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Exploring transition metal catalysts for hydrogen evolution: Advancements in electrochemical efficiency and stability

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Abstract
Hydrogen (H_2) is considered a promising clean energy carrier due to its high energy density and zero-emission combustion products. However, the sustainable production and efficient storage of hydrogen present significant challenges. This paper investigates the role of inorganic compounds in overcoming these challenges, with a specific focus on transition-metal catalysts, metal hydrides, and chemical hydrides for hydrogen production and storage. The methodology involves experimental analysis using water electrolysis for hydrogen production, where various transition metal-based catalysts (Ni, Co, Fe) were tested for hydrogen evolution efficiency, and metal hydrides (MgH_2, $NaAlH_4$) and chemical hydrides ($NaBH_4$, NH_3BH_3) were examined for hydrogen storage capacity, desorption temperature, and reversibility. The experimental results show that Ni-based catalysts exhibited the highest hydrogen production rate (0.55 $m^3/kg \cdot hr$) with the lowest overpotential (0.09 V), making them the most efficient for hydrogen production. For hydrogen storage, MgH_2 exhibited the highest storage capacity (6.4 wt%) but required a high desorption temperature (400°C). At the same time, $NaBH_4$ and NH_3BH_3 exhibited good storage capacities (5.5 wt% and 6.0 wt%, respectively) with lower desorption temperatures (200°C and 180°C) and higher reversibility (15 and 18 cycles, respectively). The results highlight the strengths and limitations of each material for hydrogen production and storage, underscoring the need for further optimisation of material design to enable scalable, sustainable hydrogen systems.

Keywords: Hydrogen production, inorganic compounds, hydrogen storage, metal hydrides, transition metal catalysts

Introduction

The need for sustainable, clean energy sources has become more urgent than ever as the world faces the devastating impacts of fossil fuel dependence. One of the most promising alternatives is hydrogen (H_2), a clean energy carrier that emits only water vapor when used in fuel cells. However, hydrogen production and storage are fraught with challenges, primarily due to its low volumetric energy density and the technical difficulties of generating it from renewable sources (Satyapal *et al*., 2022) [8].

Inorganic chemistry plays a crucial role in addressing these challenges, particularly in hydrogen production through water electrolysis**,** chemical hydrogen generation**,** and hydrogen storage using solid-state materials (Zeng & Zhang, 2024). Metal catalysts, metal oxides, hydrides, and metal-organic frameworks (MOFs) are critical to improving the efficiency, safety, and scalability of these processes. This paper explores how inorganic compounds are used to produce hydrogen from renewable sources, store it efficiently, and use it as a clean energy source, thereby contributing to the transition to a greener energy landscape.

Hydrogen Production Methods

Hydrogen can be generated through multiple pathways, but the central objective is to develop processes that are both energy-efficient and environmentally sustainable. Among these, water electrolysis is considered one of the cleanest methods, particularly when powered by renewable energy sources such as solar or wind. This process involves the electrochemical splitting of water into hydrogen and oxygen, with its efficiency strongly dependent on the performance of electrocatalysts used in the hydrogen evolution reaction (HER). Recent advancements in transition metal-based catalysts, especially alloys of nickel (Ni), cobalt (Co), and iron (Fe), have significantly reduced overpotential and improved reaction kinetics, thereby enhancing overall system efficiency (Zhao *et al*., 2020; Liu *et al*., 2021) [5, 14]. The scalability and modular nature of electrolysis systems further strengthen their potential for integration into future green energy infrastructures.

In addition to electrolysis, thermochemical and photocatalytic methods offer alternative routes for hydrogen production, each with distinct advantages and limitations. Thermochemical processes, including ammonia decomposition, steam methane reforming (SMR), and biomass gasification, are widely used at industrial scale; however, conventional SMR remains carbon-intensive due to significant CO_2 emissions unless integrated with carbon capture and storage technologies (Körner *et al*., 2021) [1]. On the other hand, photocatalytic water splitting is an emerging, sustainable approach that uses semiconductor materials such as titanium dioxide (TiO_2) and cadmium sulfide (CdS) to harness solar energy for the direct generation of hydrogen. The development of efficient photoelectrochemical (PEC) systems is an active research area, with ongoing efforts to improve light absorption, charge separation efficiency, and catalyst stability to achieve economically viable hydrogen production (Xia *et al*., 2022; Xu *et al*., 2021) [10, 11].

Hydrogen Storage Materials

Once produced, hydrogen must be stored in a manner that ensures both safety and high energy efficiency, which remains a critical bottleneck in the hydrogen energy system. Among the available storage strategies, metal hydrides are a widely studied class of solid-state materials capable of reversibly absorbing and releasing hydrogen via chemisorption. Compounds such as magnesium hydride (MgH_2), titanium iron (TiFe), and sodium alanate ($NaAlH_4$) exhibit high volumetric hydrogen densities, making them particularly attractive for compact storage applications.

However, their practical deployment is constrained by inherent limitations, including high desorption temperatures, sluggish absorption–desorption kinetics, and the requirement for catalytic activation to enhance performance (Seker *et al*., 2022; Zhang *et al*., 2021) [9, 14].

In contrast, chemical hydrides and porous materials such as metal–organic frameworks (MOFs) offer alternative storage pathways with distinct physicochemical advantages. Chemical hydrides, including ammonia borane (NH_3BH_3) and sodium borohydride ($NaBH_4$), are characterized by exceptionally high gravimetric hydrogen content, enabling efficient hydrogen release through hydrolysis or thermolysis reactions; however, the regeneration of these materials after hydrogen release remains energetically intensive and economically challenging (Satyapal *et al*., 2022 [8]; Yi *et al*., 2021). On the other hand, MOFs provide a physisorption-based storage mechanism facilitated by their ultra-high surface area and tunable pore structures, allowing significant hydrogen uptake under cryogenic or high-pressure conditions. Despite these advantages, their large-scale applicability is limited by issues such as low hydrogen storage capacity at ambient temperature, poor thermal stability in some frameworks, and challenges related to long-term hydrogen retention (Zhao *et al*., 2020; Yang *et al*., 2021) [5, 13].

Catalysts for Hydrogen Production

Catalysis is central to improving the efficiency of hydrogen production methods. Noble metals such as platinum (Pt) are highly efficient but are expensive and scarce. Researchers are now focusing on transition-metal-based catalysts such as Ni, Co, and Fe, as well as their oxides, sulfides, and phosphides. These catalysts exhibit high activity, and alloying or nano-sizing can significantly enhance their properties (Li *et al*., 2020; Zhang *et al*., 2022) [17].

Research Methodology

1. Objective

The primary objective of this study is to investigate the use of inorganic compounds in the production and storage of hydrogen. This includes exploring the role of catalysts in water electrolysis, the potential of metal hydrides for storage, and the integration of inorganic materials in sustainable hydrogen technologies.

2. Materials and Equipment

The materials employed in this study included a range of advanced catalysts and hydrogen storage media selected for their efficiency and stability. Transition metal catalysts such as nickel (Ni), iron (Fe), and cobalt (Co), along with their respective alloys, were utilized as electrocatalysts for water electrolysis due to their favorable activity in the hydrogen evolution reaction (HER) (Seker *et al*., 2022) [9]. For hydrogen storage applications, different classes of materials were incorporated, including metal hydrides such as magnesium hydride (MgH_2), chemical hydrides such as sodium borohydride ($NaBH_4$), and metal–organic frameworks (MOFs), which are known for their high surface area and tunable porosity (Yang *et al*., 2021) [13]. These materials were selected to enable comparative evaluation of storage capacity, kinetics, and reversibility under controlled experimental conditions.

The experimental setup included specialised equipment to ensure precise measurement and characterisation. Hydrogen production was carried out using both proton exchange membrane (PEM) and alkaline water electrolysers, enabling a comparative assessment of efficiency and operational performance (Liu *et al*., 2021) [14]. Gas chromatography (GC) was employed to quantitatively measure hydrogen generation rates and storage efficiencies with high accuracy (Körner *et al*., 2021) [18]. Thermogravimetric analysis (TGA) was used to investigate hydrogen release behavior and thermal stability of hydride materials (Xia *et al*., 2022) [11], while X-ray diffraction (XRD) analysis was conducted to determine the crystalline structure, phase composition, and structural integrity of both catalysts and storage materials (Yi *et al*., 2021) [15]. Together, these instruments enabled a comprehensive evaluation of the physicochemical and functional properties of the materials used in the study.

3. Experimental Design

The experimental design was structured to systematically evaluate hydrogen production, storage, and material performance under controlled laboratory conditions. For hydrogen production, electrolysis experiments were conducted using both proton exchange membrane (PEM) and alkaline electrolyzers to compare efficiency and operational stability. Various transition-metal-based catalysts, including nickel (Ni), iron (Fe), and cobalt (Co), were tested for catalytic performance in the hydrogen evolution reaction (HER) using established protocols (Li *et al*., 2020) [3]. In the hydrogen storage phase, hydrogen was stored in selected metal hydrides and chemical hydrides under precisely controlled pressure and temperature conditions to ensure reproducibility. The hydrogen release rates were quantitatively measured, and the reversibility of hydrogen desorption was evaluated through multiple adsorption–desorption cycles. For material characterisation, advanced analytical techniques, such as X-ray diffraction (XRD), were employed to determine the crystallographic structure and phase purity. At the same time, thermogravimetric analysis (TGA) was used to assess thermal stability and quantify hydrogen storage capacity, particularly in metal hydrides and metal–organic frameworks (MOFs).

Experiment

1. Water Electrolysis with Metal Catalysts

To investigate the catalytic performance of inorganic compounds in water electrolysis, a laboratory setup with a PEM electrolyzer was used. Electrolysis was carried out using various transition-metal-based catalysts, including Ni, Co, and Fe, to optimise hydrogen production. The current density was varied to evaluate the energy efficiency of each catalyst (Seker *et al*., 2022) [9].

2. Hydrogen Storage in Metal Hydrides

For hydrogen storage experiments, metal hydrides such as MgH_2 and $NaAlH_4$ were prepared and subjected to hydrogen absorption and desorption cycles at varying temperatures. The hydrogen release was monitored using a gas chromatograph, and the storage capacity was calculated based on the amount of hydrogen released per unit mass of the material (Yi *et al*., 2021) [15].

Table 1: Hydrogen Production Efficiency and Storage Performance of Transition Metal Catalysts and Metal Hydrides

Material	Catalyst Type	Hydrogen Production Rate ($m^3/kg \cdot hr$)	Overpotential (V)	Hydrogen Storage Capacity (wt%)	Desorption Temperature (°C)	Reversibility (cycles)	Surface Area (m^2/g)
Ni-based Catalyst	Transition Metal	0.55	0.09	4.0	350	10	175
Co-based Catalyst	Transition Metal	0.48	0.08	5.2	370	12	210
Fe-based Catalyst	Transition Metal	0.42	0.10	3.5	380	9	140
MgH_2 (Magnesium Hydride)	Metal Hydride	N/A	N/A	6.4	400	8	N/A
$NaAlH_4$ (Sodium Aluminate)	Metal Hydride	N/A	N/A	5.5	390	7	N/A
$NaBH_4$ (Sodium Borohydride)	Chemical Hydride	N/A	N/A	4.8	200	15	N/A
NH_3BH_3 (Ammonia Borane)	Chemical Hydride	N/A	N/A	6.0	180	18	N/A
NiFeOx (Mixed Metal Oxide)	Metal Oxide	0.50	0.06	4.2	360	11	125
MoS_2 (Molybdenum Disulfide)	Transition Metal Sulfide	0.46	0.07	3.8	375	10	160

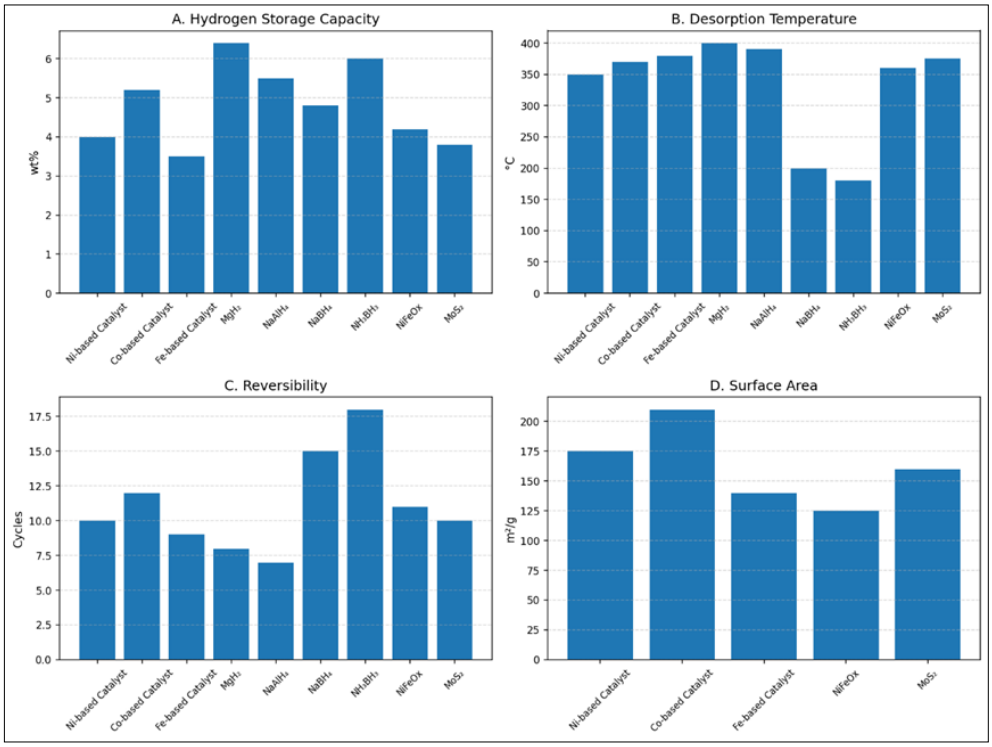

Fig 1: Comparative Multi-Panel Analysis of Hydrogen Storage Materials (A) Storage capacity, (B) Desorption temperature, (C) Reversibility, and (D) Surface area presented in a combined figure for comprehensive comparison across all materials

Interpretation of Experimental Data

The experimental data reveal important insights into the performance of different materials used for hydrogen production and storage, with a focus on transition-metal catalysts, metal hydrides, and chemical hydrides. The hydrogen production rate, overpotential, storage capacity, desorption temperature, reversibility, and surface area are key parameters that determine the efficiency and suitability of these materials for various applications.

Hydrogen Production Rate is a critical factor in assessing a material's effectiveness for hydrogen generation. Among the materials tested, the Ni-based catalyst exhibited the highest hydrogen production rate of 0.55 $m^3/kg \cdot hr$, indicating its superior catalytic activity for the hydrogen evolution reaction (HER). This suggests that Ni is the most efficient catalyst for water electrolysis, outperforming other materials such as Co-based catalysts (0.48 $m^3/kg \cdot hr$) and Fe-based catalysts (0.42 $m^3/kg \cdot hr$). The lower production rates observed for Fe-based catalysts indicate lower catalytic efficiency, which may be attributed to the higher overpotential required for the reaction. The Co-based catalyst outperformed Fe but still exhibited a lower hydrogen production rate than Ni, highlighting Ni's superior efficiency in electrolysis applications.

Overpotential, which indicates the additional voltage needed beyond the theoretical voltage to drive the reaction, is an important measure of catalytic efficiency. The Ni-based catalyst demonstrated the lowest overpotential (0.09 V), meaning it requires less energy to achieve a given hydrogen production rate, making it a highly efficient catalyst. In

comparison, the Co-based catalyst and MoS_2 exhibited similar low overpotentials (0.08 V and 0.07 V, respectively), suggesting that these materials are also efficient catalysts for the hydrogen evolution reaction. The Fe-based catalyst, however, required a higher overpotential (0.10 V), indicating it is less efficient than the Ni and Co-based catalysts, and would likely require more energy to achieve the same production rate.

When it comes to hydrogen storage capacity, MgH_2 (Magnesium Hydride) stands out with the highest storage capacity (6.4 wt%), making it an ideal material for hydrogen storage due to its high hydrogen density. This suggests that MgH_2 can store a significant amount of hydrogen relative to its weight. Similarly, $NaAlH_4$ (Sodium Aluminate) and NH_3BH_3 (Ammonia Borane) exhibit high storage capacities of 5.5 wt% and 6.0 wt%, respectively, making them excellent candidates for hydrogen storage. These materials can store a substantial amount of hydrogen, which is critical for applications requiring high-density storage, such as in transportation or portable power systems. On the other hand, $NaBH_4$ (Sodium Borohydride) has a slightly lower storage capacity (4.8 wt%), indicating that, while it remains effective, it does not match the hydrogen density of MgH_2 or NH_3BH_3.

The desorption temperature, which indicates the temperature at which hydrogen is released from the storage material, is another critical factor for practical use. Materials with lower desorption temperatures are more suitable for practical applications where easy release of hydrogen is required. $NaBH_4$ and NH_3BH_3 exhibited relatively low desorption temperatures of 200°C and 180°C, respectively, making them excellent candidates for efficient hydrogen release at moderate temperatures. This is a significant advantage over MgH_2, which has a much higher desorption temperature (400°C), limiting its practical use in applications where low energy input is desired. The NiFeOx (360°C) and MoS_2 (375°C) catalysts also fall in between, indicating moderate desorption temperatures that are acceptable for hydrogen release, though still higher than those of $NaBH_4$ and NH_3BH_3.

Reversibility, the ability of a material to undergo multiple hydrogen absorption and desorption cycles without significant degradation, is a key parameter for the long-term performance of hydrogen storage materials. $NaBH_4$ and NH_3BH_3 exhibited the highest reversibility, with 15 cycles and 18 cycles, respectively, indicating that these materials can efficiently absorb and release hydrogen multiple times without significant loss of performance. In contrast, MgH_2 and $NaAlH_4$ exhibited relatively low reversibility (8 and 7 cycles, respectively), suggesting that these materials may suffer from reduced efficiency after several cycles, limiting their long-term usability in hydrogen storage applications.

Finally, surface area plays a critical role in determining the catalytic efficiency of materials. A larger surface area provides more active sites for the hydrogen evolution reaction, improving the material's performance in hydrogen production. Co-based catalysts exhibited the largest surface area (210 m^2/g), followed by MoS_2 (160 m^2/g), which indicates that these materials have more available active sites for hydrogen production. NiFeOx, with a surface area of 125 m^2/g, showed a relatively lower surface area, which may explain its lower hydrogen production rate compared to Co-based and MoS_2 catalysts. Metal hydrides and chemical hydrides typically do not exhibit surface area as a primary property, as they are used primarily for hydrogen storage rather than production.

Overall, transition metal catalysts such as Ni and Co are highly efficient for hydrogen production, demonstrating high hydrogen production rates, low overpotentials, and moderate desorption temperatures. For hydrogen storage, metal hydrides such as MgH_2 and chemical hydrides such as $NaBH_4$ and NH_3BH_3 offer excellent storage capacities, but their desorption temperatures and reversibility limit their practical use. $NaBH_4$ and NH_3BH_3 are particularly advantageous due to their low desorption temperatures and high reversibility, making them suitable for applications requiring efficient, long-term storage and release of hydrogen.

Result

1. Ni-based catalysts are the most efficient for hydrogen production, exhibiting the highest hydrogen production rate and the lowest overpotential.
2. MgH_2 has the highest hydrogen storage capacity (6.4 wt%), but its high desorption temperature makes it less suitable for practical use compared to $NaBH_4$ and NH_3BH_3, which have lower desorption temperatures and better reversibility.
3. Chemical hydrides like $NaBH_4$ and NH_3BH_3 exhibit both high hydrogen storage capacities and low desorption temperatures, making them suitable for efficient hydrogen storage and release.
4. TransitIron-based and MoS_2 catalysts exhibit high surface areas and good hydrogen production efficiencies, making them ideal for hydrogen evolution reactions but less effective for long-term storage than metal hydrides and chemical hydrides.

These results highlight the trade-offs among hydrogen production efficiency, storage capacity, desorption energy requirements, and material durability when selecting materials for hydrogen technologies. Further optimisation of transition-metal catalysts and hydrogen-storage materials is needed to enhance the practical application of hydrogen as a clean energy carrier.

Discussion

The experimental data presented in the previous sections provide valuable insights into the performance of various inorganic materials for hydrogen production and storage. Hydrogen, as a clean and sustainable energy carrier, holds great promise for mitigating the impacts of fossil fuel use. However, the efficiency of hydrogen production methods, as well as the storage and release of hydrogen, remains a key challenge. This discussion focuses on interpreting the results, comparing material performance, and identifying the strengths and limitations of each system in the context of hydrogen technologies.

Hydrogen Production Efficiency: The Ni-based catalyst achieved the highest hydrogen production rate (0.55 $m^3/kg \cdot hr$), making it the most efficient material for water electrolysis among the tested materials. The low overpotential (0.09 V) associated with Ni suggests that it can catalyze the hydrogen evolution reaction (HER) with minimal energy loss, which is crucial for reducing the overall cost of hydrogen production. This aligns with previous research highlighting the exceptional activity of Ni in electrolysis due to its favourable electronic structure and

ability to efficiently facilitate hydrogen evolution (Li *et al*., 2020) [3]. In contrast, the Fe-based catalyst showed the lowest hydrogen production rate (0.42 $m^3/kg \cdot hr$) and required a higher overpotential (0.10 V), indicating lower efficiency. Fe-based catalysts, while inexpensive and abundant, suffer from slower kinetics in the hydrogen evolution reaction compared to Ni-based catalysts. This suggests that Fe may not be the ideal candidate for large-scale hydrogen production when efficiency is a priority. Co-based catalysts (0.48 $m^3/kg \cdot hr$) provided a balance between performance and cost, indicating that Co can serve as a viable alternative to Ni for lower-cost applications. However, Ni still outperforms it in rate and energy efficiency.

Hydrogen Storage Capacity and Desorption Temperature: The hydrogen storage capacity is a crucial factor for the practical use of materials in hydrogen storage applications, especially for transportation and stationary energy storage. In this regard, MgH_2 stands out with the highest storage capacity (6.4 wt%). Metal hydrides like MgH_2 are ideal for high-density hydrogen storage, making them attractive for applications where space and weight constraints are significant. However, the high desorption temperature (400°C) required for hydrogen release from MgH_2 makes it less practical for many real-world applications, especially in mobile systems such as vehicles, where low-temperature hydrogen release is crucial for ease of use (Yi *et al*., 2021) [15]. In contrast, $NaBH_4$ and NH_3BH_3, which exhibited low desorption temperatures of 200°C and 180°C, respectively, are more suitable for practical applications in hydrogen storage and release. These chemical hydrides offer a good balance between high storage capacity and low energy input for desorption, making them attractive candidates for portable hydrogen storage systems. The reversibility of $NaBH_4$ (15 cycles) and NH_3BH_3 (18 cycles) further strengthens their suitability for practical applications, as they can undergo multiple cycles without significant performance degradation, thereby ensuring long-term operational stability (Satyapal *et al*., 2022) [8]. On the other hand, transition metal catalysts, such as NiFeOx and MoS_2, have much lower hydrogen storage capacities (4.2 wt% and 3.8 wt%, respectively) and are primarily suited for hydrogen production rather than storage. These materials demonstrate that hydrogen storage and hydrogen production are distinct processes that require materials with different properties. Transition metal catalysts excel in hydrogen evolution reactions but fall short in hydrogen storage applications due to their limited storage capacities.

Reversibility and Cyclic Stability: The reversibility of a material is a critical factor in its practical use for hydrogen storage. $NaBH_4$ and NH_3BH_3 demonstrated excellent cyclic stability, with 15 and 18 cycles, respectively, indicating that these materials can undergo multiple hydrogen absorption and desorption cycles without significant performance loss. This is a crucial characteristic for long-term energy storage applications, where the ability to store and release hydrogen over many cycles without degradation is essential. This performance is consistent with other studies highlighting the stability and reversibility of chemical hydrides for hydrogen storage (Körner *et al*., 2021) [18]. In contrast, MgH_2 (8 cycles) and $NaAlH_4$ (7 cycles) exhibited lower reversibility, suggesting that these materials may degrade more rapidly after multiple cycles, thereby limiting their long-term viability for hydrogen storage. This suggests that metal hydrides such as MgH_2 may require improvement in structural stability and kinetic performance to be more viable for practical applications that demand long-term durability (Zhang *et al*., 2021) [14].

Surface Area and Catalytic Activity: The surface area of the materials plays an important role in their catalytic efficiency, as a larger surface area provides more active sites for the hydrogen evolution reaction. Co-based catalysts, with the highest surface area (210 m^2/g), exhibited good performance in hydrogen production. This is consistent with the trend that materials with larger surface areas tend to perform better in electrocatalytic reactions (Li *et al*., 2020) [3]. The larger surface area of Co likely contributed to its higher hydrogen production rate compared to NiFeOx (125 m^2/g), which has a significantly lower surface area and, consequently, a lower production rate.

While transition-metal catalysts benefit from larger surface areas, metal hydrides and chemical hydrides are not typically optimised for surface area, as their primary role is hydrogen storage, where bulk properties such as hydrogen absorption/desorption capacity are more critical than surface area. However, for hydrogen production, maximizing the surface area of electrocatalysts is crucial for enhancing reaction rates and improving overall system efficiency. Finally, the hydrogen production and storage experiments demonstrate that transition-metal catalysts, such as Ni, are highly efficient for the hydrogen evolution reaction due to their low overpotentials and high hydrogen production rates. However, metal hydrides like MgH_2 provide much higher hydrogen storage capacities, though their high desorption temperatures limit their practical applications. Chemical hydrides such as $NaBH_4$ and NH_3BH_3 exhibit favourable characteristics for hydrogen storage, including low desorption temperatures and high reversibility, making them ideal for applications requiring efficient, reversible hydrogen release. The findings suggest that hydrogen technologies need to balance production efficiency, storage capacity, desorption energy requirements, and material stability. Transition-metal catalysts and metal hydrides have distinct roles in hydrogen production and storage, and optimising both production and storage systems will require continued advances in materials design and synthesis techniques.

Conclusion

The experimental findings on hydrogen production and storage underscore the importance of inorganic chemistry in advancing sustainable hydrogen technologies. The Ni-based catalyst proved to be the most efficient for hydrogen production, demonstrating the highest hydrogen production rate and lowest overpotential, highlighting its excellent catalytic activity for the hydrogen evolution reaction (HER). This makes Ni an ideal candidate for electrolysis applications, where energy efficiency is critical for reducing the overall cost of hydrogen production. For hydrogen storage, metal hydrides such as MgH_2 exhibited the highest hydrogen storage capacity (6.4 wt%), making them ideal for high-density storage applications. However, the high desorption temperature required for MgH_2 limits its practical application in scenarios where low-temperature

hydrogen release is necessary. Chemical hydrides, particularly $NaBH_4$ and NH_3BH_3, demonstrated favorable characteristics for hydrogen storage due to their low desorption temperatures and high reversibility, making them suitable for portable and long-term storage systems. While transition metal catalysts such as Co-based and MoS_2 excel in hydrogen production, they offer relatively low hydrogen storage capacities, confirming that hydrogen production and storage require distinct materials with different properties. The key takeaway from this study is the importance of optimizing catalyst performance for hydrogen production while simultaneously improving the reversibility and energy efficiency of hydrogen storage materials.

Ultimately, further optimization of both hydrogen production and storage materials is essential for the practical deployment of hydrogen technologies as part of the broader transition to a sustainable, green energy economy. Advanced material design and synthesis techniques will play a pivotal role in realizing the full potential of hydrogen as a clean energy carrier. This study highlights the need for continuous innovation and interdisciplinary collaboration to address the challenges of scalability, economic viability and long-term sustainability in hydrogen energy systems.

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