditions, making them suitable for industrial applications. In the future, these outcomes will be expected to support the development of cost-effective, scalable, and environmentally friendly hydrogen production systems. Overall, the study will contribute to advancing sustainable energy solutions and promoting the global transition toward a hydrogen-based economy.

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