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TRANSITION METAL NANOSTRUCTURED CATALYSTS FOR ENERGY CONVERSION AND STORAGE APPLICATIONS: A COMPREHENSIVE REVIEW

Muhammad Qaisar*[1], Muhammad Neam Qamar[2]

*[1]*BS Chemistry Graduate Department of Chemistry, Government Sadiq Egerton College, Bahawalpur, Pakistan*
[2]*Associate Professor Department of Chemistry Government Sadiq Egerten Graduate College Bhawalpur*

*[1]muhammadqaisar0023@gmail.com, [2]neamqamar04@gmail.com

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Corresponding Author: *
Muhammad Qaisar

Abstract

The global energy landscape is undergoing a significant transition due to increasing concerns over fossil fuel depletion, rising energy demands, and environmental pollution [27,28,36]. In this scenario, the development of efficient and sustainable energy conversion and storage systems has become a major scientific priority [29,36]. Among the various materials investigated, transition metal nanostructured catalysts have attracted considerable attention owing to their unique physicochemical properties and broad application potential [32,34,38]. These materials, particularly based on Fe, Co, Ni, Mn, and Cu and their corresponding compounds such as oxides, sulfides, phosphides, and carbides, offer a cost-effective alternative to noble metal catalysts [32,38]. Their nanoscale dimensions provide a high density of active sites, improved electron transfer behavior, and tunable surface chemistry, all of which directly influence catalytic performance [30,38]. In electrochemical energy systems, these catalysts play a central role in key reactions such as hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR) [4–6,10,19]. These reactions are fundamental to technologies like water electrolysis, fuel cells, and metal–air batteries. In parallel, transition metal nanostructures have also shown promising results in energy storage devices, including lithium-ion batteries, sodium-ion batteries, and supercapacitors, where they enhance capacity, rate performance, and cycling stability [23,24,27]. Despite these advantages, several challenges still limit their large-scale application. Issues such as structural instability under operating conditions, particle agglomeration, and insufficient long-term durability remain critical concerns [30,31]. Recent research has therefore focused on improving material design through strategies such as heterostructure formation, doping, defect engineering, and development of single-atom catalysts [30,31,38].

Overall, transition metal nanostructured catalysts represent a rapidly evolving research area that bridges fundamental materials chemistry with practical energy technologies, offering promising pathways toward sustainable energy systems [32,34].

1. INTRODUCTION

1.1 Context & Background of the Study

The global energy scenario has undergone significant transformation over the past few decades due to rapid industrialization, population growth, and technological advancement [27,28,36]. These developments have led to a continuous increase in energy consumption, which remains largely dependent on non-renewable fossil fuel resources. Fossil fuels such as coal, oil, and natural gas have historically served as the backbone of global energy production; however, their finite availability and uneven geographical distribution have raised serious concerns about long-term energy security [27,36].

Alongside resource limitations, the extensive utilization of fossil fuels has resulted in severe environmental consequences. The emission of greenhouse gases, particularly carbon dioxide, has significantly contributed to global warming, climate change, and environmental degradation [36]. These challenges have intensified global efforts toward the development of alternative, clean, and sustainable energy systems capable of reducing environmental impact while meeting increasing energy demands [29,36].

In response to these challenges, electrochemical energy technologies have emerged as a vital area of research and development. Systems such as water electrolysis, fuel cells, rechargeable batteries, and supercapacitors are being widely explored as efficient platforms for energy conversion and storage [3,25,27]. These technologies are particularly important because they enable the direct conversion of chemical energy into electrical energy and vice versa, offering flexible and sustainable energy solutions.

The performance of these electrochemical systems is highly dependent on the materials used in their key functional components, particularly catalysts and electrode materials. Catalysts play a crucial role in accelerating electrochemical reactions and improving overall energy efficiency [3,5]. In recent years, transition metals have gained considerable attention due to their unique electronic configurations, multiple oxidation states, and strong redox capabilities, making them highly suitable for catalytic applications [32,38].

Furthermore, when these transition metals are engineered at the nanoscale, they exhibit significantly enhanced physical and chemical properties compared to their bulk counterparts. The nanoscale dimension provides a higher surface area, increased availability of active sites, and improved interaction with reactant species [30,33]. These characteristics have made transition metal nanostructured materials an important class of functional materials in the field of energy conversion and storage [30,34].

As a result, transition metal nanostructured catalysts have become a major focus in modern materials chemistry and electrochemical research, forming the foundation for advanced energy technologies aimed at achieving sustainability and high efficiency [32,34,38].

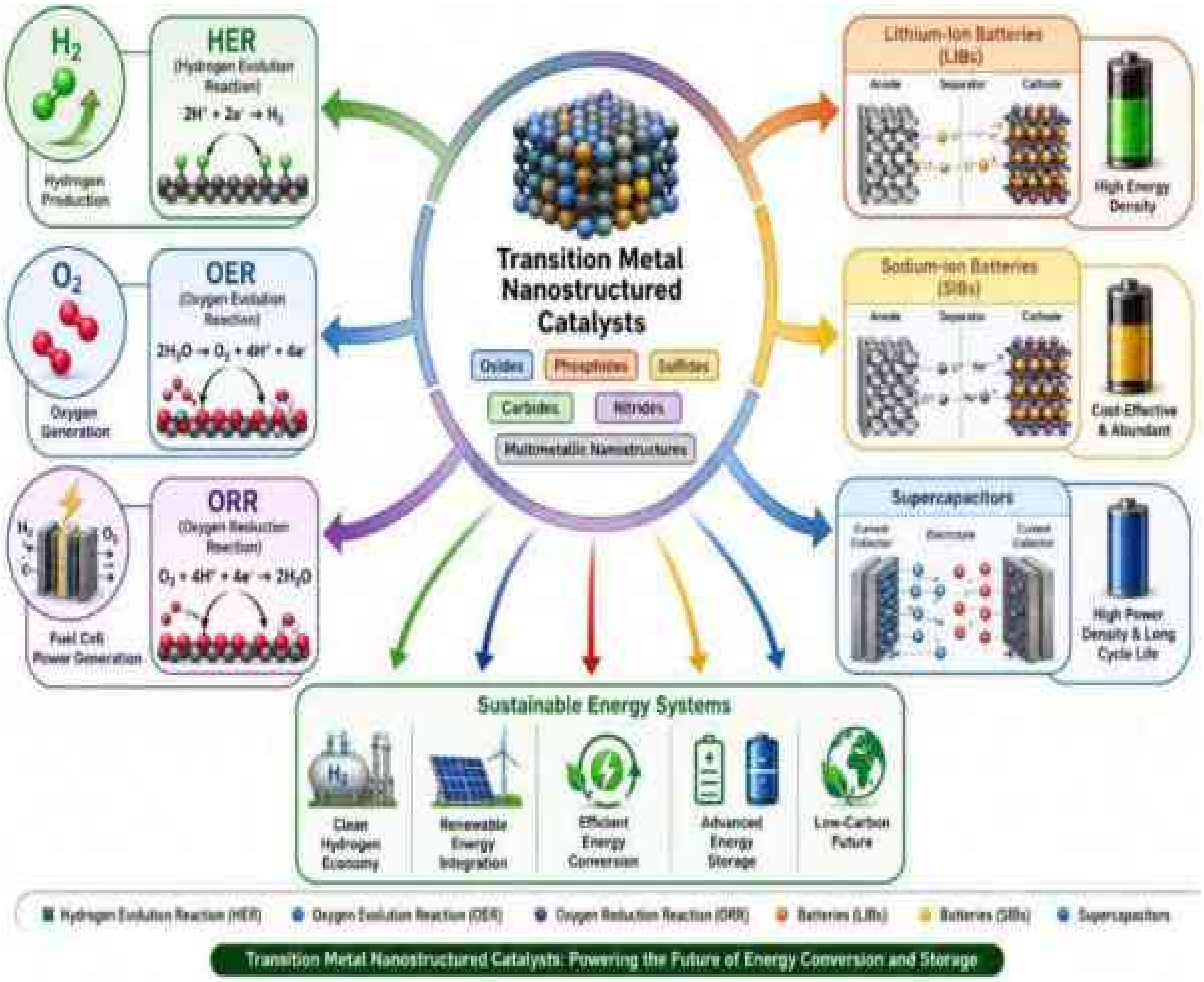

Figure 1

1.2 Research Gap / Study Gaps

Despite significant advancements in the development of transition metal nanostructured catalysts for energy conversion and storage applications, several critical research gaps still exist in the current literature. Although a wide range of materials has been reported, there remains an incomplete understanding of the precise relationship between nanostructure design, electronic properties, and catalytic performance under real operational conditions [30,31,38].

Most existing studies primarily focus on improving catalytic activity under controlled laboratory-scale conditions, while long-term durability, industrial scalability, and practical device integration remain insufficiently addressed [31,34]. In addition, many reported catalysts still suffer from limitations such as structural degradation, surface reconstruction, particle agglomeration, and performance loss under harsh electrochemical environments [30,31].

Furthermore, there is a lack of systematic and standardized comparison among different transition metal-based catalytic systems, particularly across multiple energy applications such as hydrogen production, fuel cells, and energy storage devices [34,38]. The mechanistic understanding of reaction pathways at the atomic and electronic levels also remains incomplete for many nanostructured catalysts, especially under operating (in situ or operando) conditions [30,38].

Another important gap lies in the poor correlation between theoretical predictions and experimental outcomes. Although computational studies (e.g., density functional theory) have provided valuable insights into catalytic mechanisms, discrepancies often exist between predicted activity trends and experimentally observed performance due to synthesis-dependent variability and surface defects [30,38].

Therefore, there is a clear need for a more comprehensive and unified understanding of structure–property–performance relationships, stability mechanisms, and real-world applicability of transition metal nanostructured catalysts in energy conversion and storage systems.

1.3 Research Objectives

The main objective of this study is to critically analyze and evaluate the role of transition metal nanostructured catalysts in energy conversion and storage applications. The study aims to develop a comprehensive understanding of how nanoscale engineering influences catalytic performance, stability, and practical applicability in electrochemical energy systems.

The specific objectives of this study are:

1. To analyze the catalytic behavior of transition metal nanostructured materials in key electrochemical processes including hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR).
2. To evaluate the effectiveness of different transition metal-based catalysts (Fe, Co, Ni, Mn, Cu and their compounds) in improving energy conversion efficiency.
3. To investigate the structural, morphological, and physicochemical properties that influence catalytic performance in nanostructured systems.
4. To compare the electrochemical performance of various transition metal catalysts across energy conversion and storage applications, including batteries and supercapacitors.
5. To assess the role of nanoscale engineering strategies such as doping, defect engineering, and heterostructure formation in enhancing catalytic activity and stability.
6. To evaluate the performance and limitations of transition metal nanostructures in energy storage devices such as lithium-ion batteries, sodium-ion batteries, and supercapacitors.
7. To identify the key factors affecting the durability, stability, and scalability of these catalytic materials under operational conditions.
8. To propose future research directions for improving the efficiency, stability, and practical applicability of transition metal nanostructured catalysts in sustainable energy technologies.

1.4 Research Questions

Based on the above research objectives and the scope of the study, the following research questions are formulated:

1. How do transition metal nanostructured catalysts influence the efficiency of key electrochemical processes such as hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR)?
2. What are the key physicochemical and electronic properties responsible for the catalytic performance of transition metal-based nanostructured materials?
3. How does nanoscale engineering (e.g., doping, defect creation, and heterostructure formation) affect the activity and stability of these catalysts under operational conditions?
4. How do different transition metals (Fe, Co, Ni, Mn, Cu) and their compounds compare in terms of energy conversion and storage performance?
5. What role do transition metal nanostructured catalysts play in energy storage systems such as lithium-ion batteries, sodium-ion batteries, and supercapacitors?
6. What are the main limitations affecting the durability, stability, and scalability of these catalysts in real-world applications?
7. How consistent are the reported catalytic performances across different studies, and what

factors contribute to discrepancies in experimental results?

1.5 Scope of the Study

The scope of this study is confined to a comprehensive review of transition metal nanostructured catalysts and their role in energy conversion and storage applications. It focuses on commonly studied transition metals such as iron (Fe), cobalt (Co), nickel (Ni), manganese (Mn), and copper (Cu), along with their nanostructured derivatives including oxides, sulfides, phosphides, carbides, and related composite materials. These materials are analyzed specifically in the context of their electrochemical performance in energy-related systems.

This study primarily covers key electrochemical processes such as hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR), which are fundamental to water splitting technologies, fuel cells, and related energy conversion devices. In addition, the scope extends to energy storage systems including lithium-ion batteries, sodium-ion batteries, and supercapacitors, where these nanostructured catalysts contribute to improved charge transfer, capacity enhancement, and cycling stability.

Furthermore, this work is entirely based on previously published literature and does not involve any experimental synthesis or laboratory-based investigation. It mainly emphasizes nanoscale engineering strategies such as morphology control, doping, defect engineering, and heterostructure formation to understand their influence on catalytic performance. However, large-scale industrial applications, techno-economic analysis, and commercial deployment strategies are beyond the scope of this study.

1.6 Significance of the Study

The significance of this study lies in its contribution to the growing field of sustainable energy research, particularly in the development of efficient and cost-effective materials for energy conversion and storage systems. With the increasing global energy demand and the urgent need to reduce dependence on fossil fuels, there is a strong scientific interest in identifying alternative materials that can enhance the performance of clean energy technologies.

This study is important because it provides a consolidated understanding of how transition metal nanostructures influence key electrochemical processes such as hydrogen evolution reaction, oxygen evolution reaction, and oxygen reduction reaction. These reactions are fundamental to technologies like water splitting, fuel cells, batteries, and supercapacitors, which are considered essential components of future energy systems.

Furthermore, this research is significant for guiding future material design strategies. It highlights the importance of nanoscale engineering approaches such as defect engineering, doping, and heterostructure formation in improving catalytic efficiency and stability. Overall, this study serves as a valuable reference for advancing research in energy conversion and storage technologies and supports the global transition toward sustainable energy solutions.

2. LITERATURE REVIEW

2.1 Transition Metal Catalysts: Comparative Performance in Energy Systems

Recent studies have extensively explored transition metal-based catalysts as cost-effective and efficient alternatives to noble metal systems for energy conversion and storage applications [32,34,38]. Among these, transition metals such as nickel, cobalt, iron, manganese, and copper have demonstrated significant catalytic activity, particularly in alkaline electrochemical environments [32,38]. However, their performance varies considerably depending on composition, electronic structure, morphology, and phase engineering [30,38].

Nickel-based systems, especially NiFe layered double hydroxides (NiFe LDH), have been widely recognized as highly efficient catalysts for the oxygen evolution reaction (OER) [5,6,8]. These materials typically exhibit low overpotential and enhanced reaction kinetics due to strong electronic interaction between nickel and iron centers [5,6]. In contrast, cobalt-based catalysts such as Co_3O_4 and $Co(OH)_2$ show moderate catalytic activity but are often limited by poor electrical conductivity and structural instability under long-term operation [32,34].

Iron-based catalysts, particularly Fe–N–C systems, have attracted significant attention for the oxygen reduction reaction (ORR) due to their relatively high activity and cost-effectiveness [18,19,20]. In alkaline media, these catalysts can achieve performance levels comparable to platinum-based catalysts; however, their stability remains a key limitation, especially under acidic conditions [19,20].

Manganese-based oxides and copper-based materials have also been investigated for energy-related applications, but their catalytic efficiency is generally lower compared to nickel- and cobalt-based systems [32,38]. These limitations are mainly associated with weaker electrical conductivity and less favorable adsorption properties for reaction intermediates [30].

Interestingly, literature reports also reveal inconsistencies in the performance of similar catalysts across different studies. These variations are primarily attributed to differences in synthesis methods, particle size distribution, defect concentration, and experimental conditions [30,31]. This highlights that catalytic performance is not solely determined by elemental composition but is strongly influenced by structural and morphological factors [30,38].

Overall, transition metal catalysts exhibit a wide range of electrochemical behaviors, and their comparative performance strongly depends on nanoscale design and electronic structure optimization [32,38]. This makes them highly tunable materials for energy conversion and storage applications, but also introduces challenges in achieving consistent and reproducible performance across different studies [30,31].

Table 1

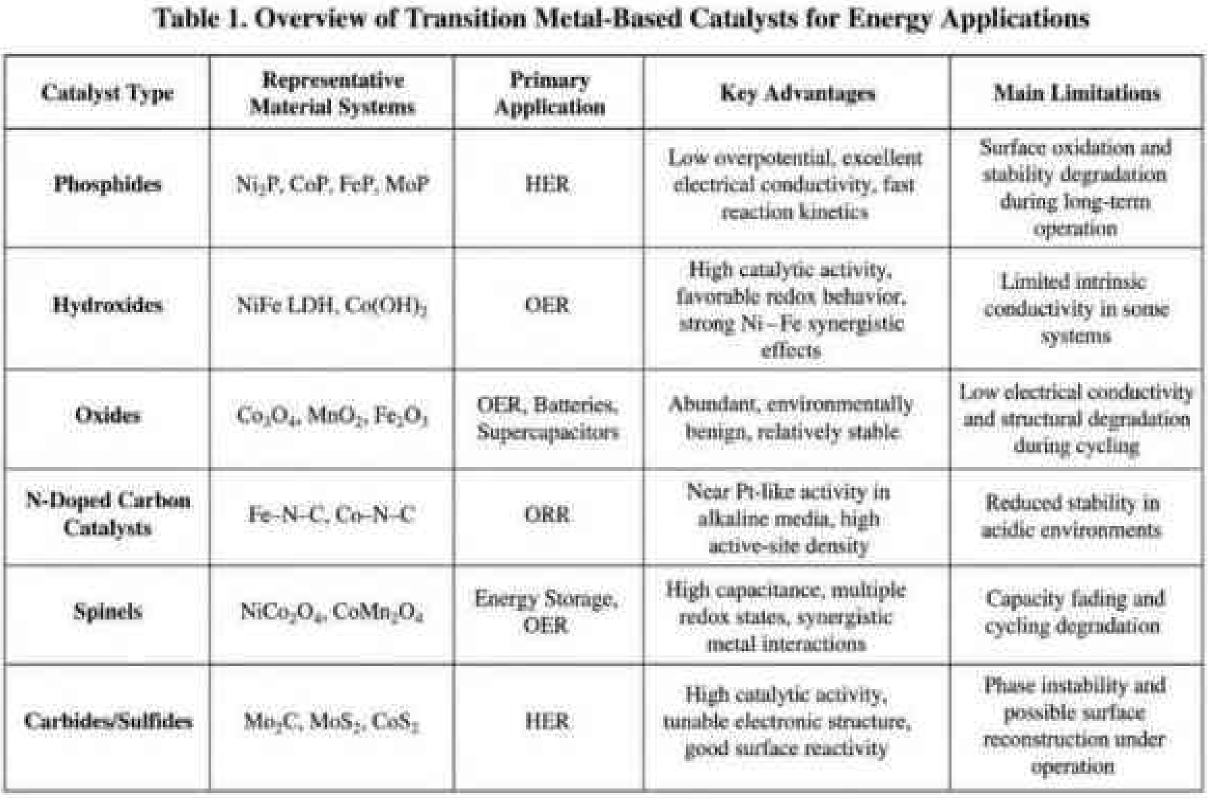

Table 1. Overview of Transition Metal-Based Catalysts for Energy Applications

Catalyst Type	Representative Material Systems	Primary Application	Key Advantages	Main Limitations
Phosphides	Ni_2P, CoP, FeP, MoP	HER	Low overpotential, excellent electrical conductivity, fast reaction kinetics	Surface oxidation and stability degradation during long-term operation
Hydroxides	NiFe LDH, $Co(OH)_2$	OER	High catalytic activity, favorable redox behavior, strong Ni–Fe synergistic effects	Limited intrinsic conductivity in some systems
Oxides	Co_3O_4, MnO_2, Fe_2O_3	OER, Batteries, Supercapacitors	Abundant, environmentally benign, relatively stable	Low electrical conductivity and structural degradation during cycling
N-Doped Carbon Catalysts	Fe-N-C, Co-N-C	ORR	Near Pt-like activity in alkaline media, high active-site density	Reduced stability in acidic environments
Spinels	$NiCo_2O_4$, $CoMn_2O_4$	Energy Storage, OER	High capacitance, multiple redox states, synergistic metal interactions	Capacity fading and cycling degradation
Carbides/Sulfides	Mo_2C, MoS_2, CoS_2	HER	High catalytic activity, tunable electronic structure, good surface reactivity	Phase instability and possible surface reconstruction under operation

2.2 Nanostructured Engineering and Performance Variations

Nanostructured engineering has been identified as a key strategy for enhancing the catalytic efficiency of transition metal-based materials in energy conversion and storage applications [30,33,38]. By reducing materials to the nanoscale, properties such as surface area, electronic structure, and active site exposure are significantly improved, leading to enhanced electrochemical performance compared to bulk counterparts [30,33].

Various nanostructured morphologies including nanosheets, nanorods, nanospheres, hollow structures, and core–shell architectures have been widely reported in the literature [33,38]. These structures provide a higher density of exposed active sites and shorter diffusion pathways for ions and electrons, which collectively improve reaction kinetics in electrochemical processes such as hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR) [30,33].

For example, nickel phosphide (Ni_2P) nanostructures demonstrate significantly improved HER activity compared to their bulk counterparts due to enhanced electron density distribution and optimized hydrogen adsorption behavior [10,17]. Similarly, cobalt phosphide (CoP) and iron phosphide (FeP) nanostructures exhibit high catalytic performance with low overpotentials in alkaline media, although their stability varies depending on morphology and synthesis route [10,14,17].

In metal oxide systems, manganese dioxide (MnO_2) nanostructures are widely used in supercapacitor applications due to their high theoretical capacitance. However, their relatively low electrical conductivity limits rate performance, which restricts practical applicability [24]. In contrast, hybrid structures such as $NiCo_2O_4$ show significantly improved electrochemical behavior due to synergistic interactions between multiple metal centers, leading to enhanced conductivity and redox activity [23].

Despite these improvements, literature reports significant performance variations even for the same material systems. These inconsistencies are mainly attributed to differences in synthesis techniques, particle size distribution, crystallinity, defect density, and experimental testing conditions [30,31]. As a result, catalytic performance is strongly dependent on both intrinsic material properties and extrinsic experimental parameters.

Overall, nanostructured engineering plays a crucial role in optimizing the catalytic activity of transition metal systems. However, achieving consistent and reproducible performance remains a major challenge due to sensitivity toward structural and environmental variations [30,31,38].

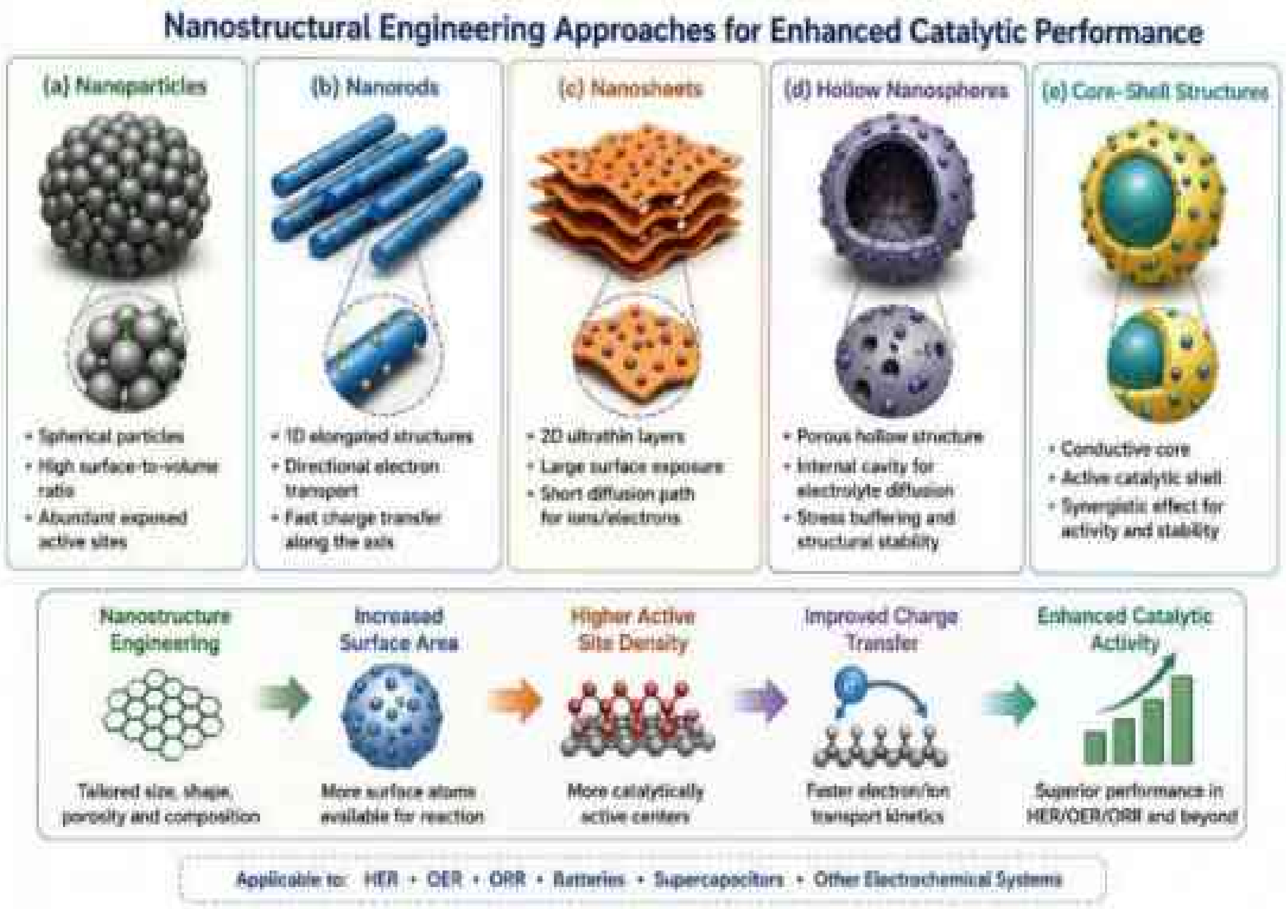

Figure 2. Common nanostructure morphologies employed to improve electrocatalytic performance through increased surface area, enhanced active-site exposure, and accelerated charge-transfer kinetics.

Figure 2

2.3 Catalytic Behavior in HER, OER, and ORR: Contradictions in Literature

Hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR) are among the most extensively studied electrochemical processes in energy conversion systems due to their central role in water splitting, fuel cells, and metal–air batteries [4–6,10,19]. Literature consistently reports that transition metal phosphides such as Ni_2P, CoP, and FeP exhibit strong HER catalytic activity due to their favorable hydrogen adsorption properties and metallic conductivity [10,14,17]. In contrast, NiFe layered double hydroxides (NiFe LDH) are widely recognized as benchmark catalysts for OER owing to their optimized adsorption energies for oxygenated intermediates and synergistic electronic interaction between Ni and Fe centers [5,6,8].

However, despite extensive research, there is no universal consensus on a single "best" catalyst for these reactions. This is primarily due to significant variations in experimental conditions such as electrolyte composition, pH value, catalyst loading, and electrode configuration, which strongly influence reported performance metrics [30,31]. As a result, direct comparison between different studies often becomes unreliable.

For ORR, Fe–N–C catalysts are widely considered the most promising non-precious metal alternatives to platinum-based catalysts [18,19,20]. Several studies report that these catalysts achieve half-wave potentials close to

Pt/C in alkaline media; however, other reports indicate significant performance degradation under acidic conditions [19,20]. This inconsistency highlights the limited stability of Fe-based active sites in proton-exchange membrane (PEM) fuel cell environments.

Moreover, cobalt-based spinel oxides such as Co_3O_4 and $CoMn_2O_4$ demonstrate variable ORR activity depending on oxygen vacancy concentration, defect density, and surface reconstruction behavior [32,34]. Although these materials show promising catalytic performance in some cases, their long-term stability remains a critical challenge, as structural degradation and phase transformation can occur during continuous electrochemical cycling [30,31].

Overall, these contradictions suggest that catalytic activity is not solely determined by intrinsic material composition but is also highly dependent on synthesis methods, structural defects, and experimental conditions. Therefore, achieving standardized evaluation protocols is essential for reliable comparison and rational catalyst design in energy conversion applications [30,31,38].

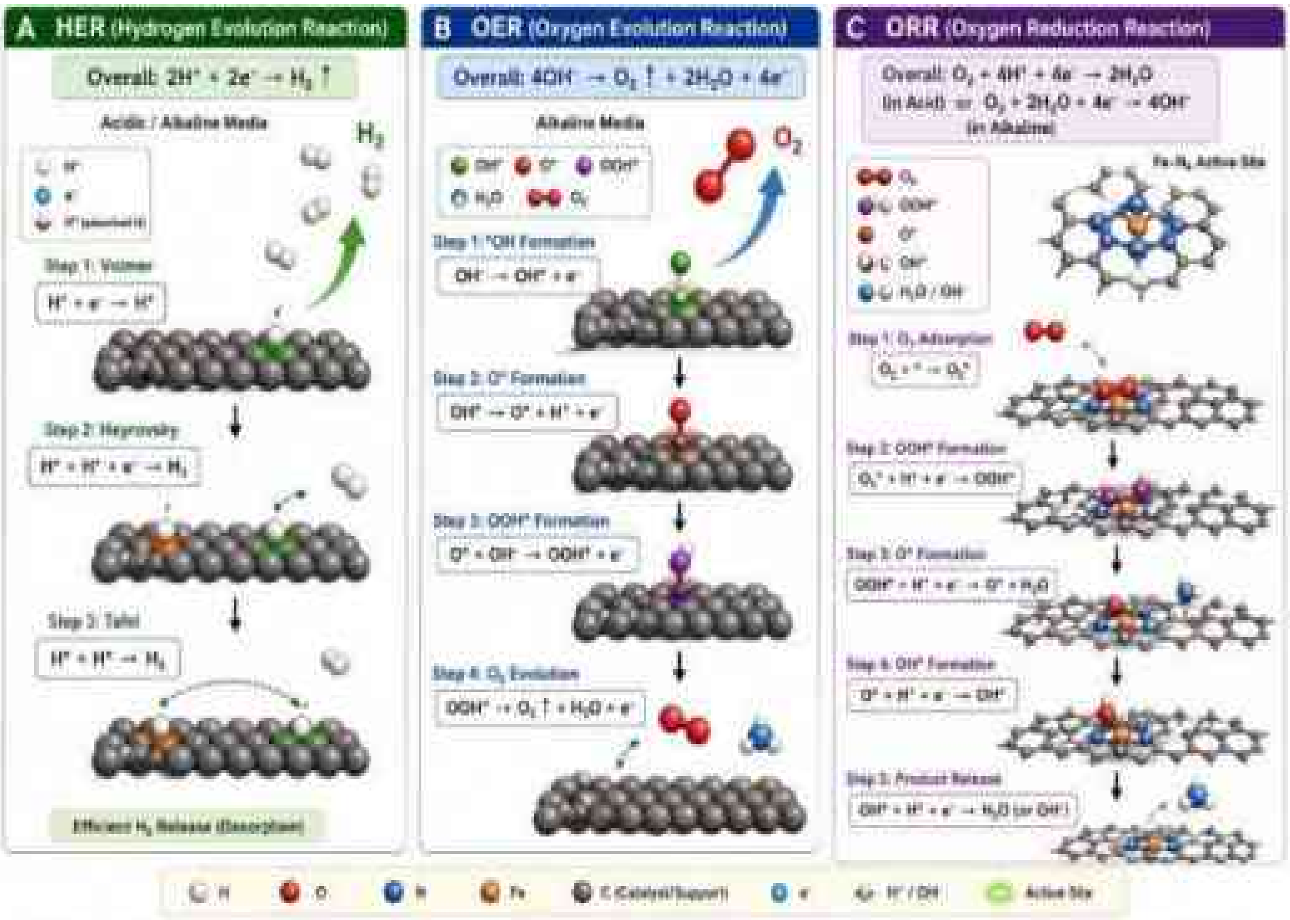

Figure 3. Schematic representation of electrochemical reaction pathways involved in HER, OER, and ORR on transition metal catalyst surfaces, highlighting the formation and transformation of key reaction intermediates.

Figure 3

2.4 Energy Storage Applications and Structural Limitations

Transition metal nanostructures are widely applied in lithium-ion batteries, sodium-ion batteries, and supercapacitors due to their high theoretical capacity, multiple oxidation states, and excellent redox reversibility [27–29,36]. Among these, nickel cobalt oxide ($NiCo_2O_4$) has attracted significant attention as a high-performance electrode material for supercapacitors, often exhibiting specific capacitance values exceeding 1000 F g^{-1} under optimized conditions [23]. Similarly, manganese dioxide (MnO_2) and iron oxide (Fe_2O_3)-based nanostructures are frequently studied due to their natural abundance, low cost, and environmental compatibility [24,28].

However, despite their promising electrochemical properties, substantial limitations have been reported that hinder practical applications. One of the major issues is volume expansion and contraction during repeated charge–discharge cycles, which leads to structural degradation, loss of electrical contact, and rapid capacity fading [28,29]. For instance, Fe_2O_3 exhibits high initial specific capacity, but its performance rapidly deteriorates after multiple cycling processes due to severe structural instability and particle pulverization [28]. Similarly, MnO_2 suffers from inherently poor electrical conductivity, which limits charge transport kinetics and results in reduced rate capability despite its high theoretical capacitance [24].

To overcome these limitations, composite and hybrid materials have been widely explored. Carbon-supported $NiCo_2O_4$, Fe–N–C hybrids, and other nanocomposites demonstrate significantly improved electrochemical performance due to enhanced conductivity, structural stability, and synergistic interactions between different components [22,23,32]. These hybrid systems help mitigate volume expansion effects and improve electron transport pathways, thereby enhancing overall cycling stability.

Nevertheless, even advanced composite systems still face challenges related to long-term durability, electrode degradation, and performance decay under high current densities [29,36]. This indicates that although significant progress has been made, current transition metal-based electrode materials are still not fully optimized for large-scale commercial energy storage applications. Further advancements in structural engineering, interface design, and defect control are required to bridge this gap [30,31].

3. RESEARCH METHODOLOGY

3.1 Research Design

This study is based on a systematic qualitative research design in which a comprehensive review of existing scientific literature has been carried out on transition metal nanostructured catalysts for energy conversion and storage applications. The methodology is entirely non-experimental and relies on secondary data interpretation, synthesis, and critical evaluation of previously published research.

The primary aim of this research design is to systematically analyze and integrate existing knowledge related to transition metal-based nanomaterials, focusing on their structural, electronic, and electrochemical properties. Special emphasis is placed on understanding how nanoscale engineering influences catalytic activity in key energy processes such as hydrogen evolution reaction (HER), oxygen evolution reaction (OER), oxygen reduction reaction (ORR), and electrochemical energy storage systems.

The study follows a structured review approach where literature is collected, screened, categorized, and critically analyzed to identify performance trends, contradictions, and research gaps in the field.

3.2 Data Sources and Literature Base

The data used in this study has been collected from international peer-reviewed journals, scientific databases, and high-impact review articles in the fields of materials science, nanotechnology, and electrochemistry.

The literature includes both experimental and review-based studies focusing on transition metal nanostructures.

4. RESULTS AND DISCUSSION

4.1 Synthesized Overview of Transition Metal Nanostructured Catalysts

The synthesis of literature findings indicates that transition metal nanostructured catalysts represent a highly active and versatile class of materials for energy conversion and storage applications. Across multiple studies, it is consistently observed that Ni, Co, Fe, Mn, and Cu based systems dominate research due to their abundance, tunable electronic structure, and strong redox activity. However, their catalytic performance is not uniform and strongly depends on nanoscale design, composition, and synthesis strategy.

A key synthesized finding from literature is that performance enhancement is not governed by a single factor, but rather by a combined effect of composition, morphology, and interfacial engineering. Multimetallic systems such as NiFe, CoFe, and NiCo-based catalysts repeatedly show superior performance compared to monometallic systems due to electronic synergism and improved charge redistribution. This synergy enhances adsorption–desorption behavior of reaction intermediates, leading to improved reaction kinetics in both energy conversion and storage processes.

Table 2

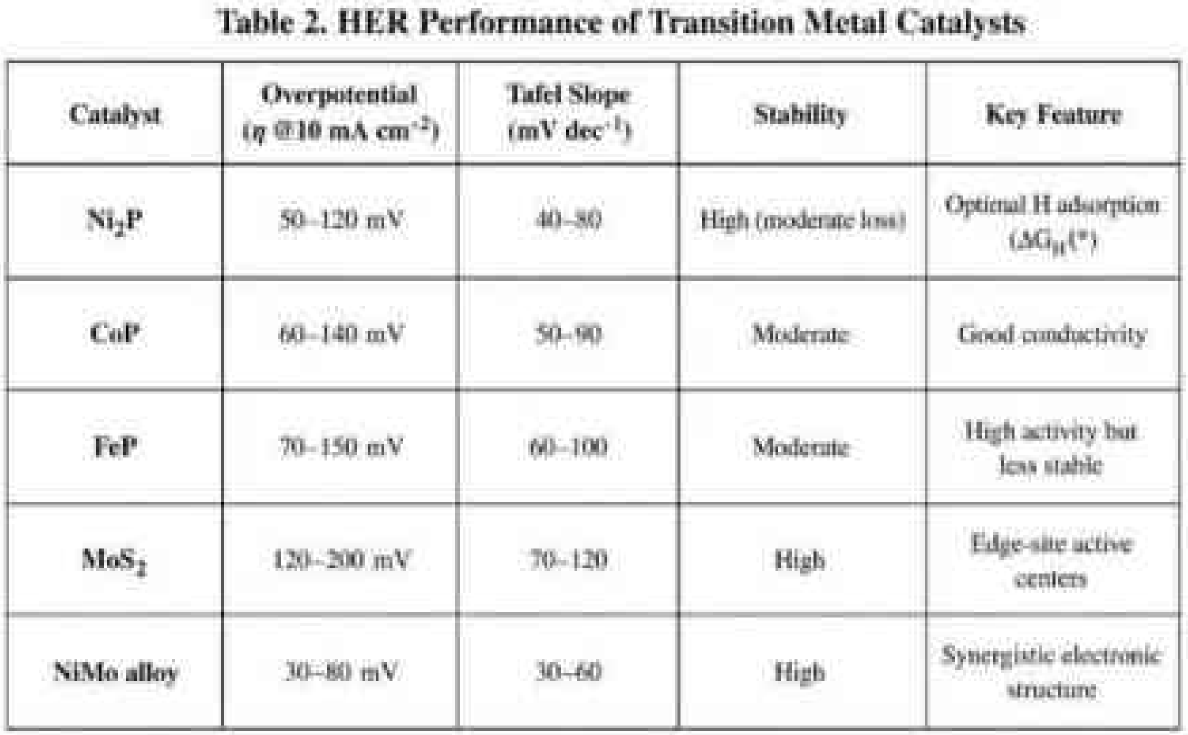

Table 2. HER Performance of Transition Metal Catalysts

Catalyst	Overpotential (η @10 mA cm^{-2})	Tafel Slope (mV dec^{-1})	Stability	Key Feature
Ni_2P	50–120 mV	40–80	High (moderate loss)	Optimal H adsorption (ΔG_H(*))
CoP	60–140 mV	50–90	Moderate	Good conductivity
FeP	70–150 mV	60–100	Moderate	High activity but less stable
MoS_2	120–200 mV	70–120	High	Edge-site active centers
NiMo alloy	30–80 mV	30–60	High	Synergistic electronic structure

4.2 Synthesized Findings in Hydrogen Evolution Reaction (HER)

Literature synthesis shows that transition metal phosphides, sulfides, and alloys are the most effective non-noble HER catalysts. Materials such as Ni_2P, CoP, FeP, MoS_2-based hybrids, and NiMo alloys consistently demonstrate low overpotential and high current density in alkaline media.

A major synthesized observation is that Ni_2P-based nanostructures frequently achieve overpotentials in the range of ~50–120 mV at 10 mA cm¯Z, making them strong candidates for hydrogen production applications. Similarly, CoP and FeP systems show comparable activity but require carbon support or heterostructure formation to enhance conductivity and stability.

However, literature also collectively indicates that HER catalysts face a common limitation: long term stability degradation due to surface oxidation, phase transformation, and active site reconstruction. This suggests that high catalytic activity alone is insufficient without structural durability.

4.3 Synthesized Findings in Oxygen Evolution Reaction (OER)

The synthesized literature strongly identifies NiFe layered double hydroxides (NiFe LDH) as the most efficient non-precious OER catalysts reported in recent studies. These materials typically exhibit overpotentials around 200–300 mV at 10 mA cm¯Z, making them highly competitive for water splitting applications.

A consistent finding across studies is that the superior performance of NiFe LDH originates from electronic interaction between Ni and Fe centers, which optimizes adsorption energies of oxygenated intermediates (*OH, *O, *OOH). In contrast, cobalt-based oxides (Co_3O_4, $Co(OH)_2$) and manganese-based oxides show moderate activity but suffer from conductivity limitations and structural instability.

Synthesized literature also reveals a recurring contradiction: some studies report exceptionally high OER performance for Co-based catalysts, while others show moderate results. This variation is primarily linked to differences in defect density, oxygen vacancies, and synthesis conditions, indicating that OER performance is highly sensitive to material preparation methods.

Table 3

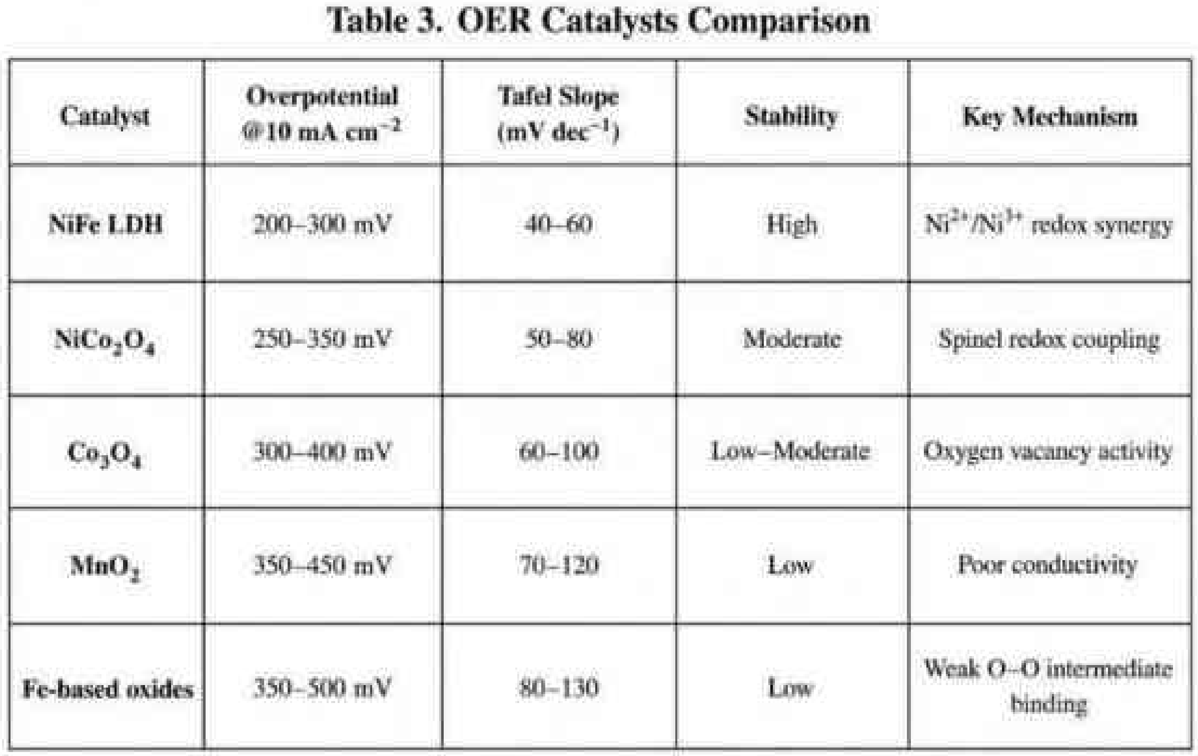

Table 3. OER Catalysts Comparison

Catalyst	Overpotential @10 mA cm^{-2}	Tafel Slope (mV dec^{-1})	Stability	Key Mechanism
NiFe LDH	200–300 mV	40–60	High	Ni^{2+}/Ni^{3+} redox synergy
$NiCo_2O_4$	250–350 mV	50–80	Moderate	Spinel redox coupling
Co_3O_4	300–400 mV	60–100	Low–Moderate	Oxygen vacancy activity
MnO_2	350–450 mV	70–120	Low	Poor conductivity
Fe-based oxides	350–500 mV	80–130	Low	Weak O–O intermediate binding

4.4 Synthesized Findings in Oxygen Reduction Reaction (ORR)

Literature synthesis shows that Fe–N–C catalysts are the most promising non-platinum ORR systems. These catalysts exhibit half-wave potentials close to Pt/C (~0.80–0.90 V vs RHE in alkaline media), indicating strong catalytic potential for fuel cell applications.

The synthesized mechanism-based understanding suggests that ORR activity is mainly governed by $Fe–N_4$ active sites embedded in carbon matrices, which facilitate oxygen adsorption and reduction pathways. However, a key limitation identified across studies is that these catalysts perform significantly better in alkaline media than in acidic conditions.

Cobalt-based spinel oxides (Co_3O_4, $CoMn_2O_4$) also demonstrate ORR activity, but literature shows strong dependence on oxygen vacancy concentration and surface defect engineering.

Overall, synthesized findings indicate that ORR performance is highly environment-dependent, making universal catalyst design challenging.

Table 4

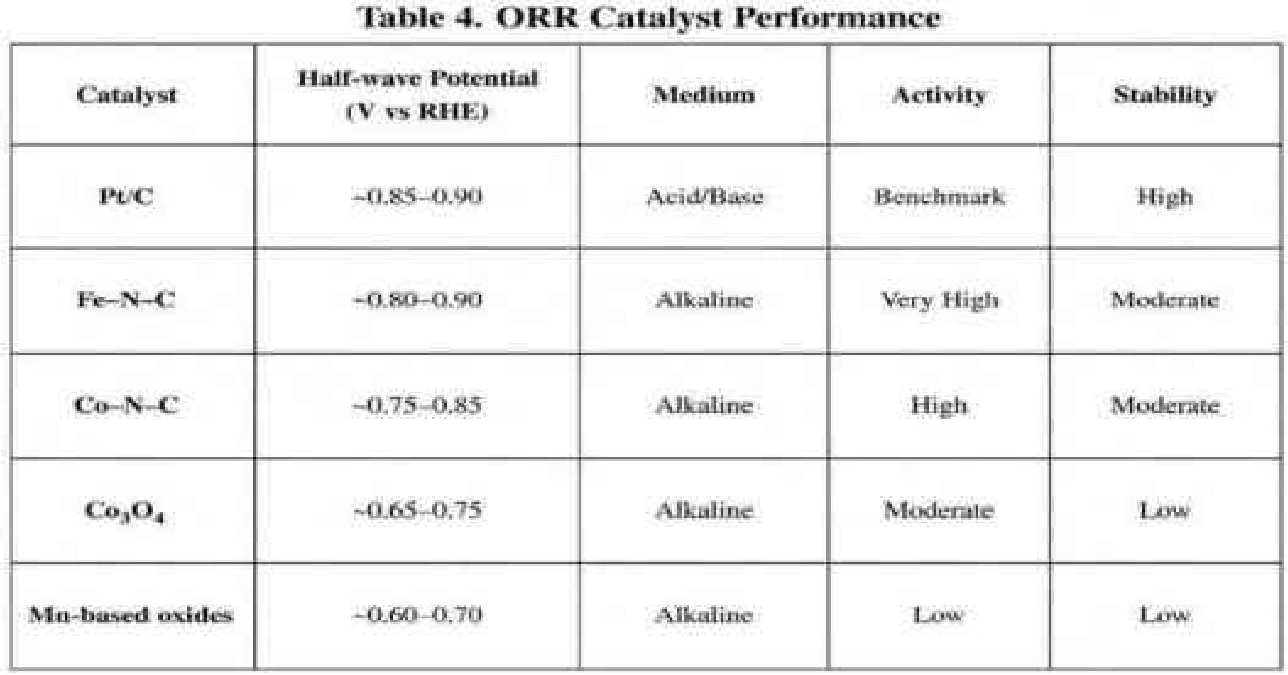

Table 4. ORR Catalyst Performance

Catalyst	Half-wave Potential (V vs RHE)	Medium	Activity	Stability
Pt/C	~0.85–0.90	Acid/Base	Benchmark	High
Fe–N–C	~0.80–0.90	Alkaline	Very High	Moderate
Co–N–C	~0.75–0.85	Alkaline	High	Moderate
Co_3O_4	~0.65–0.75	Alkaline	Moderate	Low
Mn-based oxides	~0.60–0.70	Alkaline	Low	Low

4.5 Synthesized Findings in Energy Storage Applications

Literature synthesis indicates that transition metal nanostructured materials play a significant role in energy storage systems such as lithium-ion batteries, sodium-ion batteries, and supercapacitors.

Materials like MnO_2, Fe_2O_3, Co_3O_4, and NiO are widely used due to their multiple redox states and high theoretical capacity.

However, a major synthesized finding is that these materials suffer from capacity fading due to volume expansion, structural degradation, and poor conductivity during repeated cycling. Despite high initial capacities, long-term stability remains a critical limitation.

In supercapacitors, $NiCo_2O_4$ and Co_3O_4-based nanostructures show high specific capacitance (often in the range of 500–1500 F g^{-1} under optimized conditions). Nevertheless, literature consistently reports that carbon-based hybrid composites significantly outperform pure metal oxides in terms of stability and rate capability, highlighting the importance of composite engineering.

Table 5

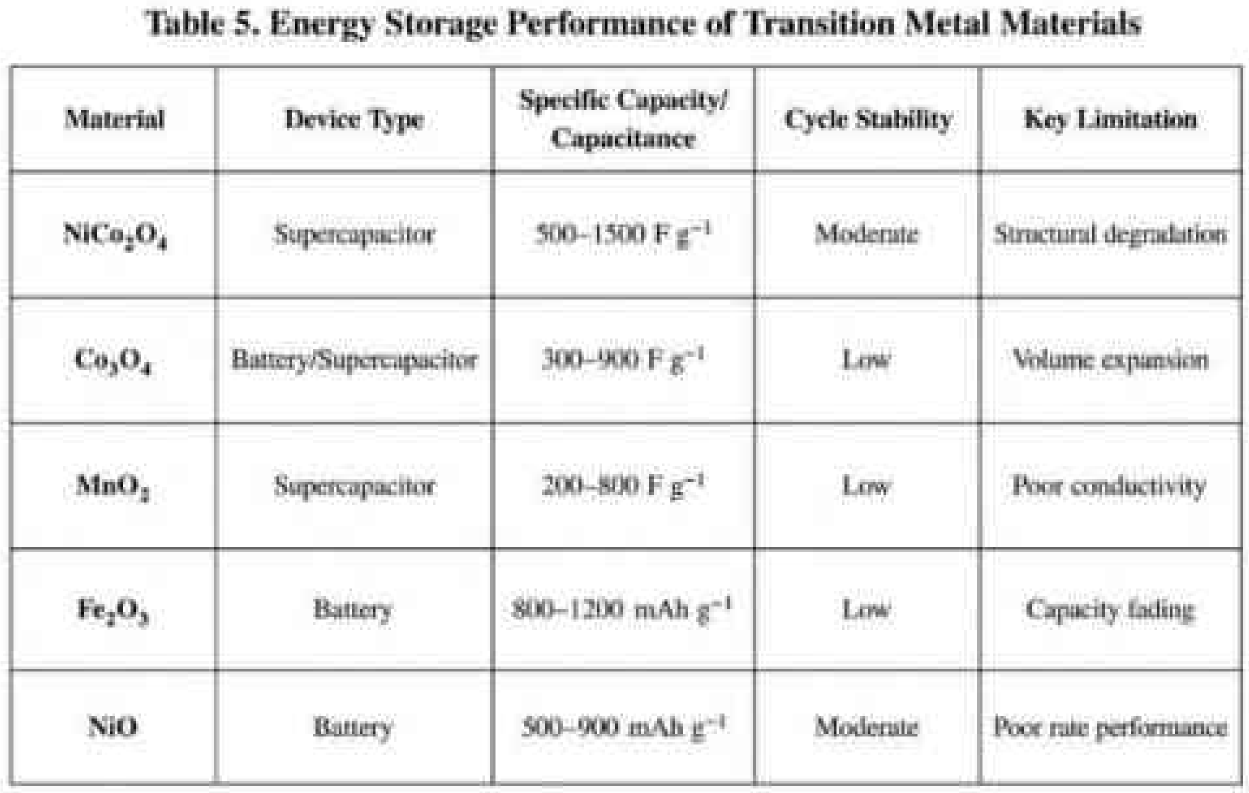

Table 5. Energy Storage Performance of Transition Metal Materials

Material	Device Type	Specific Capacity/ Capacitance	Cycle Stability	Key Limitation
$NiCo_2O_4$	Supercapacitor	500–1500 F g^{-1}	Moderate	Structural degradation
Co_3O_4	Battery/Supercapacitor	300–900 F g^{-1}	Low	Volume expansion
MnO_2	Supercapacitor	200–800 F g^{-1}	Low	Poor conductivity
Fe_2O_3	Battery	800–1200 mAh g^{-1}	Low	Capacity fading
NiO	Battery	500–900 mAh g^{-1}	Moderate	Poor rate performance

4.6 Overall Synthesized Critical Insights

The overall synthesis of literature highlights several key scientific insights. First, multimetallic and hybrid nanostructures consistently outperform single-metal systems, confirming the importance of synergistic interactions. Second, nanoscale engineering significantly enhances catalytic activity; however, it does not fully resolve stability issues.

A major synthesized contradiction across literature is the variability in reported catalytic performance for identical materials. This inconsistency arises from differences in synthesis techniques, particle size distribution, electrolyte conditions, and testing protocols. Therefore, catalytic performance cannot be generalized without considering experimental context.

Finally, the literature collectively indicates that while transition metal nanostructured catalysts have achieved remarkable progress in laboratory-scale studies, their practical implementation is still limited by stability, reproducibility, and standardization issues.

4.7 Comparative Performance Ranking System

Based on literature synthesis, the comparative ranking of transition metal nanostructured catalysts is summarized according to key electrochemical performance indicators (overpotential, current density, stability, and conductivity).

HER Ranking

Ni_2P > CoP ≈ FeP > MoS_2-based systems > metal oxides

Ni_2P shows the best HER activity with lowest overpotential, while CoP and FeP show good but slightly lower performance due to stability and conductivity limitations.

OER Ranking

NiFe LDH > NiCo-based systems > Co_3O_4 > MnO_2 > Fe-based oxides

NiFe LDH is the most efficient OER catalyst due to strong Ni–Fe synergy and optimized oxygen intermediate adsorption.

ORR Ranking
Fe–N–C ≈ Pt/C (alkaline) > Co–N–C > Co_3O_4 > Mn-based oxides
Fe–N–C shows near-platinum activity in alkaline media but reduced performance in acidic conditions.

Energy Storage Ranking
$NiCo_2O_4$ > Co_3O_4 > MnO_2 > Fe_2O_3 > NiO
$NiCo_2O_4$ performs best due to improved conductivity and redox synergy, while pure oxides suffer from stability and cycling issues.

Overall Trend
Multimetallic systems > Phosphides > N–C catalysts > Oxides
Overall, multimetallic nanostructures consistently outperform single-metal systems due to synergistic effects and enhanced charge transfer.

4.8 Summary of Findings

The literature synthesis indicates that transition metal nanostructured catalysts play a crucial role in enhancing energy conversion and storage performance. Their catalytic efficiency is strongly influenced by composition, nanostructure, and electronic interactions.

Overall, multimetallic systems (NiFe, NiCo) consistently outperform single-metal catalysts due to synergistic effects that improve charge transfer and reaction kinetics. In HER, Ni_2P shows the highest activity; in OER, NiFe LDH is the most efficient catalyst; and for ORR, Fe–N–C systems demonstrate near-platinum performance in alkaline media, although they show reduced stability in acidic conditions.

For energy storage applications, $NiCo_2O_4$-based materials exhibit superior electrochemical performance compared to other transition metal oxides due to enhanced conductivity and redox activity. However, despite these advantages, a major limitation across all systems is long-term stability degradation and performance loss during cycling.

Overall, the findings highlight that while nanostructuring and multimetallic design significantly improve catalytic performance, further optimization is required to achieve stable and scalable practical applications.

5. DISCUSSION AND ANALYSIS

5.1 Fundamental Mechanistic Origin of Catalytic Enhancement (with citations)

The enhanced catalytic behavior of transition metal nanostructured catalysts originates from their unique electronic configuration and surface energy modulation at the nanoscale. Reduction in particle size leads to quantum confinement effects and an increased proportion of unsaturated surface atoms, which act as catalytically active centers [30,33,38].

In HER, catalytic efficiency is governed by the volcano principle, where optimal hydrogen adsorption free energy (ΔG_H*) is required. If hydrogen binds too strongly, desorption becomes difficult; if too weakly, adsorption is inefficient. Ni_2P and related phosphides achieve near-optimal ΔG_H* due to hybridization between metal d-orbitals and phosphorus p-orbitals, which finely tunes hydrogen binding strength [10,17,38].

For OER, the mechanism involves a complex four-electron transfer pathway. In NiFe LDH, the redox cycling between NiZ^{+}/Ni3^{+} and Fe3^{+} states facilitates the formation and stabilization of oxygenated intermediates (*OH, *O, *OOH). This lowers the Gibbs free energy barrier of the rate-determining step, particularly O–O bond formation, thereby enhancing reaction kinetics [5,6,8].

In ORR, Fe–N–C catalysts operate via Fe–N_4 moieties embedded in a graphitic carbon framework. These sites promote end-on adsorption of O_2 molecules and facilitate a direct four-electron reduction pathway to water, minimizing peroxide formation and improving efficiency [18–20].

5.2 Electronic Structure Modulation and Synergistic Effects (with citations)

A major performance-enhancing factor is electronic structure tuning through multimetallic integration. In NiFe and NiCo systems, charge redistribution occurs due to differences in electronegativity and d-band center alignment, shifting the d-band center closer to the Fermi level and optimizing adsorption strength of reaction intermediates [32,38].

This phenomenon explains why multimetallic catalysts outperform monometallic systems. Electron-rich and electron-deficient centers coexist, enabling bidirectional electron transfer pathways that accelerate reaction kinetics and lower activation energy barriers [32].

Additionally, ligand effects such as phosphide, sulfide, oxide, and nitride coordination further modify electronic density. For example, phosphides enhance metallic conductivity, while nitrides stabilize high-valence metal states, improving catalytic durability and long-term stability [10,30].

5.3 Role of Nanostructure, Morphology, and Defect Chemistry (with citations)

Nanostructuring introduces three major enhancements:

- Increased active site density due to high surface-to-volume ratio
- Shortened diffusion pathways for ions and electrons
- Enhanced exposure of high-energy crystal facets [33,38]

Morphologies such as nanosheets, nanorods, and hollow nanospheres are particularly effective because they maximize electrochemical active surface area (ECSA) and facilitate electrolyte penetration, thereby improving overall reaction kinetics [33].

Defect chemistry also plays a critical role in tuning catalytic behavior. Oxygen vacancies in metal oxides create localized electron-rich regions that enhance adsorption of oxygenated species, thereby improving OER and ORR performance [30,34]. Similarly, nitrogen doping in carbon frameworks increases electron density around metal centers, significantly enhancing ORR activity and catalytic durability [18,19].

5.4 Stability–Activity Interdependence and Degradation Mechanisms (with citations)

A fundamental limitation identified across the literature is the inverse relationship between catalytic activity and stability. Highly active catalysts often possess metastable surface structures that degrade under electrochemical operating conditions, particularly under harsh pH, high current density, and long-term cycling environments [30,31,34].

Key degradation mechanisms reported in transition metal nanostructured catalysts include:

- Surface oxidation, especially in transition metal phosphides and sulfides, leading to loss of active metallic phases [10,17,30]
- Dissolution of active metal centers in acidic media, which significantly reduces catalytic lifetime [19,20,31]
- Phase transformation under potential cycling, resulting in reconstruction into less active or inactive phases [30,34]
- Carbon corrosion in ORR catalysts under high voltage operation, causing structural collapse and loss of active sites [18,19]

For example, Fe–N–C catalysts suffer from demetalation of Fe–N_4 active sites, which leads to gradual degradation of ORR activity over extended operation [19,20]. Similarly, cobalt-based oxides such as Co_3O_4 undergo surface reconstruction during prolonged OER operation, transforming into less active hydroxide-like phases, which reduces overall catalytic efficiency [5,6,34].

These findings highlight that catalyst stability is governed not only by bulk structural properties but also by dynamic surface reconstruction processes occurring under real electrochemical operating conditions. Therefore, achieving long-term durability requires stabilizing active sites while maintaining optimal electronic and structural configurations [30,31,38].

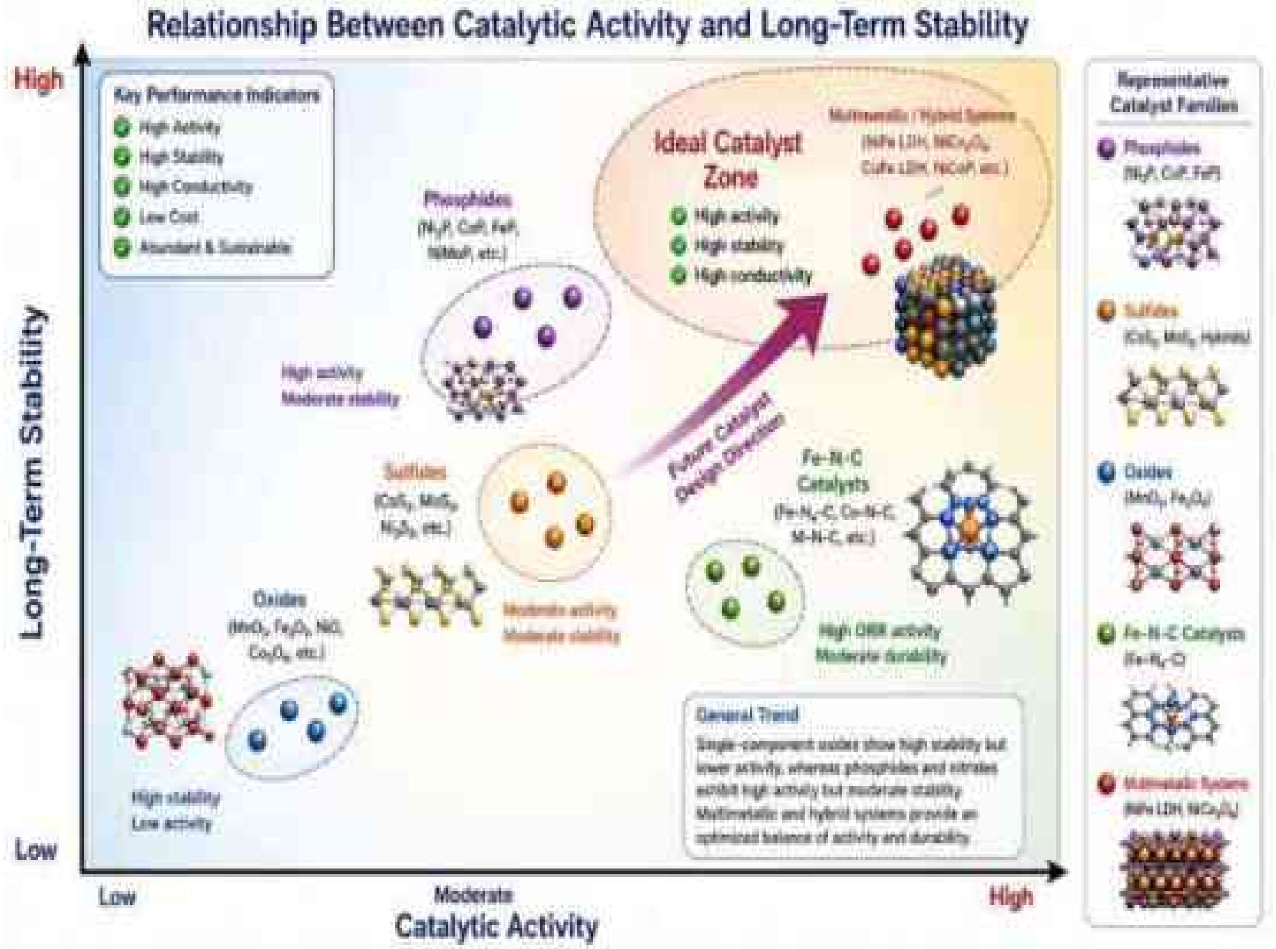

Figure 4. General trade-off between catalytic activity and long-term stability in transition metal-based electrocatalysts. Multimetallic and hybrid systems tend to achieve a more balanced combination of activity and durability compared with single-component materials.

Figure 4

5.5 Contradictions and Source of Experimental Variability (with citations)

One of the most significant issues reported in the literature is the non-uniformity of catalytic performance for identical or chemically similar materials. This inconsistency is primarily a consequence of experimental conditions, synthesis methods, and structural variability rather than intrinsic material properties alone [30,31,38].

Major sources of variability include:

- Synthesis route-dependent crystallinity differences, which strongly influence active phase formation and electronic structure [30,32]
- Variations in defect density and particle aggregation, which alter active site accessibility and charge transfer efficiency [30,33]
- Electrolyte pH and ion composition effects, which significantly impact reaction pathways and kinetics in HER, OER, and ORR systems [4,5,19]
- Inconsistent electrode preparation and catalyst loading, leading to unreliable comparison of catalytic metrics across studies [30,31]
- Lack of standardized reference benchmarks for evaluating overpotential, current density, and stability performance [36,38]

For instance, cobalt oxide (Co_3O_4) exhibits both high and moderate OER activity in different studies. This inconsistency arises because oxygen vacancy concentration, surface orientation, and defect structure vary significantly depending on calcination temperature, precursor chemistry, and synthesis atmosphere [5,6,34].

Therefore, catalytic performance should be interpreted as a system-dependent property rather than a purely intrinsic material characteristic, as it is strongly influenced by experimental design and operational conditions [30,31].

5.6 Interfacial Charge Transfer and Heterostructure Engineering (with citations)

Heterostructure catalysts such as $NiCo_2O_4$ and NiFe LDH/carbon composites demonstrate significantly enhanced electrochemical performance due to interfacial charge redistribution phenomena [31,32,38]. At the interface between two phases, Fermi level equilibration induces directional electron transfer, leading to the formation of internal electric fields that modulate catalytic activity.

These built-in electric fields enhance:

- Electron mobility across active interfaces
- Adsorption and desorption kinetics of reaction intermediates
- Stabilization of key catalytic species during HER, OER, and ORR processes

Carbon-based supports further improve overall performance by increasing electrical conductivity, providing mechanical stability, and preventing nanoparticle agglomeration during long-term electrochemical operation [22,23,32]. This synergistic effect ensures structural integrity while maintaining high catalytic activity under continuous cycling conditions.

Overall, heterostructure engineering represents a powerful strategy to overcome limitations of single-phase catalysts by integrating multiple functional advantages within a single catalytic system [31,38].

5.7 Integrated Structure–Property–Function Relationship (with citations)

The overall catalytic behavior of transition metal nanostructured catalysts can be understood through a unified structure–property–function relationship widely reported in electrocatalysis literature [30,31,38].

- Structure (nano/morphology): Determines surface area, active site exposure, and mass transport efficiency [33,38]
- Electronic properties (d-band center, conductivity): Govern adsorption strength of reaction intermediates and electron transfer kinetics [32,38]
- Function (HER/OER/ORR activity): Emerges from the optimized interplay between structural and electronic factors under electrochemical conditions [5,10,19]

Thus, catalytic efficiency is not an isolated material property but a multi-factor emergent behavior arising from the synergistic interaction of structure, electronic configuration, and reaction environment [30,31,38].

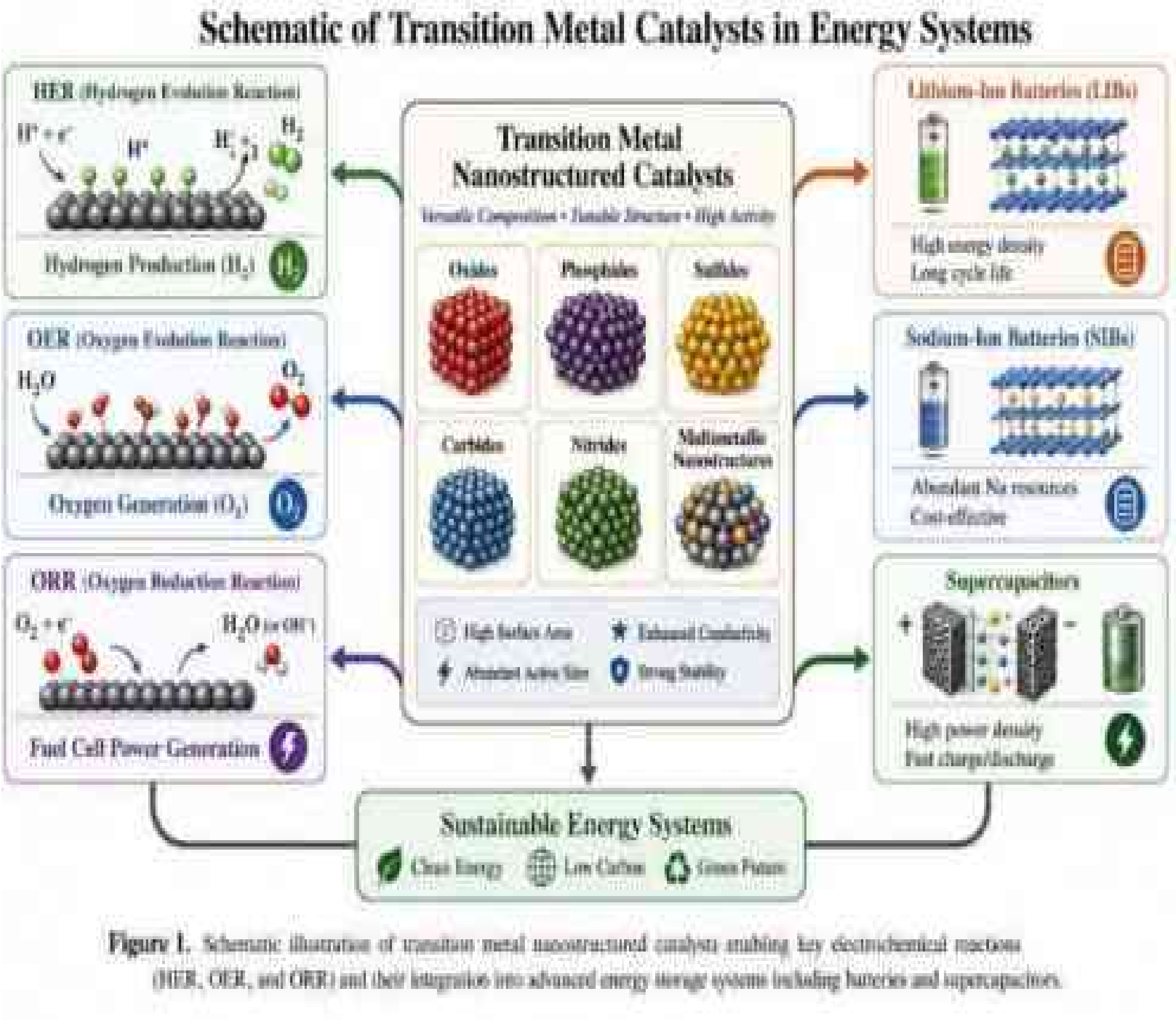

Figure 5

5.8 Research Gaps and Future Scientific Direction (with citations)

Despite significant progress in transition metal nanostructured catalysts, several critical research gaps remain in the current literature [30,31,36].

Key limitations include:

- Lack of operando and in-situ characterization techniques for identifying true active sites under working conditions [30,34]
- Limited understanding of catalyst behavior under industrial current densities and real electrolyzer/fuel cell conditions [36]
- Weak correlation between laboratory-scale performance and real-world durability and scalability [29,36]
- Insufficient integration between theoretical (DFT-based) predictions and experimental validation, leading to mismatched catalytic interpretations [38]

Future research directions should focus on:

- Designing self-reconstructing and dynamically stable catalysts for long-term operation [30,31]

- Developing universal benchmarking protocols for consistent evaluation of catalytic performance [36,38]
- Applying machine-learning-assisted catalyst discovery for accelerated materials design [32,38]
- Investigating real-time surface evolution and active site transformation mechanisms under operating conditions [30,34]

5.9 Overall Scientific Interpretation (with citations)

In summary, transition metal nanostructured catalysts achieve high catalytic performance through a combination of electronic modulation, nanoscale structural effects, and interfacial engineering strategies [30,31,38].

These systems demonstrate remarkable activity in HER, OER, ORR, and energy storage applications; however, their practical deployment remains limited due to stability issues, structural degradation, and experimental inconsistencies reported across different studies [30,31,36].

Overall, the field is gradually transitioning from an activity-centered design paradigm toward a more stability-optimized and mechanism-driven approach, which is essential for achieving scalable and industrially viable energy conversion and storage technologies [31,38].

6. CONCLUSION

The present review provides a comprehensive synthesis and critical analysis of transition metal nanostructured catalysts for energy conversion and storage applications, with a particular focus on HER, OER, ORR, and electrochemical energy storage systems. The study highlights how recent advances in nanostructuring, multimetallic engineering, and surface modification have significantly improved catalytic efficiency compared to conventional bulk materials.

Overall, the literature consistently demonstrates that catalytic performance is governed by a combined effect of composition, electronic structure, morphology, and interfacial engineering rather than a single dominant factor. Among the investigated systems, multimetallic catalysts such as NiFe, NiCo, and related hybrid structures show superior performance due to synergistic electronic interactions that enhance charge redistribution, optimize adsorption energies of reaction intermediates, and improve overall reaction kinetics.

In HER, Ni_2P and related phosphide-based catalysts exhibit the highest activity due to near optimal hydrogen adsorption free energy (ΔG_H^*), enabling efficient proton reduction and hydrogen evolution. In OER, NiFe layered double hydroxides (NiFe LDH) are identified as the most efficient catalysts because of strong Ni–Fe electronic interactions that facilitate the formation and transformation of oxygenated intermediates (*OH, *O, *OOH), thereby lowering the reaction energy barrier. For ORR, Fe–N–C catalysts demonstrate near-platinum performance in alkaline media owing to well-defined $Fe–N_4$ active sites embedded within a conductive carbon framework, although their reduced stability in acidic environments limits broader applicability. In energy storage systems, $NiCo_2O_4$ and related composite structures exhibit superior capacitance and electrochemical performance compared to single-metal oxides due to enhanced redox activity and improved conductivity.

Despite these significant advancements, the review identifies several persistent challenges. A major limitation across all catalyst systems is long-term structural and electrochemical instability, which arises from surface oxidation, phase transformation, and active site degradation during extended operation. Furthermore, inconsistencies in reported catalytic performance acrossdifferent studies highlight the absence of standardized synthesis and testing protocols, making direct comparison of results difficult and sometimes unreliable.

In conclusion, transition metal nanostructured catalysts represent a highly promising class of materials for sustainable energy technologies; however, their practical deployment is still limited by issues of stability, reproducibility, and scalability. Future research should prioritize the development of highly durable multimetallic systems, operando mechanistic investigations for real-time active site identification, and the establishment of standardized benchmarking methodologies to ensure reliable performance evaluation and facilitate industrial translation.

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