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**REVIEW**

# A review of hydrogen production and storage materials for efficient integrated hydrogen energy systems

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**Abstract**

The rapidly growing global need for environmentally friendly energy solutions has inspired extensive research and development efforts aimed at harnessing the potential of hydrogen energy. Hydrogen, with its diverse applications and relatively straightforward acquisition, is viewed as a promising energy carrier capable of tackling pressing issues, such as carbon emissions reduction and energy storage. This study conducts a preliminary investigation into effective hydrogen generation and storage systems, encompassing methods like water electrolysis, biomass reforming, and solar-driven processes. Specifically, the study focuses on assessing the potential of nanostructured catalysts and innovative materials to enhance the productivity and versatility of hydrogen energy systems. Additionally, the utilization of novel materials not only improves hydrogen storage capacity and safety but also opens up possibilities for inventive applications, including on-demand release and efficient transportation. Furthermore, critical factors such as catalyst design, material engineering, system integration, and techno-economic viability are examined to identify challenges and chart paths for future advancements. The research emphasizes the importance of fostering interdisciplinary collaborations to advance hydrogen energy technologies and contribute to a sustainable energy future.

**KEYWORDS**

advanced materials, integrated energy systems, material innovations, nanostructured catalysts, sustainable future

## 1 | INTRODUCTION

Hydrogen energy has emerged as a significant contender in the pursuit of clean and sustainable fuel sources. With the increasing concerns about climate change and the depletion of fossil fuel reserves, hydrogen offers a

promising alternative that can address these challenges.<sup>1,2</sup> As an abundant element and a versatile energy carrier, hydrogen has the potential to revolutionize various sectors, including transportation, power generation, and industrial processes. The significance of hydrogen energy lies in its ability to produce energy

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without harmful emissions. When hydrogen is used as a fuel, the only by-product is water, making it a clean and environmentally friendly option. Unlike fossil fuels, hydrogen does not contribute to greenhouse gas emissions, air pollution, or the generation of harmful particulate matter.<sup>3,4</sup> These characteristics position hydrogen energy as a key player in the global transition to a low-carbon economy. However, despite its immense potential, several challenges and limitations need to be addressed for hydrogen energy to become a widespread reality.<sup>4,5</sup> The primary challenges revolve around the production and storage of hydrogen. As shown in Figure 1, the global demand for hydrogen had surged to over 94 million tons (Mt) in 2021, marking a notable 5% rise from the previous year's levels.<sup>6</sup> This increase was particularly evident in traditional applications of hydrogen since 2000, specifically in chemical processes and a significant rebound from the impacts of the Covid-19 pandemic. Within the framework of the IEA's Stated Policies Scenario, the potential escalation of hydrogen demand will reach 115 Mt by 2030.<sup>7,8</sup>

In 2021, the collective worldwide production of hydrogen amounted to 94 Mt and met the hydrogen demand, compare to 86 Mt in 2019 which was less than the demand, as seen in Figure 2. Currently, the most common methods for hydrogen production involve the reforming of natural gas. The requirement for

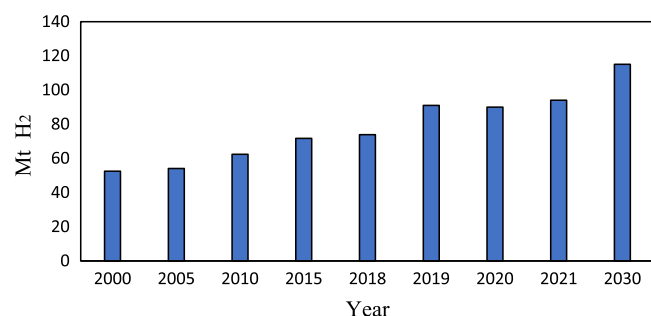


FIGURE 1 Global hydrogen demand.

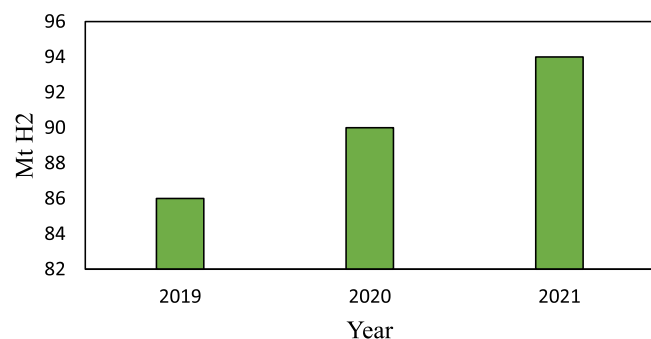


FIGURE 2 Global hydrogen production.

hydrogen is predominantly fulfilled through the utilization of unabated fossil fuel-based hydrogen production. While these methods are well-established, they have limitations in terms of cost, efficiency, and carbon footprint.<sup>8,9</sup>

As the global demand for hydrogen continues to rise, driven by its multifaceted applications across industries, there is a growing emphasis on advancing hydrogen production methods that align with sustainability goals. Efforts to optimize and enhance hydrogen production have led to the exploration of innovative catalysts and materials such as nanostructured catalysts that can expedite reactions and improve efficiency. In addition, hydrogen has a low volumetric energy density, requiring large storage volumes or high-pressure containment systems. Safety concerns related to hydrogen storage and handling also need to be effectively addressed to ensure public acceptance and confidence in its use. To overcome these challenges, novel approaches are essential to improve efficiency, reduce costs, and enhance the safety of hydrogen production and storage technologies. Advanced catalysts and materials play a vital role in enhancing the performance and efficiency of hydrogen production processes, enabling the development of more sustainable and cost-effective methods. Furthermore, breakthroughs in hydrogen storage materials and techniques are needed to improve storage capacity, safety, and practicality. Given the emerging but promising developments in this domain, a comprehensive review focusing on the application of nanostructured catalysts and advanced materials for efficient hydrogen production becomes imperative. The potential of hydrogen as an environment-friendly and sustainable energy solution is studied. Exploring various hydrogen production methods, considering the advantages, disadvantages, and economic dimensions, while highlighting the importance of renewable energy sources. As the global energy landscape shifts towards a greener future, hydrogen's role as an energy carrier and storage modality becomes progressively significant, making collaborative multidisciplinary research essential for the effective integration of hydrogen-based energy systems.<sup>10–13</sup>

Investigating the enhancement of heat transfer within metal hydride (MH) reactors using graphene oxide (GO) nanofluids. By leveraging numerical simulations and machine learning techniques, the study aims to optimize hydrogen storage rates and reactor performance.<sup>14</sup> The focus shifts to biohydrogen production as a sustainable alternative fuel source. The study highlights the economic and environmental benefits of biohydrogen, along with the challenges associated with preprocessing and

scalability. Machine learning models are proposed to optimize biohydrogen production processes.<sup>15</sup> Undertaking a comprehensive assessment of hydrogen energy systems, emphasizing their potential to transform the global energy landscape. Despite numerous advantages, significant challenges remain in storage, manufacturing, distribution, and cost. The study underscores the need for collaborative efforts and breakthrough technologies to realize the full potential of hydrogen energy.<sup>16</sup> Exploring into optimizing biohydrogen production through multivariate analysis. By employing a multi-input and single-output framework, the study identifies key factors influencing biohydrogen yield and proposes optimal operating parameters for maximum efficiency.<sup>17</sup> Therefore, this work aims to highlight the need for innovative approaches and advancements in hydrogen energy. It will explore the current challenges and limitations in hydrogen production and storage technologies, emphasizing the importance of developing novel methods to enhance efficiency, reduce costs, and improve safety. Throughout this study, we explored a wide range of methodologies and approaches for hydrogen production, including water electrolysis, biomass reforming, and solar-driven processes, all optimized using state-of-the-art nanostructured catalysts. Moreover, throughout this study, we explore a wide range of methodologies and approaches for hydrogen storage, including advanced techniques, such as metal-organic frameworks (MOFs), carbon nanomaterials, complex hydrides, and nanostructured alloys, all optimized using state-of-the-art nanostructured materials. As one of the first investigations in this exciting and rapidly evolving area, this review paper serves as a valuable resource for researchers, policymakers, and industry professionals seeking to understand the latest developments in efficient hydrogen production and storage. By critically analyzing the existing literature and experimental findings, we provide a comprehensive overview of the current state-of-the-art in efficient hydrogen production and storage. This work aims to make significant contributions to the field of hydrogen energy by addressing the challenges of hydrogen production and storage through the innovative use of nanostructured catalysts and advanced materials. The main contributions of this paper are manifested through the objectives and the novelty as follows:

#### Objectives:

- *Introducing effective hydrogen production and storage techniques:* This review offers a comprehensive exploration of various techniques for hydrogen production and storage, including water electrolysis, biomass reforming, and solar-driven processes.

- *Highlighting the potential of nanostructured catalysts and advanced materials:* The paper emphasizes the significance of nanostructured catalysts and advanced materials in optimizing hydrogen production and storage processes. It demonstrates how these materials can enhance efficiency and safety in hydrogen-related technologies.
- *Identifying key challenges and opportunities:* By analyzing existing literature and experimental findings, the review aims to recognize key challenges in hydrogen production and storage based on nanostructured catalysts and advanced materials. Furthermore, it aims to identify opportunities for further advancements in catalyst design, material engineering, system integration, and techno-economic feasibility.

#### Novelty:

- The novelty of this paper lies in its comprehensive approach to addressing challenges in hydrogen production and storage through the innovative use of nanostructured catalysts and advanced materials. While previous studies have examined hydrogen-related technologies, this review uniquely focuses on the potential of nanostructured materials to optimize efficiency and safety. Additionally, by identifying key challenges and opportunities, the paper contributes to the advancement of hydrogen energy research and informs stakeholders about the latest developments in the field.

## 2 | REVIEW METHODOLOGY

This paper's review methodology entails an exhaustive examination of the pertinent literature and research studies on two main groups: hydrogen production and storage, as shown in Figure 3. By embracing these viewpoints, our paper attempts to provide knowledge of effective hydrogen production and storage using nanostructured catalysts and cutting-edge materials. This review paper presents a comprehensive synthesis of numerous research findings in the field, showcasing the progress and significant contributions made in the subject of efficient hydrogen production and storage using nanostructured catalysts and advanced materials. By consolidating these studies, the paper offers a comprehensive overview of the advances, challenges, and potential applications in harnessing the potential of nanostructured catalysts and advanced materials for efficient hydrogen production and storage, as presented in Figure 3.

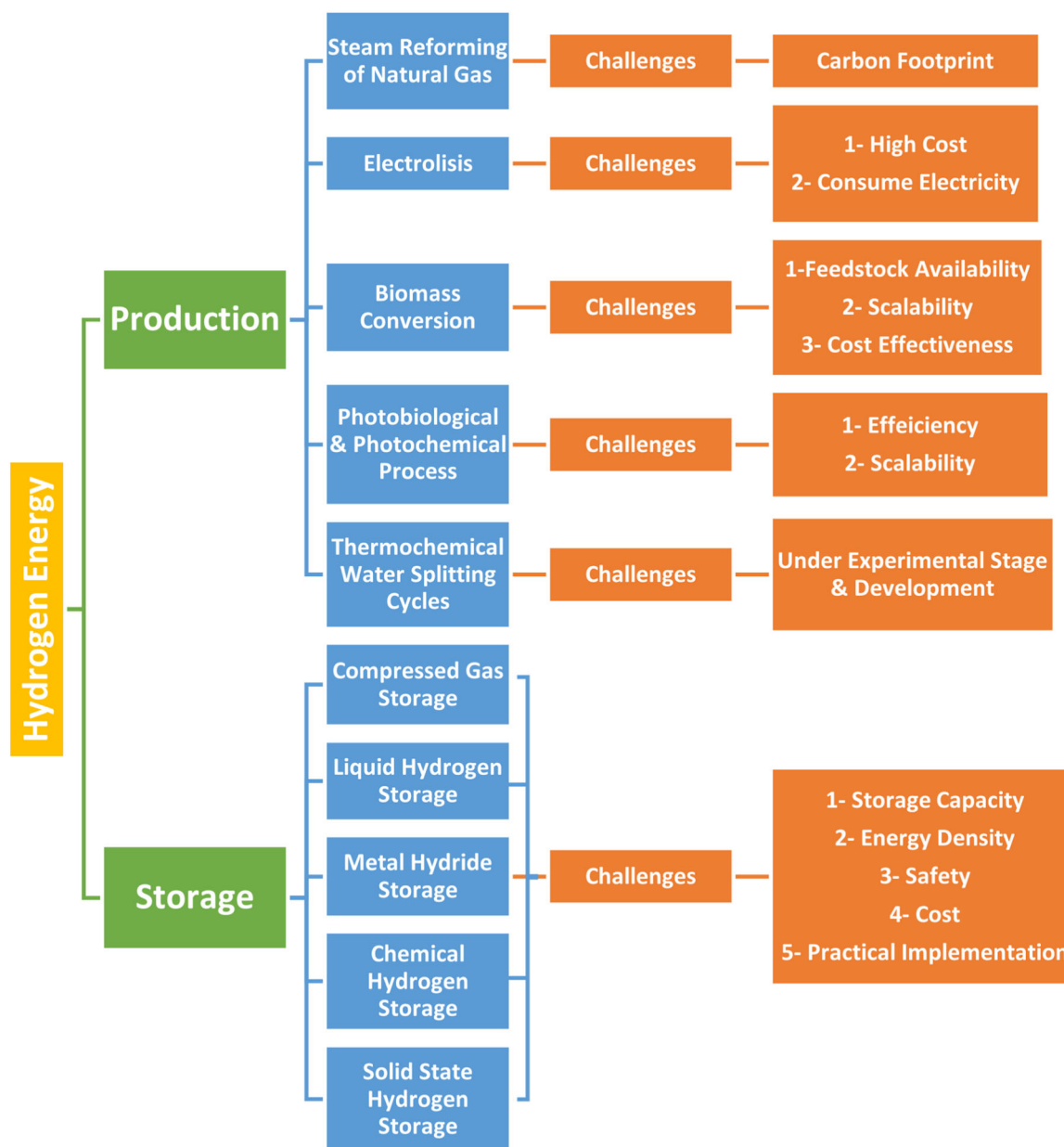


FIGURE 3 Hydrogen energy production and storage challenges.

### 3 | NANOSTRUCTURED CATALYSTS FOR HYDROGEN PRODUCTION

In 2021, global hydrogen production reached a total of 94 million metric tons, as illustrated in Figure 2. The primary method of production, depicted in Figure 4, predominantly relied on natural gas, contributing to 62% of hydrogen production, followed by coal and naphtha reforming at 19% and 18%, respectively. The International Energy Agency (IEA) reported that the production of low-emission hydrogen, accounting for only 1%, was primarily sourced from fossil fuels with carbon capture utilization and storage.<sup>8,9</sup> A smaller portion of

approximately 35 thousand metric tons was generated through water electrolysis powered by electricity. Notably, the quantity of hydrogen produced via water electrolysis, albeit relatively small in scale, exhibited nearly a 20% growth compared with 2020. This expansion can be attributed to the increasing adoption of water electrolyzers.

According to the IEA's monitoring of hydrogen production projects, a notable increase in initiatives targeting the production of low-emission hydrogen is evident. This surge indicates a significant rise in projects announced with the goal of producing hydrogen through water electrolysis or by integrating fossil fuels with carbon capture processes. Successful implementation of

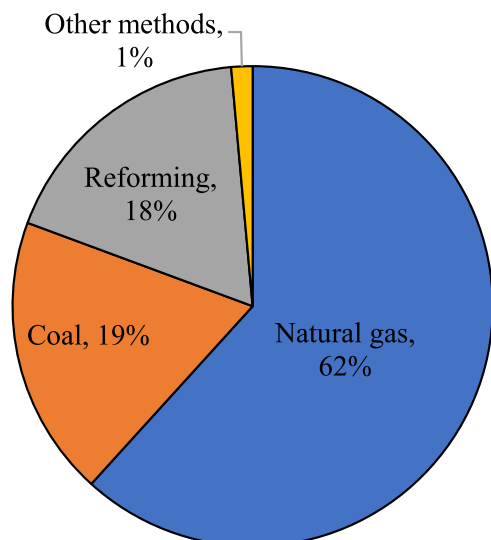


FIGURE 4 Hydrogen energy methods.

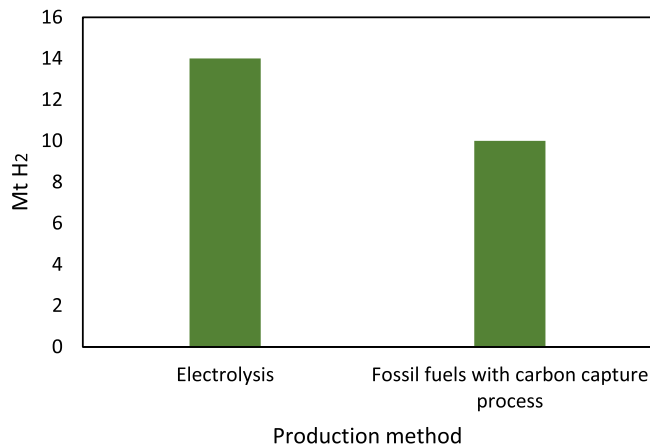


FIGURE 5 Low-emission hydrogen energy production methods.

these ongoing initiatives, aimed at low-emission hydrogen production, could lead to an estimated annual output exceeding 24 million metric tons by 2030, as depicted in Figure 5.

Hydrogen has emerged as a promising and pivotal alternative energy carrier with the potential to significantly contribute to global decarbonization efforts and tackle pressing energy challenges. The escalating demand for clean and sustainable energy solutions has prompted extensive research into a wide array of hydrogen production methods, as depicted in Figure 5. In this section, we offer a comprehensive overview of the current state-of-the-art hydrogen production techniques, encompassing steam reforming, electrolysis, biomass conversion, photobiological and photoelectrochemical processes, along with other emerging methodologies, as discussed in Table 1:

- **Steam reforming:** is the dominant method for producing hydrogen globally. It involves reacting steam with hydrocarbons, mainly natural gas, using a catalyst. This process yields carbon dioxide and hydrogen gas. While steam reforming offers economic advantages and high efficiency, it heavily depends on fossil fuels, as shown in Figure 6.<sup>18</sup>
- **Electrolysis:** It presents as a highly promising technique for the production of hydrogen, through the electrochemical separation of water molecules into hydrogen and oxygen such as fuel cells promoted by catalysts.<sup>19</sup> Nanostructured catalysts, including platinum nanoparticles, nickel-iron hydroxide nanosheets, and cobalt-based nanostructures, play a vital role in improving the efficiency and kinetics of this process by providing a high surface area and tailored active sites for the electrochemical reactions. These nanostructured catalysts offer significant advantages in terms of improved reaction kinetics, reduced overpotential, and enhanced durability, thereby contributing to the overall efficiency and sustainability of water electrolysis as a method for hydrogen generation, as illustrated in Figure 7.<sup>20</sup>
- **Biomass conversion:** Biomass conversion involves turning various biomass materials, such as agricultural residues, wood, or energy crops, into hydrogen gas. This can be achieved through techniques, like, gasification, pyrolysis, or fermentation. Biomass gasification is particularly notable, where biomass is transformed into synthesis gas (syngas), containing hydrogen, carbon monoxide, and other gases. Syngas can then be further processed to produce hydrogen. One of the key advantages of biomass conversion is its use of renewable feedstock sources, supporting sustainability goals and reducing greenhouse gas emissions. However, challenges related to feedstock availability, scalability, and cost-effectiveness must be addressed. The process is illustrated in Figure 8.<sup>21,22</sup>
- **Photobiological and photoelectrochemical processes:** These processes utilize sunlight to directly produce hydrogen from water. In photobiological methods, microorganisms or algae harness sunlight's energy through photosynthesis to generate hydrogen. Photoelectrochemical processes employ specific semiconductors that produce an electrical current when exposed to light, facilitating electrolysis of water to yield hydrogen. These approaches offer sustainable hydrogen production driven by solar energy. However, they are still in early stages of development and face challenges regarding scalability and efficiency. See Figure 9 for illustration.<sup>23</sup>

TABLE 1 Advantages, challenges, used energy source, used feedstock, efficiency, cost, TRL, maturity and availability, and realization of hydrogen production methods.<sup>19–26</sup>

| Production method                                  | Advantages   | Challenges   | Used energy source                 | Feedstock                 | Efficiency (%) | Cost (\$/kg) | TRL              | Maturity        | Availability and realization                                  |
|--|--|--|------------------------------------|---------------------------|----------------|--------------|------------------|-----------------|---|
| Steam reforming                                    | <ul style="list-style-type: none"> <li>High hydrogen production</li> <li>Versatile feedstock</li> </ul>                            | <ul style="list-style-type: none"> <li>Greenhouse gas emissions</li> <li>Energy-intensive</li> </ul>                       | Fossil fuel                        | Natural gas               | 74–85          | 2.27         | High             | High            | Widely available  |
| Water splitting (electrolysis)                     | <ul style="list-style-type: none"> <li>Direct and clean hydrogen production</li> <li>Potential for renewable energy use</li> </ul> | <ul style="list-style-type: none"> <li>Energy-intensive</li> <li>High initial investment</li> </ul>                        | Wind, solar electricity generators | Water                     | 60–80          | 10.3         | Moderate to high | Increasing      | Increasing availability                                       |
| Biomass conversion                                 | <ul style="list-style-type: none"> <li>Renewable energy source</li> <li>Low environmental impact</li> </ul>                        | <ul style="list-style-type: none"> <li>Low efficiency</li> <li>Technological challenges</li> </ul>                         | Steam generated within the system  | Woody biomass             | 10–11          | 2.13         | Moderate to high | Moderate        | Available in certain regions                                  |
| Photobiological and photoelectrochemical processes | <ul style="list-style-type: none"> <li>Higher hydrogen yield</li> <li>Efficient use of light energy</li> </ul>                     | <ul style="list-style-type: none"> <li>Complex process conditions</li> <li>Sensitivity to environmental factors</li> </ul> | Solar                              | Water                     | 0.1            | 2.83         | Moderate         | Low             | Limited availability  |
| Thermal gasification                               | <ul style="list-style-type: none"> <li>Versatile feedstock use</li> <li>Produces synthesis gas (syngas)</li> </ul>                 | <ul style="list-style-type: none"> <li>High capital costs</li> <li>Environmental emissions and cleanup needed</li> </ul>   | Fossil fuel                        | Coal                      | 30–40          | 1.77–2.05    | Moderate to high | Moderate        | Available in some regions with suitable feedstocks            |
| Thermal decomposition (pyrolysis)                  | <ul style="list-style-type: none"> <li>Biochar and bio-oil production</li> <li>Minimal greenhouse gas emissions</li> </ul>         | <ul style="list-style-type: none"> <li>Complex process optimization</li> <li>Variable product quality</li> </ul>           | Steam generated within the system  | Natural gas woody biomass | 35–50          | 1.59–1.7     | Moderate         | Moderate        | Available in niche markets for biochar and bio-oil production |
| Thermal cracking (thermolysis)                     | <ul style="list-style-type: none"> <li>Rapid reaction</li> <li>High energy recovery</li> </ul>                                     | <ul style="list-style-type: none"> <li>Limited feedstock applicability</li> <li>High-temperature requirements</li> </ul>   | Nuclear Solar                      | Water                     | 20–45          | 7.98–8.4     | Low to moderate  | Low to moderate | Limited availability  |

Abbreviation: TRL, technology readiness level.

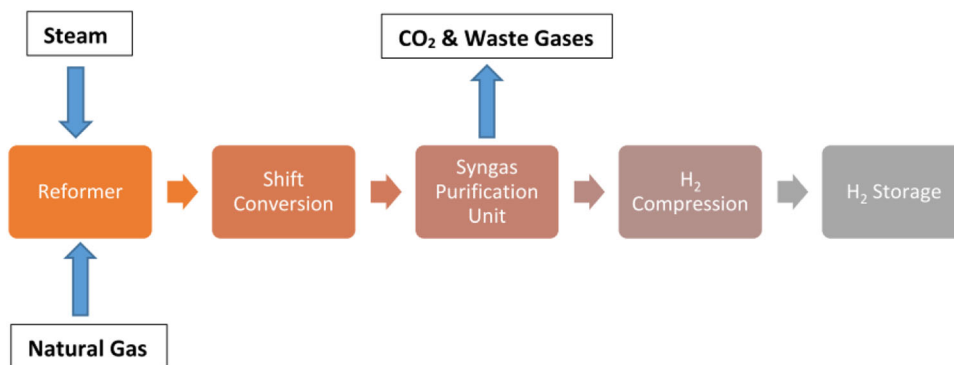


FIGURE 6 Steam reforming process for hydrogen production.

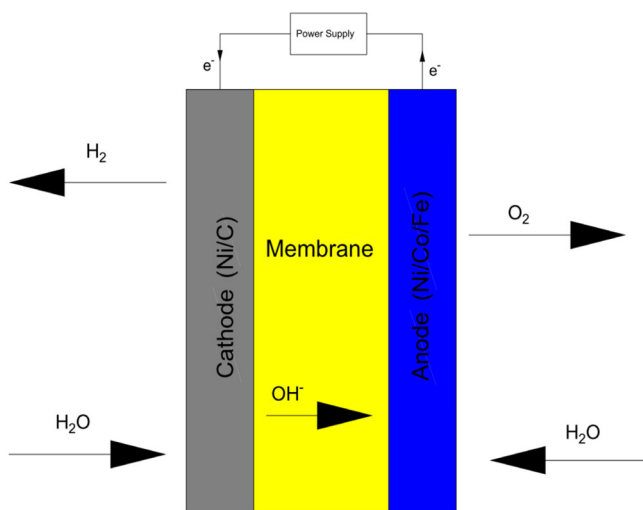


FIGURE 7 Electrolysis process for hydrogen production in fuel cells promoted by catalysts.

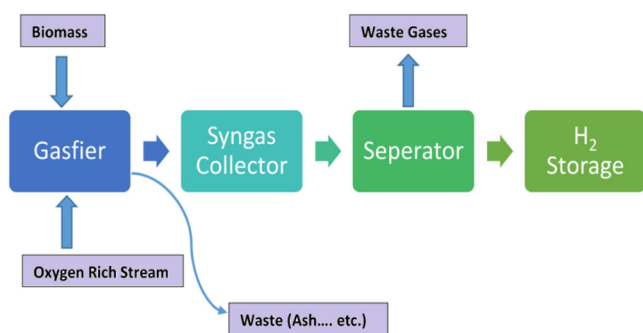


FIGURE 8 Biomass conversion process for hydrogen production.

- *Other methods:* Figure 10 showcases additional methods for hydrogen synthesis, including thermochemical water-splitting techniques such as Thermal Gasification, Pyrolysis, and Thermolysis, along with high-temperature electrolysis utilizing solid oxide electrolysis cells. These approaches offer alternative pathways

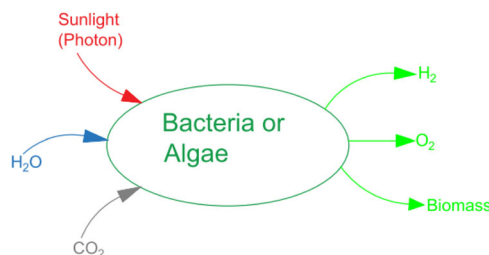


FIGURE 9 Photobiological and photoelectrical process for hydrogen production.

for hydrogen production, although they are currently in the experimental phase of development. Despite being at an early stage, they show promising potential for achieving efficient hydrogen production.<sup>24,25</sup>

- To achieve sustainable hydrogen production, a pivotal strategy involves a combination of various methods and the seamless integration of renewable energy sources. This holistic approach holds promise in ushering in a new era of environmentally friendly hydrogen generation.

Table 1 offers a thorough summary of the advantages and challenges linked to diverse hydrogen production methods. It delineates the energy origins and input materials used in each method while emphasizing their effectiveness and associated expenditures. This tabular presentation serves as a valuable tool for evaluating the relative strengths and weaknesses of distinct approaches to hydrogen generation.

Figure 11 depicts the hydrogen production techniques, which compares their cost-efficiency dynamics, offers valuable insights into the intricate landscape of hydrogen production technologies. Steam reforming is expensive yet effective and emerges as a costly approach, but its impressive efficiency range, spanning from 74% to 85%, underscores its proficiency in converting fossil fuels into hydrogen. It remains favored



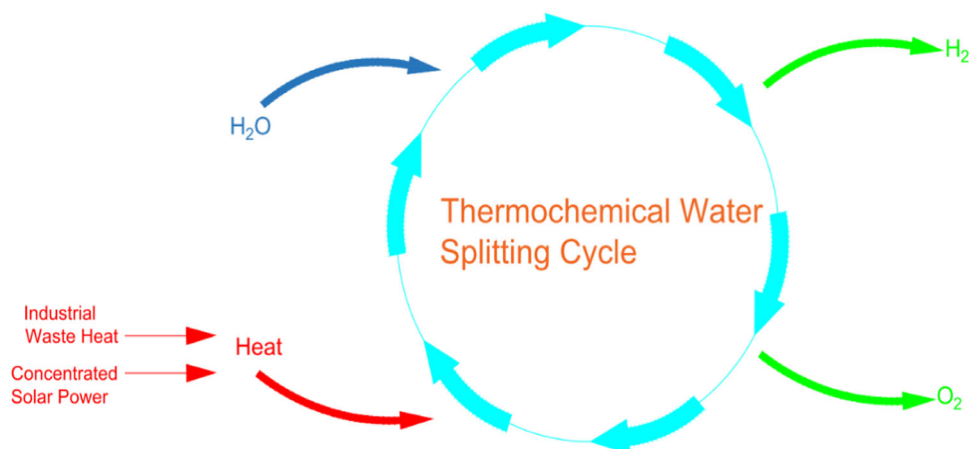


FIGURE 10 Thermochemical process for hydrogen production.

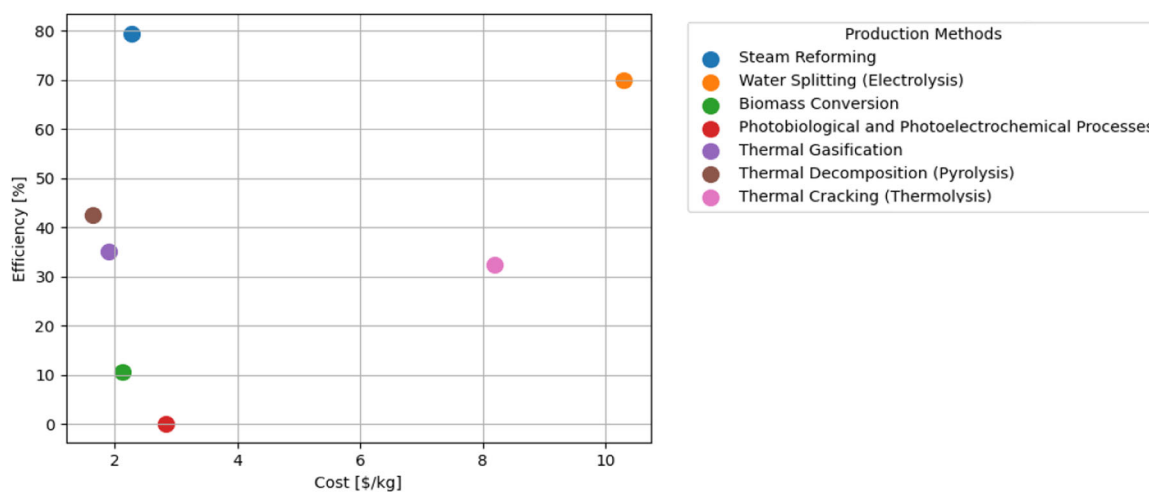


FIGURE 11 Hydrogen production methods: cost versus efficiency.

in industrial applications where efficiency outweighs cost concerns. Water splitting (electrolysis) is environmentally friendly and promising bearing in mind electrolysis, powered by renewable sources like wind and solar energy, presents an ecofriendly avenue for hydrogen production. Its efficiency range of 60%–80% is noteworthy, although the initial investment can be a deterrent. Ongoing research and development in this domain hold substantial potential for sustainable hydrogen generation. Biomass conversion is renewable, with lingering challenges, as a renewable energy source, aligns with sustainability objectives. Nevertheless, its relatively modest efficiency range of 10%–11% indicates the need for enhancements. Overcoming technological obstacles is pivotal to unlocking its full promise in the transition to clean energy. Photobiological and Photoelectrochemical processes are aspiring solar solutions, these processes harness solar energy but grapple with

intricacies and sensitivity to environmental factors. With an efficiency range as low as 0.1%, there exists a conspicuous necessity for innovative breakthroughs to render these methods more practical for real-world applications. Thermal gasification, decomposition, and cracking are versatile feedstock handling, the trio of thermal techniques offers adaptability in handling diverse feedstocks. However, their efficiency ranges, spanning from 30% to 45%, signal the potential for enhancement to compete with more efficient methodologies. Figure 11 also generates debate on the delicate balance between cost and efficiency in hydrogen production. It underscores the imperative for interdisciplinary research, technological advancements, and policy backing to expedite the shift towards sustainable hydrogen production methods, ultimately contributing to a more environmentally conscious and energy-efficient future.

### 3.1 | Introduction to nanostructured catalysts and their advantages in improving hydrogen production

Nanostructured catalysis stands at the forefront of catalytic science, representing a paradigm shift in the design and application of catalysts. At its core, nanostructured catalysis revolves around the utilization of catalysts featuring nano-sized structures, typically ranging from 1 to 100 nm in at least one dimension. This nanoscale dimensionality imparts unique properties to these catalysts, setting them apart from their conventional counterparts. Compared with traditional supported catalysts, nanostructured catalysts offer several distinct advantages. One of the most notable is their exceptionally high surface area-to-volume ratio. This heightened surface area provides an abundance of active sites for catalytic reactions, facilitating enhanced reactivity and efficiency. Moreover, the quantum size effects inherent in nanostructured materials confer them with novel electronic and geometric properties, further augmenting their catalytic performance. Nanostructured catalysts encompass a diverse array of materials, spanning metals, metal oxides, carbon-based materials, and MOFs. These materials can be precisely engineered to exhibit tailored properties, allowing for fine-tuning of catalytic activity and selectivity. Additionally, nanostructured catalysts offer improved mass transport characteristics owing to their small size and high porosity, facilitating efficient diffusion of reactant molecules to active sites and the removal of products. In the realm of hydrogen production and storage, nanostructured catalysts play a pivotal role in various processes. Reforming catalysts are employed to generate hydrogen from hydrocarbons or water, while water-splitting catalysts facilitate the electrolysis or photocatalysis of water into hydrogen and oxygen. Additionally, hydrogenation catalysts are utilized in the conversion of biomass or carbon dioxide into hydrogen-containing compounds. Meanwhile, storage materials such as MHs and chemical hydrides rely on nanostructured catalysts to enable efficient hydrogen storage. It is essential to differentiate between support materials and active components within nanostructured catalysts. Support materials, such as carbon nanotubes (CNTs) or metal oxides, provide a scaffold for anchoring active catalytic species. On the other hand, the active components, typically metallic nanoparticles or metal complexes, catalyze the desired reactions. Understanding and optimizing the interaction between these components are crucial for maximizing catalytic performance.<sup>27–32</sup> In summary, nanostructured catalysis represents a frontier in catalytic science, offering unparalleled opportunities for advancing various

industrial processes, including hydrogen production and storage. By harnessing the unique properties of nanostructured materials, researchers can pave the way for more efficient, selective, and sustainable catalytic technologies, driving progress towards a greener and more prosperous future.

### 3.2 | Exploration of novel nanostructured catalyst materials and their potential in hydrogen production

Figure 12 illustrates the prominent materials that garnered significant attention from researchers in the year 2021. A closer examination of the patterns in substance classes within this chronological progression reveals notable research trends.<sup>8,9</sup> Researchers have shown a concentrated interest in incorporating conventional elements such as carbon, platinum, and nickel in hydrogen production processes. However, there has been a growing exploration of novel chemical domains, marked by the investigation of new polymers, alloys, and oxide materials for applications in electrocatalysis and photocatalysis.<sup>8,9</sup>

Numerous investigations have been conducted in the quest for novel nanostructured catalyst materials capable of enhancing hydrogen production. A diverse range of nanostructured catalyst materials, including metal nanoparticles, MOFs, and carbon-based substances, have emerged as promising candidates for expediting hydrogen synthesis reactions.<sup>33</sup> Metal nanoparticles like platinum (Pt), palladium (Pd), and ruthenium (Ru), as depicted in Figure 13, have been

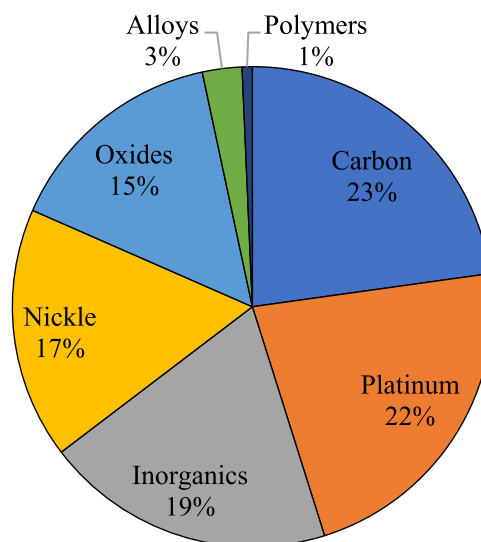


FIGURE 12 Key substances in hydrogen production by researchers in 2021.

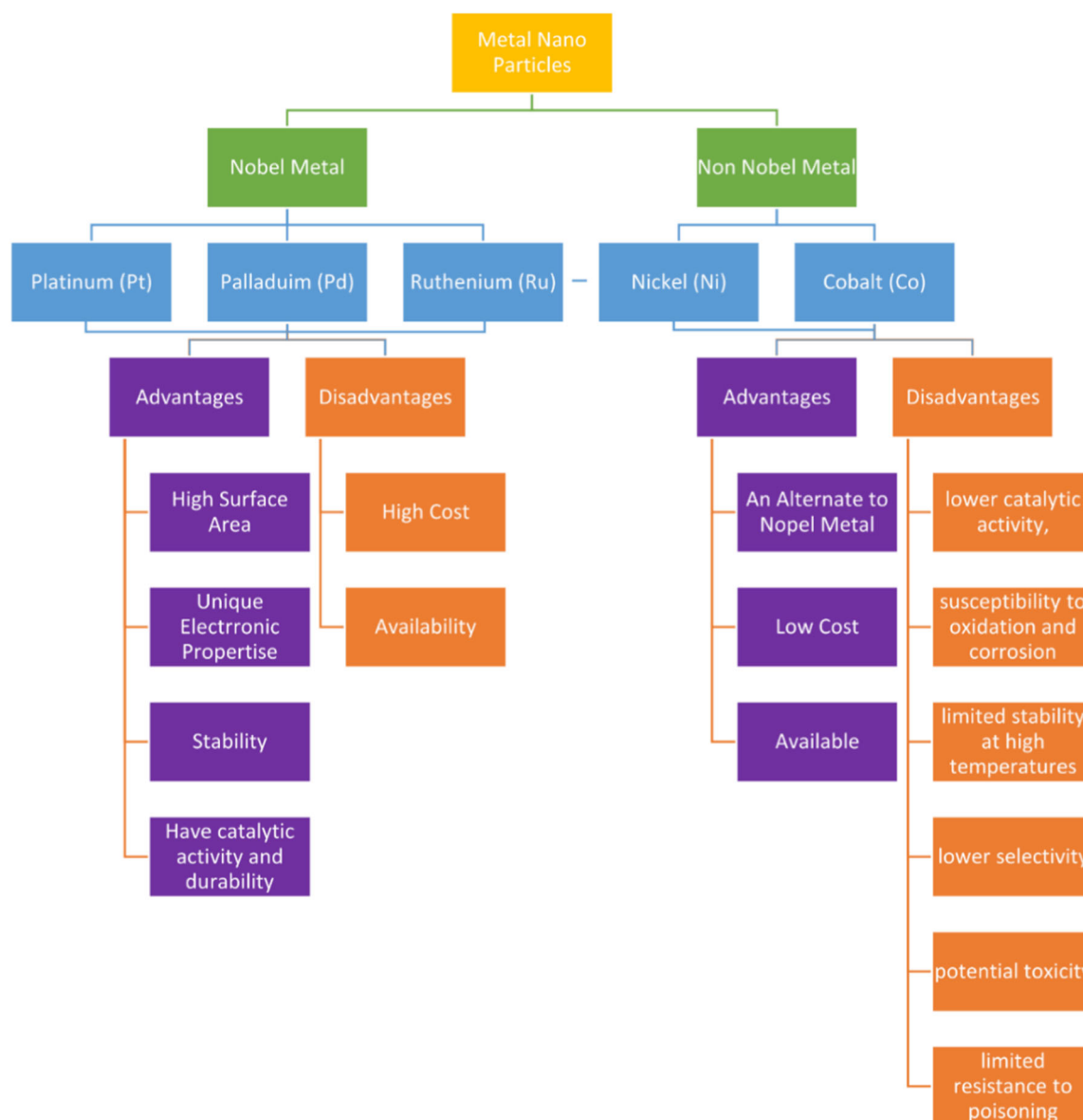


FIGURE 13 The nanostructured catalyst materials in hydrogen production with the main advantages and disadvantages.

extensively studied for their role in catalyzing hydrogen generation. Their extensive surface area and unique electrical properties contribute to their significant catalytic activity. For instance, Pt nanoparticles are commonly employed in hydrogen evolution processes (HER) due to their exceptional catalytic activity and durability. However, the exploration of nonnoble metal nanoparticles like nickel (Ni) and cobalt (Co) as alternatives to precious metals like platinum, gold, and palladium has gained momentum. These nonnoble metals do present certain drawbacks, including reduced catalytic activity, susceptibility to oxidation and corrosion, limited high-temperature stability, lower selectivity, potential toxicity, and limited resistance to poisoning. This exploration is driven by the

high cost and limited availability of noble metals.<sup>34</sup> MOFs: MOFs represent a category of crystalline materials composed of metal ions or clusters interconnected by organic ligands. These materials have garnered significant attention as prospective catalysts for hydrogen production. Their high porosity and tunability enable the inclusion of catalytic metal sites and the enhancement of mass transport properties. MOFs' versatility allows for catalytic processes like water splitting, which can produce hydrogen electrochemically or photocatalytically.

By modifying their design and synthesis, the stability and catalytic efficiency of MOFs can be further improved.<sup>35–37</sup> Carbon-based materials, including CNTs, graphene, and carbon nanofibers, have also

demonstrated potential as catalyst supports for hydrogen synthesis. These substances possess exceptional chemical stability, high thermal conductivity, and impressive mechanical strength. To enhance the catalytic activity of carbon-based materials, they can be functionalized with transition metal catalysts or metal nanoparticles. The combination of carbon-based materials and metal nanoparticles, for instance, has exhibited improved stability and catalytic activity in water-splitting and other hydrogen generation processes.<sup>38</sup> In addressing concerns related to stability, cost-effectiveness, and efficiency, researchers are actively exploring innovative nanostructured catalyst materials for hydrogen synthesis. The ability to tailor a catalyst's properties at the nanoscale holds the promise of elevating its catalytic activity, selectivity, and longevity. The advancement of hydrogen production technologies and the realization of hydrogen's potential as a clean and sustainable energy source hinge on the development of efficient and cost-effective catalyst materials.<sup>39</sup>

In summary, the investigation of metal nanoparticles, MOFs, carbon-based materials, and other emerging nanostructured catalyst materials presents exciting prospects for enhancing hydrogen generation methods and facilitating the transition to a hydrogen-based economy. To maximize the utility of these materials in hydrogen generation systems, further research is imperative to unravel their catalytic mechanisms, scale up their production, and optimize their performance.

### 3.3 | Experimental methods for catalyst synthesis, characterization, and performance evaluation

The comprehension of catalysts, encompassing their synthesis, characterization, and performance assessment, constitutes a vital aspect of elucidating the intricate interplay between their structure and activity, as well as refining their efficacy for specific catalytic reactions. To facilitate these processes, a range of experimental techniques and methodologies are enlisted. In Figure 14,<sup>40,41</sup> we can observe several commonly employed catalyst synthesis methods, each bearing distinct advantages and disadvantages, as elucidated in Table 2.

- *Wet chemical methods*: One avenue for catalyst creation involves wet chemical procedures, such as impregnation, co-precipitation, precipitation, and hydrothermal synthesis. These methods entail the meticulous mixing of precursor solutions or suspensions, culminating in the judiciously controlled

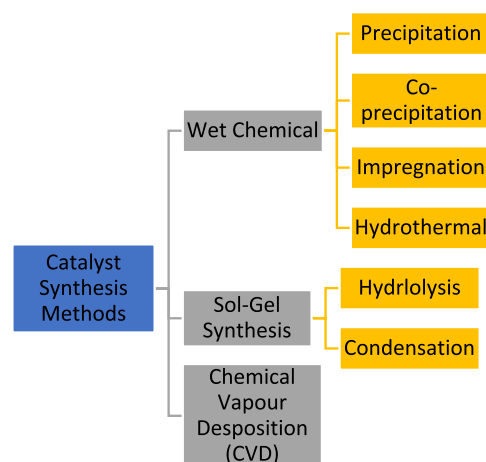


FIGURE 14 Catalyst synthesis methods.

TABLE 2 Advantages and disadvantages of catalyst synthesis methods.<sup>40,41</sup>

| Catalyst synthesis methods | Advantages           | Disadvantages          |
|----------------------------|----------------------|------------------------|
| Wet chemical methods       | Versatility          | Limited precision      |
|                            | Cost-effectiveness   | Potential contaminants |
|                            | Controlled synthesis | Energy consumption     |
|                            | Homogeneity          |                        |
| Sol-gel methods            | Tailored structure   | Complexity             |
|                            | High purity          | Precursor selection    |
|                            | Chemical stability   |                        |
| Chemical vapor deposition  | High precision       | Equipment cost         |
|                            | Conformal coating    | High temperatures      |
|                            | Efficiency           | Limited thickness      |

chemical reactions necessary to fashion the catalyst material.

- *Sol-gel methods*: The production of a gel commences with the hydrolysis and condensation of metal alkoxides or precursors. Subsequently, the gel is subjected to drying and thermal treatment, ultimately yielding the desired catalyst material.
- *Chemical vapor deposition (CVD)*: CVD operates by depositing precursor molecules onto a substrate at elevated temperatures, resulting in the formation of a thin-film catalyst.
- In essence, these catalyst synthesis methodologies constitute indispensable tools in the arsenal of catalyst research, enabling the systematic exploration of

catalyst structure–activity relationships and the enhancement of their performance tailored to specific catalytic reactions.

A thorough comprehension of catalyst materials requires the application of a variety of characterization techniques, as illustrated in Figure 15.<sup>42</sup> These methods provide insights into various aspects of catalyst properties, elucidating their structure and composition. Below are the key characterization techniques employed:

- *X-ray diffraction (XRD)*: XRD is instrumental in unveiling the crystal structure and phase composition of catalyst materials. It offers detailed information regarding the crystalline nature of the catalyst and can identify impurities or phase transitions.
- *Scanning electron microscopy (SEM) and transmission electron microscopy (TEM)*: SEM and TEM techniques enable the observation of catalyst particles' shapes, sizes, and distributions. They provide high-resolution images and facilitate the characterization of catalyst nanostructures.
- *X-ray photoelectron spectroscopy (XPS)*: XPS delves into the surface chemical composition of catalyst materials.

It discerns the oxidation states and chemical environments of the catalyst's constituent elements.

- *Fourier transform infrared spectroscopy (FTIR)*: FTIR identifies surface species and functional groups present on the catalyst material. It aids in comprehending the chemistry of the catalyst's surface and the interactions between reactants and the catalyst.
- *Brunauer–Emmett–Teller (BET) analysis*: BET analysis serves to assess the specific surface area and porosity of catalyst materials. It provides critical insights into the surface area available for reactant adsorption.
- To achieve a comprehensive grasp of catalyst materials, a combination of these diverse methodologies is often employed. Furthermore, the advantages and disadvantages of these catalyst characterization techniques are expounded upon in Table 3.

Figure 16 showcases a range of techniques employed for the evaluation of catalyst performance, while Table 4 provides a summary of the principal advantages and challenges associated with these methods.<sup>43</sup> These performance evaluation techniques are vital for comprehending how catalysts behave and perform in various reactions. Here is an overview of these techniques:

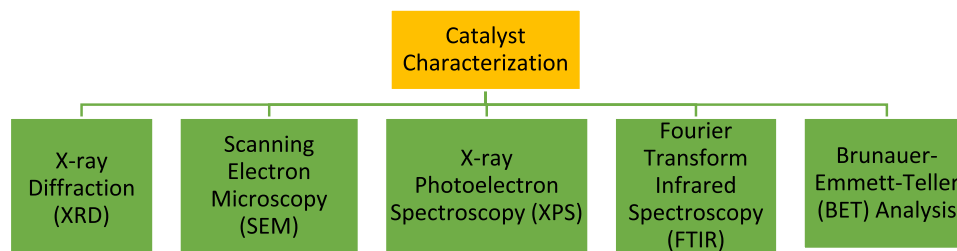


FIGURE 15 Catalyst characterization techniques.

TABLE 3 Advantages and disadvantages of catalyst characterization techniques.<sup>42</sup>

| Catalyst characterization techniques                              | Advantages   | Disadvantages                                       |
|---|--|---|
| X-ray diffraction   | Crystal structure analysis<br>Impurity detection           | Limited to crystalline materials<br>Bulk analysis   |
| Scanning electron microscopy and transmission electron microscopy | High-resolution imaging<br>Nanostructure insights          | Sample preparation<br>Limited to surface analysis   |
| X-ray photoelectron spectroscopy                                  | Surface chemical analysis<br>Nondestructive                | Limited depth profiling<br>Equipment complexity     |
| Fourier transform infrared spectroscopy                           | Surface chemistry information<br>Versatile technique       | Surface sensitivity<br>Interpretation complexity    |
| Brunauer–Emmett–Teller analysis                                   | Surface area evaluation<br>Applicable to various materials | Surface area only<br>Requires specialized equipment |

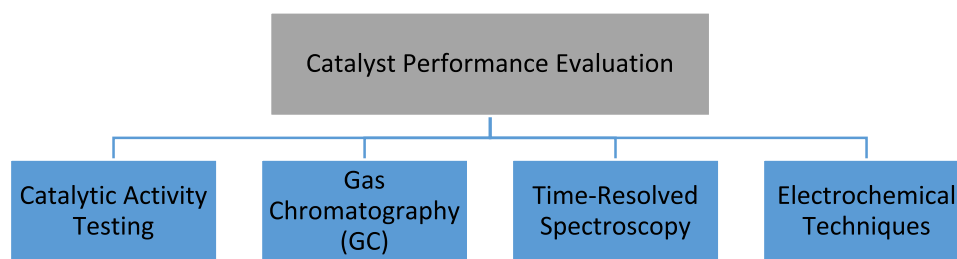


FIGURE 16 Catalyst performance evaluation techniques.

TABLE 4 Advantages and challenges of catalyst performance evaluation techniques.<sup>43</sup>

| Catalyst performance evaluation techniques | Advantages   | Challenges  |
|--|--|---|
| Catalytic activity testing                 | Direct assessment<br>Reaction parameter control                                  | Labor-intensive<br>Time-consuming                         |
| Gas chromatography                         | Product composition analysis<br>Quantitative data                                | Requires sample preparation<br>Limited surface insights   |
| Time-resolved spectroscopy                 | In situ analysis<br>Surface species identification                               | Specialized equipment<br>Limited quantitative data        |
| Electrochemical techniques                 | Applicable to electrochemical reactions<br>Electrocatalytic activity measurement | Electrochemical setup<br>Limited to specific applications |

- **Catalytic activity testing:** Involves utilizing various reactors and experimental setups. These setups can indeed vary depending on factors such as the nature of the reaction and the conditions involved. Reactors can be made of different materials such as glass or steel, and they can operate in batch or continuous mode. The parameters mentioned, like, temperature, pressure, and reactant concentrations, are indeed critical in assessing catalytic activity.
- **Gas chromatography (GC):** GC is a valuable tool for analyzing the composition of reaction products and quantifying reactant conversion rates. It offers insights into the selectivity and efficiency of the catalyst.
- **Time-resolved spectroscopy:** Time-resolved spectroscopic methods, including in situ FTIR spectroscopy and X-ray absorption spectroscopy, are employed to investigate the dynamic changes in catalyst surface species and reaction intermediates during catalytic reactions.
- **Electrochemical techniques:** In applications involving electrochemical reactions such as water splitting and fuel cells, catalyst performance is assessed using electrochemical techniques, like, cyclic voltammetry and chronoamperometry.
- These performance evaluation techniques are indispensable for characterizing catalyst behavior and optimizing catalyst performance in a variety of catalytic processes.

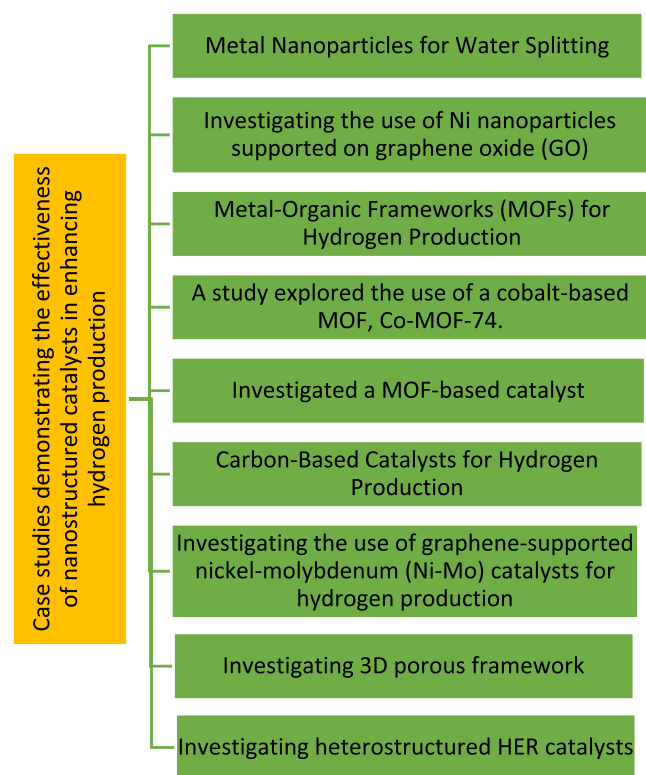
Researchers can create catalysts with specific features, describe their structure and surface characteristics, and assess how well they work in catalytic reactions with the use of these experimental procedures and approaches. Researchers can better understand catalyst behavior and direct the development of new catalyst materials for hydrogen production and other catalytic processes by integrating synthesis, characterization, and performance evaluation.

### 3.4 | Case studies that demonstrate the effectiveness of nanostructured catalysts in enhancing hydrogen production efficiency

Several case studies have demonstrated, as shown in Figure 17, the effectiveness of nanostructured catalysts in enhancing hydrogen production efficiency:

In Figure 17, emerging trends in nanostructured catalysts for hydrogen production based on the case studies are summarized as follows:

- Transition metal nanoparticles on GO supports:
  - o **Key findings:** Enhanced hydrogen production in alkaline electrolysis with Ni–Mo–N/NG catalyst.



**FIGURE 17** Case studies demonstrating the effectiveness of nanostructured catalysts for hydrogen production. HER, hydrogen evolution process.

- o *Innovative approach*: Utilization of heterostructured Ni–Mo–N nanoparticles on nitrogen-doped reduced GO for synergistic effects.
- o *New insights*: Potential of nonnoble metal catalysts for efficient hydrogen production, highlighting the importance of innovative catalyst design.<sup>44,45</sup>
- MOFs:
  - o *Key findings*: Exploration of various MOF-related electrocatalysts and consideration of MOF-based photocatalysts for hydrogen generation.
  - o *Innovative approach*: Recognition of MOFs' adaptability and diverse compositions for enhancing hydrogen production.
  - o *New insights*: Potential environmental benefits of utilizing MOFs in hydrogen production.<sup>46–48</sup>
- Carbon-based catalysts:
  - o *Key findings*: Identification of diverse carbon-based materials for hydrogen generation and discussion of techniques to enhance their photocatalytic activity.
  - o *Innovative approach*: Discussion on the promising potential and unique properties of carbon-based materials.
  - o *New insights*: Opportunities for further optimization in photocatalytic applications.<sup>49</sup>
- Nickel–molybdenum (Ni–Mo) catalysts:

- o *Key findings*: Summary of recent developments in Ni–Mo-based HER catalysts, highlighting their potential for enhanced hydrogen production.
- o *Innovative approach*: Exploration of Ni–Mo-based catalysts as alternatives to precious metal-based catalysts.
- o *New insights*: Viability of Ni–Mo-based catalysts for sustainable hydrogen production technologies.<sup>50</sup>
- Three-dimensional (3D) porous frameworks:
  - o *Key findings*: Investigation of enhanced electrocatalytic performance of 3D porous frameworks for hydrogen production.
  - o *Innovative approach*: Utilization of open 1D channels contributing to high oxygen evolution reaction (OER) activity.
  - o *New insights*: Potential of 3D porous frameworks as novel electrocatalyst architectures.<sup>51</sup>
- Heterostructured catalysts:
  - o *Key findings*: Discussion of advancements in heterostructured catalysts for HER and OER, emphasizing cost-effectiveness and efficiency.
  - o *Innovative approach*: Development of precious-metal-free heterostructures.
  - o *New insights*: Potential for sustainable energy conversion technologies.<sup>52</sup>

From the provided case studies, the emerging trend in the discussed field of nanostructured catalysts for hydrogen production appears to be the development and exploration of alternative, nonnoble metal catalysts. Several case studies highlight the utilization of materials such as nickel, molybdenum, cobalt-based MOFs, and carbon-based materials for catalyzing hydrogen evolution and water-splitting reactions. These materials offer promising alternatives to precious metal catalysts like platinum and iridium, which are expensive and less abundant. Additionally, there is a focus on innovative catalyst design approaches, including heterostructuring, nanoparticle decoration, and utilization of support materials, such as GO and MOFs. These approaches aim to enhance catalytic activity, stability, and efficiency while reducing costs and environmental impact. Overall, the trend in the discussed field involves the development of cost-effective, efficient, and environmentally sustainable catalysts for hydrogen production, with a particular emphasis on nonnoble metal catalysts and innovative catalyst design strategies. This trend reflects the ongoing efforts to address the challenges associated with traditional catalysts and advance the field towards practical applications in sustainable energy technologies. Table 5 offers a comparison of oxides, sulfides, and other materials for hydrogen production, along with specific examples and their respective strengths and weaknesses.

**TABLE 5** Comparing oxides, sulfides, and other materials for hydrogen production, along with specific examples and their advantages and disadvantages.

| <b>Oxides</b>   |  |                  |
|---|--|------------------|
| <b>Examples</b>   | <b>Properties</b>  | <b>Reference</b> |
| Ceria (CeO <sub>2</sub> )   | Used as a catalyst support and in redox cycling processes for solar-driven water splitting.                                      | [53]             |
| LaCoO <sub>3</sub>  | Exhibits excellent oxygen exchange and catalytic activity for thermochemical water splitting. However, it is a rare earth metal. | [54]             |
| Cobalt oxide (Co <sub>3</sub> O <sub>4</sub> )  | Effective in electrochemical water-splitting and photoelectrochemical cells.   | [55]             |
| <b>Advantages</b>   |  |                  |
| <i>Stability:</i> Oxides are often thermally stable and chemically robust, suitable for high-temperature processes.     |  |                  |
| <i>Tunability:</i> Electronic and surface properties of oxides can be engineered for enhanced catalysis.                |  |                  |
| <b>Disadvantages</b>  |  |                  |
| <i>High activation energy:</i> Some oxides require substantial energy input to initiate catalytic reactions.            |  |                  |
| <i>Limited kinetics:</i> Certain oxide catalysts have slower reaction kinetics, affecting overall reaction rates.       |  |                  |
| <i>Coking:</i> Prone to carbon deposition, diminishing catalytic activity.  |  |                  |
| <b>Sulfides</b>   |  |                  |
| <b>Example</b>  | <b>Properties</b>  | <b>Reference</b> |
| MoS <sub>2</sub>  | Used as an efficient catalyst for hydrogen evolution in electrochemical processes.   | [56]             |
| Cobalt sulfide (CoS)  | Exhibits good activity for hydrogen evolution, commonly used in electrocatalysis.  | [57]             |
| Nickel sulfide (NiS)  | Shows promising catalytic activity for hydrogen generation in various conditions.  | [58]             |
| <b>Advantages</b>   |  |                  |
| <i>Catalytic activity:</i> Sulfides often display strong catalytic activity, especially in alkaline conditions.         |  |                  |
| <i>Low cost:</i> Many sulfide materials are economically viable due to abundant raw materials.                          |  |                  |
| <i>Fast kinetics:</i> Sulfides can offer rapid reaction kinetics, leading to efficient hydrogen production.             |  |                  |
| <b>Disadvantages</b>  |  |                  |
| <i>Stability:</i> Some sulfides face challenges in maintaining stability over time.                                     |  |                  |
| <i>Sensitivity:</i> Susceptible to pH and other environmental changes, impacting performance.                           |  |                  |
| <i>Sulfur poisoning:</i> Vulnerable to sulfur adsorption, reducing catalytic effectiveness.                             |  |                  |
| <b>Other materials (nitrides, carbides, etc.)</b>   |  |                  |
| <b>Examples</b>   | <b>Properties</b>  | <b>Reference</b> |
| Molybdenum nitride (Mo <sub>2</sub> N)  | Demonstrates promising hydrogen evolution activity in acidic conditions.   | [59]             |
| Tungsten carbide (WC)   | Used as a catalyst in hydrothermal processes for hydrogen production.  | [60]             |
| Titanium nitride (TiN)  | Under investigation for its electrocatalytic properties in hydrogen evolution.   | [61]             |
| <b>Advantages</b>   |  |                  |
| <i>Diverse properties:</i> Materials like nitrides and carbides offer diverse catalytic behaviors.                      |  |                  |
| <i>Enhanced activity:</i> Some materials exhibit high activity under specific conditions.                               |  |                  |
| <i>Potential multifunctionality:</i> Can catalyze multiple reactions, enhancing versatility.                            |  |                  |
| <b>Disadvantages</b>  |  |                  |
| <i>Synthesis complexity:</i> Production methods for these materials can be complex, affecting scalability.              |  |                  |
| <i>Catalyst poisoning:</i> Susceptible to surface contamination or poisoning, reducing efficiency.                      |  |                  |
| <i>Performance variation:</i> Performance can be sensitive to composition, crystal structure, and synthesis techniques. |  |                  |



The choice between oxides, sulfides, or other materials for hydrogen production depends on factors, such as stability, activity, cost, and operational conditions. Each material category possesses inherent advantages and limitations, necessitating a careful consideration of these attributes tailored to specific applications.

#### 4 | ADVANCED MATERIALS FOR HYDROGEN STORAGE

Hydrogen storage is considered a crucial means of energy storage due to its exceptionally high energy content per unit mass, measuring at an impressive 142 kJ/g, surpassing that of other fuels. However, hydrogen exhibits relatively low density at standard temperatures, resulting in a reduced energy capacity per unit volume. Therefore, the development of advanced, dependable, and efficient storage methods is essential to achieve a substantial energy density.<sup>62,63</sup> Despite the growing research focus on green hydrogen production, with over 10,000 publications in 2021, the study presented in Osman et al.<sup>62</sup> and Baum et al.<sup>63</sup> highlights a consistent number of scholarly publications dedicated to hydrogen storage each year. On average, around 1500 articles were published between 2019 and 2021, as depicted in Figure 18.

Hydrogen storage plays a pivotal role in harnessing and transporting hydrogen as an energy carrier. Diverse techniques have been devised to securely and effectively store hydrogen. Below is an overview of contemporary hydrogen storage methods, as depicted in Figure 19.

Hydrogen can be stored through various methods, each with its own set of advantages and limitations given in Table 6.

- **Compressed gas storage:** This method involves compressing hydrogen gas to high pressures (typically between 350 and 700 bar). While it offers a high energy

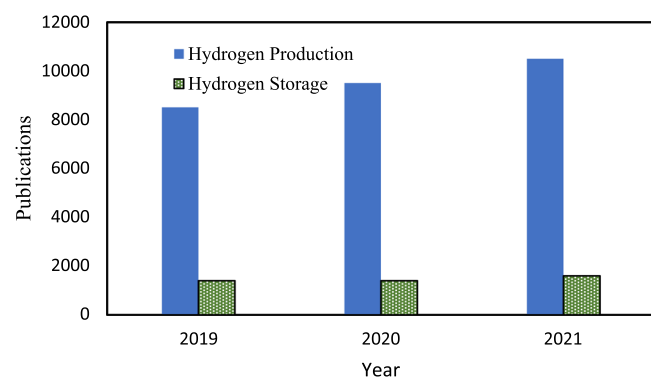


FIGURE 18 Publication trends by year in terms of green hydrogen production and storage research.

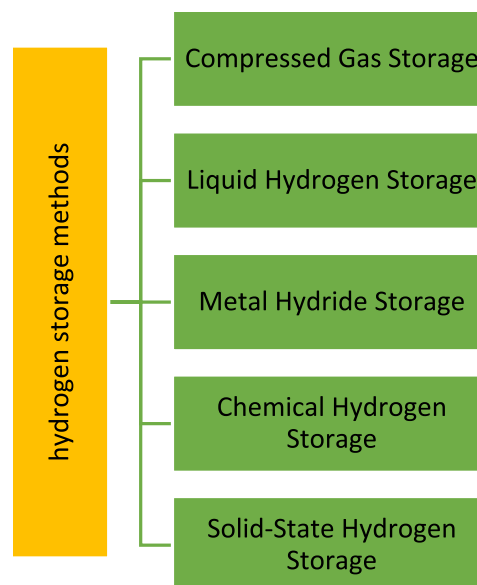


FIGURE 19 The main hydrogen storage methods.

density, it requires robust storage containers, often made of lightweight composite materials, like, carbon fiber-reinforced polymers. This storage approach is better suited for stationary applications and local transportation.<sup>64,65</sup>

- **Liquid hydrogen storage:** Hydrogen can be converted into a liquid state at extremely low temperatures ( $-253^{\circ}\text{C}$ ). Liquid hydrogen storage provides a higher energy density compared with compressed gas storage. However, it demands specialized cryogenic storage tanks with efficient insulation to maintain the low temperatures, presenting logistical challenges.<sup>65,66</sup>
- **MH storage:** MHs, such as complex metal alloys like  $\text{LaNi}_5$  (1.5–2.0 wt% at ambient conditions),  $\text{NaBH}_4$  or  $\text{TiFe}$  (1.0–1.5 wt%), are more commonly used for reversible hydrogen storage due to their ability to absorb and release hydrogen under certain conditions. These MHs operate based on the absorption and desorption of hydrogen into their lattice structure, which allows for safe and efficient hydrogen storage.<sup>64</sup>
- **Chemical hydrogen storage:** Methylcyclohexane (MCH) is a promising chemical for hydrogen storage. It belongs to a group of organic compounds capable of releasing hydrogen reversibly, making them potential carriers for hydrogen-powered applications like fuel cells. MCH undergoes a reversible reaction where it can be hydrogenated to form  $\text{MCH}_2$  and then dehydrogenated to release hydrogen gas, typically catalyzed by suitable catalysts. One of MCH's advantages is its relatively high hydrogen content by weight, around 6.5%, making it more efficient than many other chemical hydrogen storage materials.<sup>65</sup>

TABLE 6 Advantages and disadvantages of hydrogen storage methods.<sup>64–66</sup>

| Hydrogen storage methods     | Advantages  | Disadvantages   |
|------------------------------|---|---|
| Compressed gas storage       | High energy density<br>Mature technology                | The need for heavy-duty storage containers<br>Limited range   |
| Liquid hydrogen storage      | Higher energy density<br>Long-term storage              | Cryogenic storage<br>Boil-off loss                            |
| Metal hydride storage        | Higher storage capacity<br>Safer storage                | Hydrogen release rate<br>Temperature and pressure constraints |
| Chemical hydrogen storage    | High energy density<br>Potential for tailored solutions | Hydrogen release efficiency<br>Reaction conditions            |
| Solid-state hydrogen storage | High storage capacity<br>Customizable features          | Technical challenges<br>Cost and scalability                  |

TABLE 7 Characteristics of hydrogen storage in various solid-state materials.<sup>67–73</sup>

| Advanced material   | Temperature (°C) | Pressure (MPa) | Hydrogen capacity (wt%) |
|---|------------------|----------------|-------------------------|
| Combination of magnesium hydride and titanium trichloride ( $\text{MgH}_2\text{TiCl}_3$ )                           | 278              | 2              | 6.70                    |
| Composite of $\text{MgH}_2$ and multilayer $\text{Ti}_3\text{C}_2$ (ML- $\text{Ti}_3\text{C}_2$ )                   | 142              | –              | 6.56                    |
| Alpha magnesium oxycarboxylate, $\alpha\text{-}[\text{Mg}_3(\text{O}_2\text{CH})_6]$                                | –196             | 2.7            | 1.2                     |
| Composite material involving magnesium hydride, silicon carbide, and nickel, $\text{MgH}_2\text{-(SiC-Ni)}$         | 300              | 3              | 5.10                    |
| Reduced graphene oxide with aluminum oxide and palladium nanoparticles, rGO ( $\text{Al}_2\text{O}_3 + \text{Pd}$ ) | 24.9             | 1              | 0.31                    |
| Composite material comprising magnesium hydride and cobalt, $2\text{MgH}_2\text{-Co}$                               | 300              | 3              | 4.43                    |
| Magnesium Iron hexahydride, $\text{Mg}_2\text{FeH}_6$   | 370–500          | –              | 5.4                     |
| Activated carbon derived from cellulose, AC (cellulose)   | –196             | 2              | 8.1                     |
| Graphene nanosheets with magnesium hydride and nickel phosphide GNs ( $\text{MgH}_2\text{-Ni}_2\text{P}$ )          | 325              | –              | 6.1                     |
| Polystyrene/silicon-modified graphene oxide with palladium nanoparticles, PS/Si-GO(Pd)                              | 25               | –              | 2.1                     |

- *Solid-state hydrogen storage*: In solid-state hydrogen storage, hydrogen is absorbed within a solid matrix, such as porous materials or nanostructures. Materials like MOFs, porous carbons, and other nanostructured substances offer high storage capacity and customizable features. However, technical issues related to kinetics, reversibility, and stability of hydrogen uptake and release must be addressed for broader practical use.<sup>66,67</sup>
- The choice of hydrogen storage method depends on specific application requirements, considering factors like portability, range, and duration of hydrogen use. Ongoing research and development efforts aim to enhance the performance, efficiency, and

commercial viability of hydrogen storage systems, facilitating the widespread adoption of hydrogen as a sustainable and clean energy source. In the context of solid-state hydrogen storage, nanomaterials and nanocomposites show promise, but achieving significant hydrogen performance typically requires extremely low temperatures, presenting a challenge for practical implementation.<sup>67–73</sup>

Information extracted from Table 7 suggests that the loading conditions for materials such as  $\text{MgH}_2\text{TiCl}_3$  and  $\text{MgH}_2\text{-(SiC-Ni)}$  necessitate high temperatures and pressures to effectively load hydrogen into pores. Conversely, materials like  $\alpha\text{-}[\text{Mg}_3(\text{O}_2\text{CH})_6]$  require

lower temperatures and moderate pressures due to their distinct chemical properties.

Regarding storage conditions, it is generally observed that room temperature and moderate pressure are suitable for safely storing hydrogen in porous materials, although specific requirements may vary based on material characteristics and hydrogen adsorption properties. For releasing hydrogen, elevated temperatures or the presence of catalysts are often required to overcome binding energies. This requirement is exemplified in entries like  $\text{MgH}_2\text{TiCl}_3$ , where elevated temperatures are essential for efficient release. In terms of necessary equipment, high-pressure autoclaves and gas storage vessels are essential for safely conducting loading, storage, and release experiments.

Figure 20 visually portrays the correlation between temperature and the hydrogen storage capacity of a variety of advanced materials. The following key findings can be derived from the plot like temperature impact on hydrogen capacity. As anticipated, there exists a notable fluctuation in hydrogen storage capacity as temperatures vary. Moreover, distinct materials display different levels of hydrogen storage capacity at various temperature points. Besides, material diversity is also shown because the scatter plot encompasses a spectrum of materials (indicated on the plot) alongside their respective hydrogen storage capacities. Some materials exhibit elevated hydrogen storage capacities, while others demonstrate lower capacities. Additionally, the significance of temperature emerges as a pivotal factor influencing hydrogen storage capacity. For instance, materials like “Activated carbon derived from cellulose” showcase heightened capacity at extremely low temperatures (approximately  $-196^\circ\text{C}$ ). Conversely, materials like “ $\text{MgH}_2\text{-TiCl}_3$ ” perform optimally at higher temperatures,

around  $278^\circ\text{C}$ . Pressure Variations: It is noteworthy that certain data points lack pressure-related information, suggesting that pressure might not exert a critical influence on hydrogen storage within these materials. This is notably evident in materials such as “ $\text{MgH}_2\text{-ML-Ti}_3\text{C}_2$ ” and “GNs ( $\text{MgH}_2\text{-Ni}_2\text{P}$ ).” Materials of Particular Interest: these materials, “Activated carbon derived from cellulose” defines recognized because of its important high hydrogen storage capacity at extremely low temperatures. Conversely, “Polystyrene/silicon-modified graphene oxide with palladium nanoparticles” (PS/Si-GO(Pd)) performs admirably at a temperature of approximately  $25^\circ\text{C}$ . Finally, the plot emphasizes that a diverse range of materials is employed for hydrogen storage, encompassing MHs like “ $\text{MgH}_2$ ” as well as composite materials featuring graphene and various metals.

In summary, this plot effectively illustrates the broad spectrum of hydrogen storage capacities exhibited by diverse advanced materials across varying temperature conditions. Researchers and engineers involved in hydrogen storage applications, such as fuel cells and energy storage, can leverage this data to make informed decisions regarding material selection based on specific temperature and capacity prerequisites.

#### 4.1 | Introduction to advanced materials for improved hydrogen storage capabilities

Advanced materials are pivotal in advancing hydrogen storage technologies by improving storage capacities, kinetics, and addressing current storage method challenges, as depicted in Figure 21. This section introduces

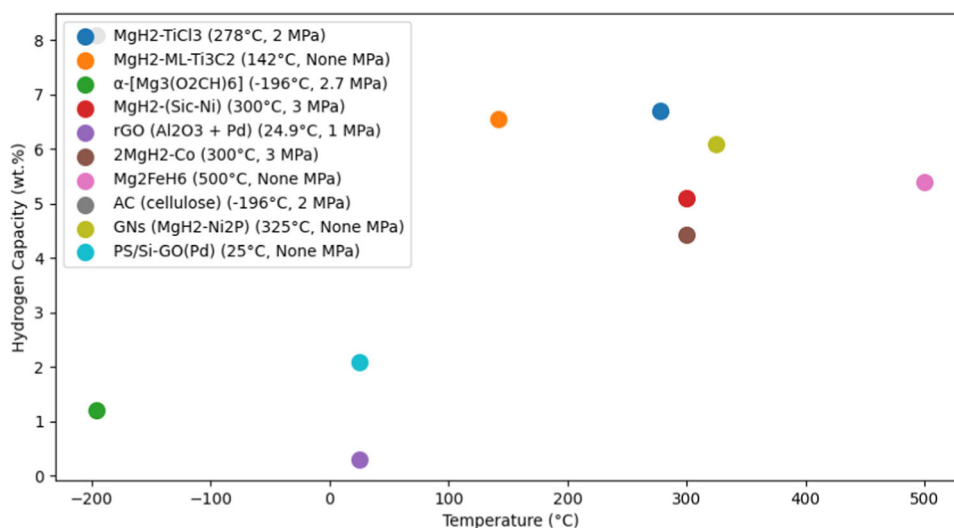


FIGURE 20 Hydrogen capacity versus temperature for advanced materials.

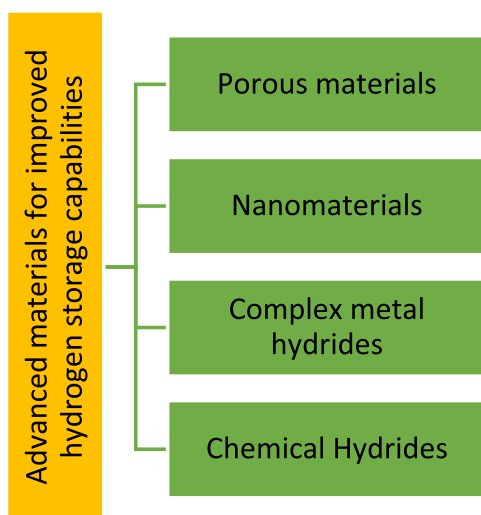


FIGURE 21 Advanced materials for improved hydrogen storage capabilities.

key cutting-edge materials aimed at enhancing hydrogen storage capabilities.

Advanced materials play a crucial role in advancing hydrogen storage technologies by addressing existing challenges and enhancing storage capacities. Here is an overview of key cutting-edge materials aimed at improving hydrogen storage capabilities:

- *Porous materials*: Porous materials such as zeolites, MOFs, and covalent organic frameworks (COFs) are known for their high surface areas and well-defined pore structures, enabling efficient hydrogen adsorption and storage. For example, MOFs, composed of metal ions or clusters and organic ligands, offer adjustable properties and large surface areas, making them highly attractive for hydrogen storage. COFs, on the other hand, feature a porous structure formed by covalent bonds between organic building blocks. Zeolites, crystalline aluminosilicate minerals, have distinct pore architectures capable of absorbing significant amounts of hydrogen.<sup>74</sup>
- *Nanomaterials*: Nanomaterials, characterized by their small size and high surface area-to-volume ratio, exhibit unique properties. Metal nanoparticles like palladium (Pd), platinum (Pt), and nickel (Ni) have shown improved hydrogen storage capabilities due to their high reactivity and catalytic qualities. Carbon-based nanomaterials such as CNTs and graphene can store hydrogen through physisorption or chemisorption. Additionally, other nanomaterials, including metal oxide nanoparticles and nanostructured alloys, hold promise for enhancing hydrogen storage.<sup>75</sup>

- *Complex MHs*: Complex MHs are stable compounds formed by combining metal cations with hydride ions, such as alanates, borohydrides, amides, and imides. These materials enable hydrogen storage through chemical bonding and possess high theoretical hydrogen capacities. However, practical challenges related to kinetics, thermodynamics, and reversibility must be overcome for real-world applications.<sup>76</sup>
- *Chemical hydrides*: Chemical hydrides, like sodium borohydride ( $\text{NaBH}_4$ ) and ammonia borane ( $\text{NH}_3\text{BH}_3$ ), release hydrogen through chemical processes. They offer high hydrogen density and stability, making them suitable for long-term storage and transportation. Overcoming obstacles related to effective hydrogen release mechanisms and material regeneration is crucial for their practical use.<sup>77</sup>
- Table 8 provides an overview of the advantages and disadvantages associated with these advanced materials for energy storage. By improving adsorption/desorption kinetics, increasing storage capacities, and addressing stability and safety concerns, advanced materials hold the potential to enhance hydrogen storage capabilities. Researchers continue to explore and develop new materials and nanostructures while optimizing existing ones to facilitate the practical application of hydrogen as a clean energy carrier.

In addition to physical storage methods, chemical hydrogen storage mechanisms merit recognition for their potential in complementing overall hydrogen storage strategies. Prominent examples include<sup>78–80</sup>:

- *Ammonia ( $\text{NH}_3$ )*: Ammonia is a well-established chemical hydrogen carrier, with a high hydrogen content by weight. It can be produced through the Haber–Bosch process and subsequently decomposed back into hydrogen and nitrogen through catalytic reactions, such as the Haber–Bosch reverse reaction.
- *Methanol ( $\text{CH}_3\text{OH}$ )*: Methanol is another viable chemical hydrogen carrier that can be synthesized from hydrogen and carbon dioxide or carbon monoxide. Catalytic processes, such as steam reforming or partial oxidation, can produce methanol from these feedstocks. Methanol can then release hydrogen through catalytic reforming or steam reforming reactions.
- *Hydrocarbons from Fischer–Tropsch synthesis*: Hydrocarbons generated through the Fischer–Tropsch synthesis, such as liquid fuels and waxes, also offer potential as chemical hydrogen carriers. These hydrocarbons can store hydrogen in chemical bonds and release it through catalytic processes, including steam reforming or thermal cracking.

**TABLE 8** Advantages and disadvantages of advanced materials used for hydrogen energy storage.<sup>73–77</sup>

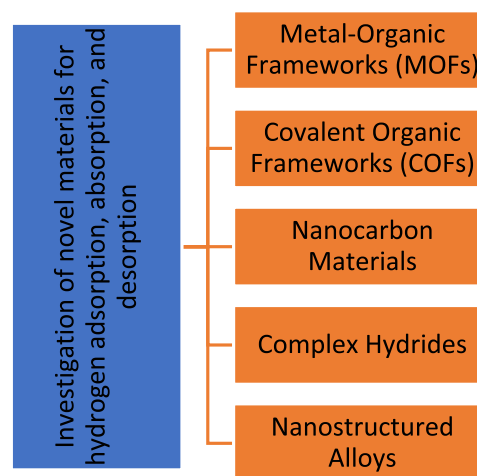
| Advanced materials     | Advantages  | Disadvantages  |
|------------------------|---|--|
| Porous materials       | High surface area<br>Tunable pore structures<br>Selective adsorption                        | Kinetic limitations<br>Stability concerns                        |
| Nanomaterials          | High surface area-to-volume ratio<br>Improved reactivity<br>Physisorption and chemisorption | Agglomeration<br>Production costs                                |
| Complex metal hydrides | Reversible hydrogen storage<br>High theoretical hydrogen capacity                           | Kinetic and thermodynamic barriers<br>Catalysis requirements     |
| Chemical hydrides      | High hydrogen density<br>Stability  | Hydrogen release mechanisms<br>Regeneration of storage materials |

These chemical compounds serve as carriers for hydrogen, undergoing reversible reactions catalyzed by specific catalysts to facilitate hydrogen release when needed. By acknowledging these chemical storage mechanisms and their reliance on catalysis, a more comprehensive perspective on the diverse approaches to hydrogen storage.

## 4.2 | Investigation of novel materials for hydrogen adsorption, absorption, and desorption

An essential research focus in the field of hydrogen storage revolves around the development of novel materials capable of effectively adsorbing, absorbing, and desorbing hydrogen. Researchers are driven to enhance the efficiency, storage capacity, and kinetics of hydrogen storage systems, prompting their exploration of innovative materials and their unique attributes. Figure 22 provides an overview of the ongoing investigation into these new materials and their potential for hydrogen adsorption, absorption, and desorption.

- **MOFs:** MOFs such as ZIF-8 (Zeolitic Imidazolate Framework-8) and MOF-5 (also known as IRMOF-1) have been extensively studied for hydrogen storage. These materials exhibit high surface areas and tunable pore sizes, making them promising candidates for efficient hydrogen adsorption and storage.<sup>81</sup>
- **COFs:** Examples of COFs investigated for hydrogen storage include COF-102 and COF-105, which have shown promising hydrogen adsorption capacities. COFs offer precise control over pore size and structure,


**FIGURE 22** Novel materials for hydrogen adsorption, absorption, and desorption.

allowing for tailored designs to optimize hydrogen storage performance.<sup>82</sup>

- **Nanocarbon materials:** CNTs have attracted significant attention for hydrogen storage applications. Functionalized CNTs, such as single-walled carbon nanotubes and multiwalled carbon nanotubes (MWCNTs), have demonstrated enhanced hydrogen adsorption capacities. Graphene-based materials, including GO and reduced GO, also exhibit potential for hydrogen storage due to their high surface area and structural flexibility.<sup>83</sup>
- **Complex hydrides:** Examples of complex hydrides explored for hydrogen storage include sodium borohydride ( $\text{NaBH}_4$ ) and ammonia borane ( $\text{NH}_3\text{BH}_3$ ). These materials offer high hydrogen storage capacities by forming stable complexes with hydrogen. Research

focuses on improving their hydrogen release kinetics and reversibility through compositional and structural modifications.<sup>84</sup>

- **Nanostructured alloys:** Nanostructured alloys such as magnesium-based alloys (e.g., MgH<sub>2</sub>) and titanium-based alloys (e.g., TiFe) have been investigated for hydrogen storage. These materials exhibit enhanced hydrogen absorption and desorption kinetics compared with their bulk counterparts. Alloy morphologies, compositions, and nanostructuring techniques play crucial roles in optimizing hydrogen storage performance.<sup>85</sup>

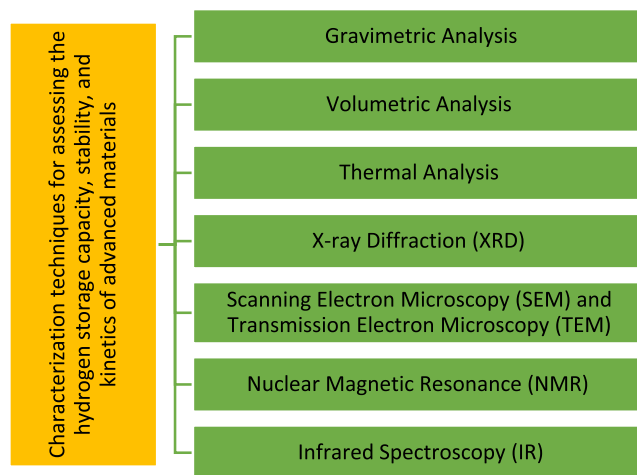
Table 9 provides an overview of the advantages and disadvantages associated with advanced materials for hydrogen adsorption, absorption, and desorption. These investigations rely on a combination of computational modeling, synthesis methodologies, and experimental characterization to assess the performance of new materials for hydrogen storage. A deep understanding of the fundamental principles and properties of these materials is crucial for developing hydrogen storage technology, thereby enabling hydrogen to serve as a widely adopted, sustainable, and clean energy source.

### 4.3 | Characterization techniques for assessing the hydrogen storage capacity, stability, and kinetics of advanced materials

The stability, kinetics, and hydrogen storage capability of advanced materials utilized in hydrogen storage systems are all evaluated using characterization approaches. These methods help in the development

and improvement of hydrogen storage technologies by offering insightful information about the functionality and characteristics of materials. Here are a few of the characterization methods that are frequently utilized, as shown in Figure 23.

- **Gravimetric analysis:** Gravimetric analysis quantifies the change in weight that occurs when a substance absorbs or releases hydrogen. This method involves precise measurements of the material's mass before and after exposure to hydrogen. Gravimetric analysis, in conjunction with parameters like equilibrium pressure and enthalpy, allows for the determination of hydrogen storage capacity.<sup>86</sup>
- **Volumetric analysis:** Volumetric analysis measures the volume of gas that undergoes changes as hydrogen is



**FIGURE 23** Characterization techniques for assessing the hydrogen storage capacity, stability and kinetics of advanced materials.

**TABLE 9** An overview of the advantages and disadvantages associated with advanced materials.

| Advanced materials          | Advantages                           | Challenges                                 |
|-----------------------------|--------------------------------------|--|
| Metal-organic frameworks    | Tunable structure                    | Kinetics                                   |
|                             | High surface area                    | Stability                                  |
|                             | Versatile applications               |  |
| Covalent organic frameworks | Precise engineering                  | Hydrogen adsorption capacity               |
|                             | Chemical stability                   | Scale-up                                   |
| Nanocarbon materials        | Extensive research base              | Kinetics and reversibility                 |
|                             | Enhanced hydrogen-carbon interaction | Cost and scalability                       |
| Complex hydrides            | Reversible hydrogen storage          | Kinetics and thermodynamics                |
|                             | High theoretical hydrogen capacity   | Catalysis and lower operating temperatures |
| Nanostructured alloys       | Improved kinetics                    | Stability and durability                   |
|                             | Tunable composition                  | Manufacturing complexity                   |

absorbed or desorbed. It entails monitoring pressure variations as hydrogen is introduced into or released from a sealed system. Volumetric analysis is employed to calculate parameters like adsorption isotherms and desorption kinetics, providing insights into hydrogen storage capacity.<sup>87</sup>

- **Thermal analysis:** Thermal analysis techniques such as differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) are employed to assess materials' thermal stability and characteristics. DSC records heat flow as a function of temperature, yielding data on reaction kinetics, phase transitions, and decomposition. TGA tracks the weight variation of a substance with temperature, facilitating evaluations of stability, desorption kinetics, and decomposition temperatures.<sup>88</sup>
- **XRD:** XRD is used to investigate materials' crystal structure and phase composition. It can detect phase changes or the emergence of new phases during hydrogen absorption or desorption, offering insights into atomic arrangements within a material. XRD is particularly effective for studying structural alterations in complex hydrides and MOFs.<sup>89</sup>
- **SEM and TEM:** SEM and TEM techniques are employed to examine materials' morphology, microstructure, and surface properties. While TEM enables nanoscale investigations of internal features, SEM provides high-resolution images of material surfaces. These methods are valuable for evaluating catalyst

distribution, pore architectures, and morphological changes induced by hydrogen interactions.<sup>90</sup>

- **Nuclear magnetic resonance (NMR):** NMR spectroscopy is utilized to study hydrogen adsorption, transport, and interactions with materials. It provides insights into hydrogen distribution, chemical modifications, and material mobility. Various NMR techniques, including solid-state NMR and pulsed-field gradient NMR, are applied for the analysis of hydrogen storage in porous materials and complex hydrides.<sup>91</sup>
- **Infrared spectroscopy (IR):** IR spectroscopy is employed to investigate hydrogen bonds and surface interactions. It furnishes information on chemical species, functional groups, and hydrogen content within materials. IR methods, such as FTIR spectroscopy, are instrumental in the analysis of hydrogen adsorption and desorption processes.<sup>92</sup>
- Table 10 summarizes the advantages and disadvantages of characterization techniques used for hydrogen storage materials. These methods, in combination with others like Raman spectroscopy, electron microscopy, and surface area analysis, facilitate comprehensive evaluations of advanced materials' hydrogen storage capacity, stability, and kinetics. Researchers improved the understanding of material characteristics and performance, achieved through the amalgamation of multiple methodologies, contributing to the design and development of efficient and dependable hydrogen storage systems.

**TABLE 10** Advantages and disadvantages of characterization techniques used for hydrogen storage materials.<sup>84–89</sup>

| Characterization techniques for hydrogen storage materials        | Advantages                              | Challenges                           |
|---|---|--------------------------------------|
| Gravimetric analysis  | Accurate quantification                 | Time-consuming                       |
|   | Equilibrium pressure and enthalpy       | Hydrogen loss                        |
| Volumetric analysis   | Direct measurement of gas volume        | Equilibrium limitation               |
|   | Relatively simple experimental setup    | Adsorption/desorption hysteresis     |
| Thermal analysis (DSC and TGA)                                    | Thermal stability evaluation            | Limited to thermodynamic information |
|   | Kinetics and phase changes              | Lack of structural details           |
| X-ray diffraction   | Crystal structure analysis              | Limitations for amorphous materials  |
|   | Study of phase changes                  |                                      |
| Scanning electron microscopy and transmission electron microscopy | Morphology and microstructure analysis  | Sample preparation                   |
|   | Visualization at nanoscale              | Limited quantitative information     |
| Nuclear magnetic resonance (NMR)                                  | Hydrogen interaction analysis           | Instrumentation and expertise        |
|   | Different NMR techniques                |                                      |
| Infrared spectroscopy   | Surface interactions                    | Surface sensitivity                  |
|   | FTIR for hydrogen adsorption/desorption |                                      |

Abbreviations: DSC, differential scanning calorimetry; FTIR, Fourier transform infrared; TGA, thermogravimetric analysis.

#### 4.4 | Case studies showcasing the potential of advanced materials in achieving efficient hydrogen storage

Several case studies have demonstrated, as shown in Figure 24, the effectiveness of advanced materials in enhancing hydrogen storage efficiency.

In Figure 24, emerging Trends in advanced Materials for Hydrogen Storage based on the case studies are summarized as follows:

- MOFs:
  - *Key findings*: Thorough characterization and high thermal stability of MOF-76 (Nd). Investigation of hydrogen storage properties and humidity-sensing capabilities.
  - *Innovative approach*: Synthesis of MOF-76 (Nd) and evaluation of its structural features and performance.
  - *New insight*: Insights into material's structural properties, thermal stability, and potential applications in hydrogen storage and humidity sensing.<sup>93</sup>
- Carbon nanomaterials:
  - *Key findings*: Development of ZnO-MWCNTs with enhanced hydrogen adsorption capacity due to ZnO nanoparticle spillover effect.
  - *Innovative approach*: Doping ZnO nanoparticles onto MWCNTs to create ZnO-MWCNTs.
  - *New insight*: Substantial advancements in hydrogen adsorption capabilities through nanoparticle doping.<sup>94</sup>
- Complex hydrides:
  - *Key findings*: Exploration of complex hydrides' adaptability and tunable properties for hydrogen storage, ion conduction, and catalysis.

- *Innovative approach*: Highlighting potential applications of complex hydrides in renewable energy technologies.
- *New insight*: Tunable physical and chemical properties of complex hydrides for various clean energy applications.<sup>95</sup>
- Porous materials:
  - *Key findings*: Exploration of solid-state porous materials as safe alternatives to high-pressure compression for hydrogen storage.
  - *Innovative approach*: Review of developments in improved porous materials and their composites.
  - *New insight*: Safer and more effective alternatives to high-pressure compression techniques through the use of solid-state porous materials.<sup>96</sup>
- Nano catalysts:
  - *Key findings*: Analysis of nanocatalysts and nanostructuring methods for improved magnesium hydride (MgH<sub>2</sub>) performance.
  - *Innovative approach*: Investigating nanocatalysts and nanostructuring techniques to improve MgH<sub>2</sub> hydrogen desorption.
  - *New insight*: Addressing kinetic and thermodynamic obstacles in using MgH<sub>2</sub> for hydrogen storage through nanocatalysts and nanostructuring.<sup>96</sup>

The new trends observed in the discussed field: Researchers are exploring MOFs for high-capacity hydrogen storage, characterizing their structural properties, thermal stability, and hydrogen adsorption capabilities, with potential applications in renewable energy technologies. Advancements in carbon nanomaterials involve doping with metal oxides to enhance hydrogen adsorption capacities, leveraging the “spillover effect” of metal oxide nanoparticles on CNTs for substantial improvements. Complex hydrides with tunable properties are being investigated for hydrogen storage, ion conduction, and catalysis, emphasizing their adaptability and potential applications in clean energy technologies.

Porous materials, particularly solid-state porous materials, are being explored as safe alternatives to high-pressure compression for hydrogen storage, with developments in improved porous materials and composites showing potential to revolutionize hydrogen storage methods. Nanocatalysts and nanostructuring techniques are being analyzed to improve the performance of magnesium hydride (MgH<sub>2</sub>) for hydrogen desorption, addressing kinetic and thermodynamic obstacles in hydrogen storage through innovative approaches.

Table 11 offers a comparison of oxides, sulfides, and other materials for hydrogen storage, complete with specific instances and their respective advantages and disadvantages. The decision regarding oxide, sulfide, or

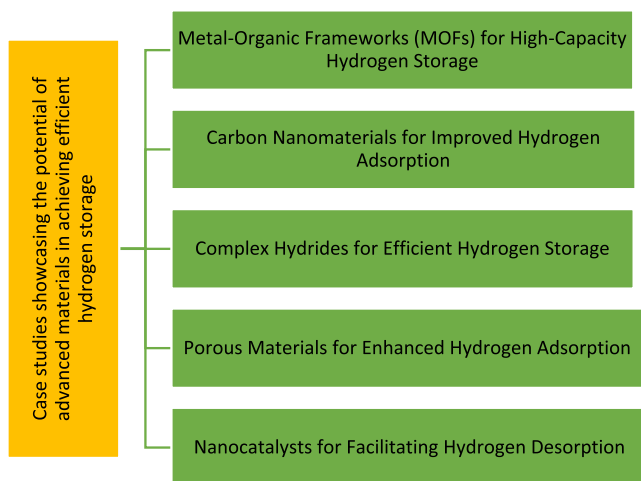


FIGURE 24 Case studies showcasing the potential of advanced materials.



**TABLE 11** Comparing oxides, sulfides, and other materials for hydrogen storage, along with specific examples and their advantages and disadvantages.

| <b>Oxides</b>  |  |                  |
|--|--|------------------|
| <b>Examples</b>  | <b>Properties</b>  | <b>Reference</b> |
| MgH <sub>2</sub> /MgO  | Combination of metal hydrides with oxides for improved reversible hydrogen storage.  | [68]             |
| Iron oxide (Fe <sub>2</sub> O <sub>3</sub> )   | Utilized in redox reactions for thermochemical hydrogen storage.   | [97]             |
| Barium titanium oxide (BaTiO <sub>3</sub> )  | Explored for its ability to absorb and release hydrogen through solid-state reactions, making it a candidate for solid oxide hydrogen storage materials. | [98]             |
| <b>Advantages</b>  |  |                  |
| <i>Thermally stable:</i> Oxides are often stable at high temperatures, suitable for certain storage methods.             |  |                  |
| <i>Compatibility:</i> Many oxide materials are chemically compatible with hydrogen, allowing reversible storage.         |  |                  |
| <i>Potential redox reactions:</i> Oxides can participate in redox reactions for reversible hydrogen storage.             |  |                  |
| <b>Disadvantages</b>   |  |                  |
| <i>Low hydrogen capacity:</i> Oxides might have limited hydrogen storage capacity compared with other materials.         |  |                  |
| <i>High operating temperatures:</i> Some oxide-based storage systems require elevated temperatures for hydrogen release. |  |                  |
| <i>Slow kinetics:</i> Reaction kinetics can be slower, affecting storage and release rates.                              |  |                  |
| <b>Sulfides</b>  |  |                  |
| <b>Example</b>   | <b>Properties</b>  | <b>Reference</b> |
| NaBH <sub>4</sub> , LiBH <sub>4</sub>  | Investigated their ability to store and release hydrogen through reversible chemical reactions.  | [99]             |
| Thiophene-based  | Organic sulfide compounds explored for hydrogen storage.   | [100]            |
| Hydrides-sulfides  | Combination of metal hydrides and sulfides for improved hydrogen storage properties.   | [101]            |
| <b>Advantages</b>  |  |                  |
| <i>Chemical reactivity:</i> Sulfides can undergo reversible reactions for hydrogen storage.                              |  |                  |
| <i>Hydrogen capacity:</i> Some sulfides exhibit relatively higher hydrogen storage capacities.                           |  |                  |
| <i>Potential low temperatures:</i> Certain sulfide-based systems can operate at moderate temperatures.                   |  |                  |
| <b>Disadvantages</b>   |  |                  |
| <i>Stability:</i> Some sulfides may suffer from chemical degradation or instability over repeated cycles.                |  |                  |
| <i>Sensitivity:</i> Sensitivity to moisture or air might impact storage reliability.                                     |  |                  |
| <i>Reaction kinetics:</i> Reaction rates can vary, influencing the efficiency of storage and release.                    |  |                  |
| <b>Other materials (nitrides, carbides, etc.)</b>  |  |                  |
| <b>Examples</b>  | <b>Properties</b>  | <b>Reference</b> |
| NaAlH <sub>4</sub>   | Well-studied hydrogen storage materials with high capacity.  | [102]            |
| NH <sub>3</sub> BH <sub>3</sub>  | A chemical hydride with good hydrogen capacity.  | [103]            |
| MOFs   | Porous materials explored for physisorption-based hydrogen storage.  | [104]            |
| <b>Advantages</b>  |  |                  |
| <i>High capacity:</i> Some materials, like, metal hydrides, offer substantial hydrogen storage capacities.               |  |                  |
| <i>Reversible reactions:</i> Many materials exhibit reversible storage and release of hydrogen.                          |  |                  |
| <i>Variable operating conditions:</i> Different materials can work under diverse temperature and pressure ranges.        |  |                  |
| <b>Disadvantages</b>   |  |                  |
| <i>Thermodynamics:</i> Certain materials require high temperatures or pressures for hydrogen release.                    |  |                  |
| <i>Desorption kinetics:</i> Kinetics of desorption can be slow for some storage materials.                               |  |                  |
| <i>Cycling stability:</i> Cycling between storage and release might impact materials' stability over time.               |  |                  |

alternative materials for hydrogen storage hinges on factors like capacity, thermodynamics, kinetics, and operating conditions. Each material category boasts its own strengths and limitations, and the selection should be tailored to the specific demands of the intended application.

## 5 | INTEGRATED SYSTEMS FOR EFFICIENT HYDROGEN ENERGY

### 5.1 | Integration of nanostructured catalysts and advanced materials in hydrogen production and storage systems

The integration of advanced materials with nanostructured catalysts, as depicted in Figure 25, is critical for enhancing hydrogen production and storage systems. Researchers aim to improve hydrogen production and storage capabilities by leveraging nanostructured catalysts alongside advanced materials. Recent research emphasizes various aspects of hydrogen production, storage, and utilization technologies: Nanomaterials such as metallic nanoparticles, MOFs, CNTs, and graphene play a transformative role in advancing hydrogen energy. They address challenges in conventional storage methods and boost hydrogen production efficiency.<sup>105,106</sup>

Different hydrogen production processes, including thermochemical and electrolytic methods, are explored. Methods for hydrogen purification, such as filtration through palladium alloy membranes and membrane catalysis, enable efficient production and purification. Moreover, conventional and novel hydrogen storage and transportation methods are discussed.<sup>63</sup> Recent advancements in catalyst materials facilitating green hydrogen

production, alongside chemical and physical storage systems and materials used in fuel cells, are reviewed. This provides an overview of the current state of development in hydrogen technologies.<sup>107</sup> Advances in porosity tunability in nanostructures for hydrogen generation and storage are highlighted. Strategies for porosity engineering in nanostructured materials improve hydrogen production efficiency and storage capacity.<sup>108</sup> Biomass hydrogen production technology is an emerging field. The review critically evaluates nanotechnology's role in green bio-H<sub>2</sub> production, summarizing the merits and limitations of different approaches. It emphasizes the crucial role of nanostructured materials, especially nanocatalysts, in enhancing biomass hydrogen production.<sup>109</sup>

Researchers are actively combining nanostructured catalysts and advanced materials to advance hydrogen production and storage systems. This integration leverages the unique properties of nanostructured catalysts and advanced materials to address challenges in hydrogen energy applications. Here are the key points:

- *Nanostructured catalysts for hydrogen production:* Nanostructured catalysts like metal nanoparticles and MOFs provide high surface areas and active sites, enabling efficient hydrogen generation. They enhance reaction kinetics and selectivity, particularly in processes of hydrocarbons, resulting in increased hydrogen yields. These catalysts can be integrated into hydrogen production systems to accelerate reactions, reduce energy consumption, and improve overall efficiency.<sup>110</sup>
- *Advanced materials for hydrogen storage:* Advanced materials, including porous materials, nanomaterials, and complex MHs, offer enhanced hydrogen storage capabilities, kinetics, and stability. Incorporating these advanced materials into hydrogen storage systems can lead to higher gravimetric and volumetric storage capacities. For instance, using materials like MOFs or carbon-based substances as adsorbents in storage tanks can increase hydrogen absorption and release rates, enhancing storage performance.<sup>111</sup>
- *Hybrid systems for integrated hydrogen production and storage:* Researchers are exploring hybrid systems that combine hydrogen production and storage functionalities. By integrating nanostructured catalysts and advanced materials, these systems can achieve higher hydrogen storage capacity and improved efficiency in hydrogen production methods, such as photoelectrochemical cells or electrolyzers. Integrated systems offer on-site solutions for hydrogen production and storage, making hydrogen more practical for various applications.<sup>112</sup>

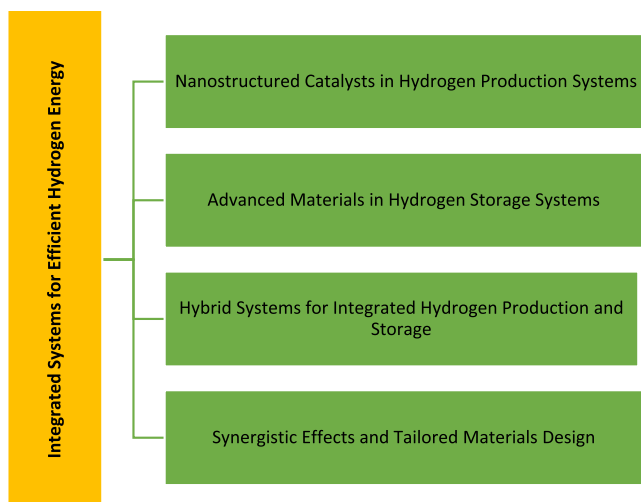


FIGURE 25 Integrated systems for efficient hydrogen energy.

- **Synergistic effects and tailored materials design:** The combination of nanostructured catalytic activity and advanced material properties can result in synergistic effects, leading to better hydrogen production and storage performance. Researchers can design catalysts and materials specifically to maximize their interactions, resulting in desired functionality, such as improved reaction kinetics, increased storage capacity, or enhanced durability.<sup>113</sup>
- In summary, the integration of nanostructured catalysts and advanced materials is a promising avenue for addressing challenges in hydrogen energy applications. This synergy opens up possibilities for innovative solutions, including photocatalysis, electrocatalysis, and hybrid systems, ultimately advancing the use of hydrogen as a sustainable and clean fuel source.

## 5.2 | Design and optimization of efficient hydrogen energy systems for various applications

The successful adoption and exploitation of hydrogen as a clean and sustainable energy source depend on the design and optimization of efficient hydrogen energy systems. These systems are adaptable enough to accommodate the needs of a variety of applications, including power generation, transportation, and more. Figure 26 illustrates important factors for constructing and enhancing effective hydrogen energy systems.

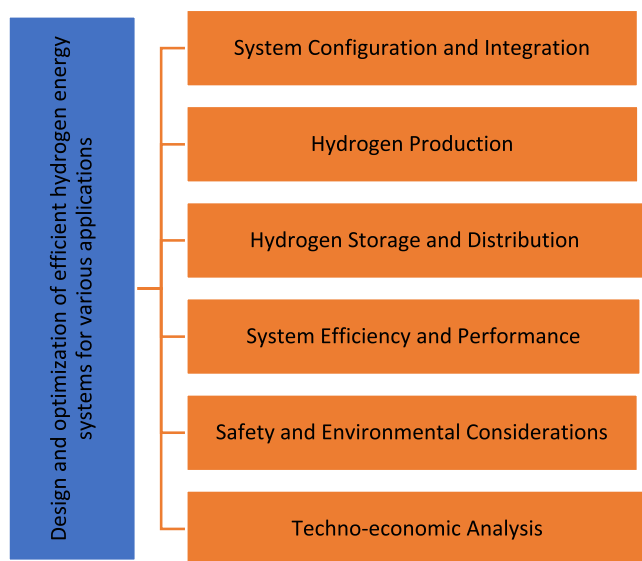


FIGURE 26 Important factors for designing and optimizing efficient hydrogen energy systems.

- **System configuration and integration:** Successful hydrogen energy systems require seamless integration of components, such as hydrogen generation, storage, delivery, and consumption. Careful planning is essential, including the selection of appropriate technologies, equipment sizing, and the establishment of an integrated infrastructure to ensure efficient hydrogen utilization.<sup>114</sup>
- **Hydrogen production:** When choosing hydrogen generation techniques like steam reforming, electrolysis, and biomass conversion, factors such as energy efficiency, cost-effectiveness, and environmental impact must be taken into account. Additionally, exploring advanced technologies such as photoelectrochemical cells, photocatalysis, and biological processes can contribute to sustainable and renewable hydrogen production.<sup>115</sup>
- **Hydrogen storage and distribution:** Optimal storage options, including compressed gas, liquid hydrogen, and advanced materials-based storage, should be selected based on considerations, like, storage capacity, security, and transportation requirements. Efficient distribution networks, pipelines, or hydrogen filling stations must be designed and optimized to ensure reliable and affordable hydrogen delivery to end-users.<sup>116</sup>
- **System efficiency and performance:** Enhancing overall energy efficiency is a primary goal in design optimization. This involves improving system performance, reducing energy losses during conversion, storage, and distribution, and enhancing component efficiency. Advanced control techniques and intelligent energy management systems can further increase system efficiency, especially in scenarios with varying load and demand.<sup>117</sup>
- **Safety and environmental considerations:** Safety measures are crucial in the design and operation of hydrogen systems to ensure safe handling, storage, and use of hydrogen. Additionally, incorporating renewable energy sources for hydrogen generation and adopting sustainable practices throughout the system's lifecycle can reduce greenhouse gas emissions and minimize the carbon footprint of the hydrogen energy system.<sup>118</sup>
- **Technoeconomic analysis:** Conducting a thorough technoeconomic analysis is essential to assess the practicality and economic viability of the proposed hydrogen energy system. Factors to consider include potential revenue from hydrogen use in different applications, capital expenditures, operational costs, and hydrogen production expenses.<sup>119</sup>
- In conclusion, the development of efficient and long-lasting hydrogen energy systems for various

applications, such as energy storage, hydrogen fuel cell vehicles, and power generation, relies on the continuous evolution of technology, materials, and system integration techniques. Careful consideration of these key aspects is essential to create effective hydrogen-based energy solutions that meet diverse energy needs.

### 5.3 | Technoeconomic analysis of integrated systems, considering factors, such as energy efficiency, scalability, and cost-effectiveness

Technoeconomic analysis is essential for determining if integrated hydrogen energy systems are feasible and economically viable. To assess the system's economic potential and competitiveness, several criteria, including energy efficiency, scalability, and cost-effectiveness, must be evaluated. The following are crucial factors to consider while conducting a technoeconomic study of integrated hydrogen energy systems, as shown in Figure 27:

- *Energy efficiency*: An essential factor in evaluating integrated systems is energy efficiency. At each stage, from hydrogen production to consumption, assessing energy losses is crucial. Employing state-of-the-art technology, efficient system design, and innovative energy management techniques can significantly enhance overall efficiency.<sup>120</sup>

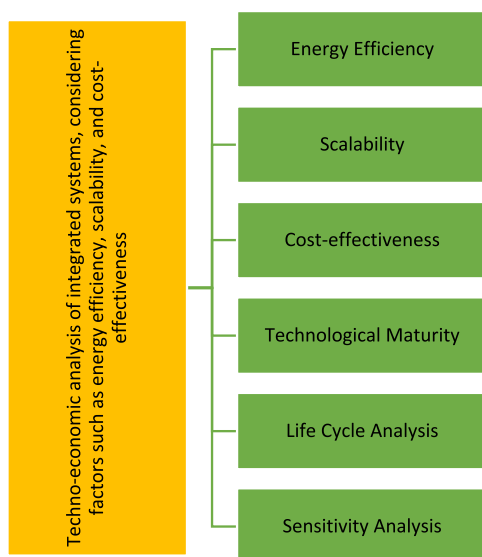


FIGURE 27 Crucial factors in the technoeconomic analysis of integrated hydrogen energy systems.

- *Scalability*: Successful deployment and commercialization of integrated systems rely on scalability. It involves considering the system's potential for expansion to meet future energy demands. Evaluation should encompass infrastructure requirements, production and storage capacities, as well as distribution networks.<sup>121</sup>
- *Cost-effectiveness*: Part of the cost-effectiveness assessment involves a comprehensive analysis of the integrated hydrogen energy system's overall expenses. This includes infrastructure, operational, maintenance costs, and raw materials. The analysis should also explore potential revenue streams from hydrogen's applications, such as power generation and transportation. It should consider strategies like economies of scale, technological advancements, and government incentives.<sup>122</sup>
- *Technological maturity*: The level of technological readiness is a critical consideration. Evaluating factors such as reliability, performance, and the availability of necessary infrastructure and support services is essential. Employing established technologies can improve cost projections and reduce the risks associated with technology development and utilization.<sup>123</sup>
- *Life cycle analysis*: Life cycle analysis assesses the environmental impact of the integrated system throughout its entire life cycle, from raw material extraction to disposal. Factors like greenhouse gas emissions, water usage, and waste generation should be taken into account. Comparing the environmental performance of the integrated system with conventional energy systems can identify areas for environmental improvements and development.<sup>124</sup>
- *Sensitivity analysis*: Sensitivity analysis plays a significant role in determining the technoeconomic feasibility of the integrated system. It identifies critical characteristics and variables that influence the system's robustness. By adjusting these parameters within realistic limits, the analysis can evaluate potential risks and uncertainties.<sup>125</sup>
- In summary, technoeconomic analysis offers valuable insights into the economic viability and potential of integrated hydrogen energy systems. It assists stakeholders in making informed decisions, optimizing system design, and identifying areas for enhancement. Factors like energy efficiency, scalability, and cost-effectiveness are crucial in the development of economically viable and sustainable hydrogen energy solutions for diverse applications.

## 5.4 | Evaluation of safety considerations and mitigation strategies for hydrogen production, storage, and utilization

Systems for the generation, storage, and use of hydrogen must be designed, operated, and implemented with safety as a top priority. To ensure the safe handling, storage, and use of hydrogen, safety considerations must be assessed, and mitigating measures must be put in place. Here are important factors to consider while assessing safety and placing the mitigation techniques, shown in Figure 28, into action.

- **Risk assessment:** A comprehensive risk assessment is imperative to identify potential hazards associated with hydrogen production, storage, and utilization. This evaluation should encompass various scenarios, including system malfunctions, leaks, ignition sources, and human errors. The assessment aims to gauge the likelihood and consequences of potential accidents or incidents.<sup>126</sup>
- **Safety codes and standards:** Adhering to established safety guidelines, rules, and regulations is paramount when dealing with hydrogen applications. International safety standards, such as those outlined in the International Fire Code and National Fire Protection Association codes, provide essential recommendations for hydrogen safety across diverse applications. Complying with these safety criteria ensures the safe planning, construction, and operation of systems.<sup>127</sup>
- **Design considerations:** Safety precautions should be integrated into the design process, encompassing



FIGURE 28 Important factors evaluating safety and implementing mitigation strategies.

aspects like system layout, material selection, and component requirements. Mitigating potential risks can be achieved through features, such as adequate ventilation, leak detection systems, and appropriate pressure relief mechanisms. Employing safety features like pressure sensors, flame arrestors, and automated shut-off valves further enhances safety.<sup>128</sup>

- **Training and education:** Personnel responsible for operating and maintaining hydrogen systems should undergo comprehensive training and instruction. It is essential that operators possess sound knowledge of safe hydrogen handling, storage, and emergency response protocols. Fostering a safety-oriented culture throughout all concerned parties is critical to raising awareness and ensuring adherence to safety standards.<sup>129</sup>
- **Leak detection and mitigation:** Prompt identification and localization of hydrogen leaks are crucial, necessitating the implementation of reliable leak detection systems. Utilizing tools like hydrogen sensors, gas detectors, and thermal imaging cameras facilitates the detection of leaks and potential hazards. Effective mitigation strategies, including isolation devices, emergency shutdown procedures, and proper ventilation systems, should be in place to minimize the impact of leaks.<sup>130</sup>
- **Fire and explosion mitigation:** Employing safety measures to mitigate the risk of fires and explosions is paramount. This includes the use of fire suppression systems, explosion-proof equipment, and flame arrestors. Technologies should ensure adequate ventilation to prevent hydrogen buildup in confined spaces. Additionally, developing emergency response plans and conducting drills prepares personnel to respond effectively in the event of a fire or explosion.<sup>131</sup>
- **Public awareness and communication:** Promoting public understanding and dispelling misconceptions regarding hydrogen safety is crucial. Educating both the public and relevant stakeholders is essential to achieve this. Effective communication channels should be established to disseminate safety information and updates related to hydrogen production, storage, and utilization systems. Collaboration and transparency with regulatory bodies, emergency response organizations, and the local community are key to addressing safety concerns adequately.<sup>132</sup>
- Sustaining the safety of hydrogen production, storage, and utilization systems necessitates continuous monitoring, routine maintenance, and periodic safety audits. By examining safety considerations and implementing appropriate mitigation strategies, the associated risks of hydrogen can be effectively managed, facilitating the widespread

adoption of hydrogen as a clean and sustainable energy source.

### 5.5 | Future prospects and challenges in the implementation of efficient hydrogen energy systems

Energy issues can be solved and a transition to a cleaner, more sustainable energy future can be facilitated using effective hydrogen energy systems. However, as shown in Figure 29, several opportunities and difficulties must be taken into account for these systems to be successfully deployed and widely used.

- *Scaling up hydrogen production: Future prospects:* Advances in renewable energy technologies, such as solar and wind, can pave the way for large-scale green hydrogen generation via electrolysis, reducing reliance on fossil fuels. *Challenges:* Expanding hydrogen production on a grand scale necessitates substantial infrastructure investments, including renewable energy capacity, electrolyzers, and hydrogen storage and distribution networks. Addressing these infrastructure challenges is pivotal before widespread adoption of hydrogen energy systems can occur.<sup>133</sup>
- *Technological developments in distribution and storage: Future Prospects:* Enhanced hydrogen storage technologies, like solid-state storage systems and improved materials, hold promise for increasing both the efficiency and safety of hydrogen storage. These advancements can facilitate the integration of hydrogen into existing energy infrastructure. *Challenges:* Developing high-capacity, affordable, and secure hydrogen storage devices remain challenging. Additionally, establishing a comprehensive hydrogen

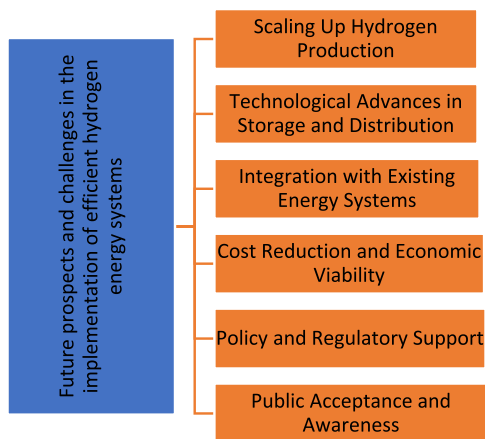


FIGURE 29 Future prospects and challenges in the implementation of efficient hydrogen energy systems.

distribution infrastructure, encompassing pipelines and filling stations, is vital to support broad hydrogen usage.<sup>134</sup>

- *Integration with current energy systems: Future Prospects:* Efficiently integrating hydrogen energy systems with current energy infrastructure, such as power grids and transportation networks, can enable diverse applications, including electricity generation, heating, and transportation. *Challenges:* Overcoming the intermittent nature of renewable energy sources used for hydrogen generation and retrofitting existing infrastructure to accommodate hydrogen are complex tasks. Careful planning and coordination are required to address the technological and regulatory aspects of hydrogen integration across various industries.<sup>135–137</sup>
- *Cost reduction and economic viability: Future prospects:* Continuous research and development efforts hold the potential to lower the cost of hydrogen production, storage, and utilization technologies, enhancing hydrogen's competitiveness compared with traditional fossil fuels. *Challenges:* Presently, hydrogen generation and storage systems are cost-intensive. To improve the economic feasibility of hydrogen technologies and hydrogen energy systems, optimization of supply chains, financial incentives for technology adoption, and enhancing technology efficiency and cost-effectiveness are imperative.<sup>138</sup>
- *Policy and regulatory support: Future prospects:* Robust policy frameworks and regulatory support in the future can significantly aid the development and adoption of effective hydrogen energy systems. Policies such as incentives, subsidies, and mandates can encourage investment and innovation in hydrogen technologies. *Challenges:* Establishing comprehensive regulatory frameworks encompassing safety, environmental standards, and infrastructure requirements is crucial. Collaboration between governments, industry stakeholders, and research organizations is vital for creating favorable policy frameworks that encourage the deployment of hydrogen energy systems.<sup>139</sup>
- *Public acceptance and awareness: Future prospects:* Boosting public acceptance and support for hydrogen energy systems can be achieved by raising awareness about hydrogen and fostering positive perceptions of it as a sustainable and clean energy source. *Challenges:* Addressing public concerns regarding safety, infrastructure expansion, and the transition from conventional energy sources to hydrogen is essential. Transparent communication, public engagement, and educational programs are key to instilling confidence and fostering universal acceptance of hydrogen energy systems.<sup>140,141</sup>

Addressing these prospects and challenges necessitates interdisciplinary collaboration, technological innovation, policy support, and public involvement. Effective hydrogen energy systems have the potential to make significant contributions to decarbonizing numerous industries and advancing a sustainable energy future.<sup>142</sup>

## 6 | CONCLUSION

In conclusion, this research has underscored the critical role of nanostructured catalysts and advanced materials in advancing hydrogen production and storage technologies. The main conclusions and contributions of this study can be summarized as follows:

- *The importance of nanostructured catalysts:* This study underscores the potential of nanostructured catalysts, such as carbon-based materials, metal nanoparticles, and MOFs, in enhancing reaction kinetics and selectivity for efficient hydrogen production. These catalysts offer high surface areas, improved reactivity, and tunable features, which are essential for optimizing hydrogen production processes.
- *The potential of advanced materials in hydrogen storage:* By exploring various advanced materials, including porous materials, nanomaterials, and complex MHs, this paper demonstrates their potential to enhance hydrogen storage capabilities. These materials exhibit high hydrogen adsorption capacities, improved stability, and enhanced kinetics, making them promising candidates for effective hydrogen production and storage.
- *Experimental methods and characterization techniques:* The research covers experimental techniques for catalyst synthesis, characterization, and performance evaluation, as well as methods for assessing the kinetics, stability, and hydrogen storage capacity of advanced materials. These techniques provide valuable insights into the structure–property relationships, aiding in the design and optimization of catalysts and materials for hydrogen energy systems.
- *Case studies and applications of advanced materials:* This study presents case examples that highlight the significant enhancement of hydrogen production and storage efficiency achieved through the use of advanced materials and nanostructured catalysts. These studies demonstrate the practical utility of these materials in real-world applications by showcasing their ability to increase hydrogen production, improve storage capacity, and boost overall system performance.

- *Potential impact and future research directions:* This research emphasizes the value of advanced materials and nanostructured catalysts in hydrogen production and storage. By adopting these materials, the effectiveness and viability of these technologies can be substantially improved, leading to reduced greenhouse gas emissions and decreased dependency on fossil fuels. Additionally, the increased efficacy, affordability, and safety offered by these materials can facilitate the wider adoption of hydrogen across various industries, including transportation, energy production, and manufacturing, thus accelerating the transition towards a cleaner, more sustainable energy landscape.

Overall, this paper highlights the significance of nanostructured catalysts and advanced materials as essential enablers for the development of hydrogen generation and storage systems. The findings presented in this study have the potential to significantly advance the field and contribute to the realization of a cleaner, more sustainable energy future.<sup>142</sup>

## NOMENCLATURE

|                                 |   |
|---------------------------------|---|
| BET                             | Brunauer–Emmett–Teller                  |
| CeO <sub>2</sub>                | ceria                                   |
| CFRPs                           | carbon fiber-reinforced polymers        |
| CNTs                            | carbon nanotubes                        |
| Co <sub>3</sub> O <sub>4</sub>  | cobalt oxide                            |
| COFs                            | covalent organic frameworks             |
| CoS                             | cobalt sulfide                          |
| CVD                             | chemical vapor deposition               |
| DSC                             | differential scanning calorimetry       |
| FTIR                            | Fourier transform infrared spectroscopy |
| GC                              | gas chromatography                      |
| HER                             | hydrogen evolution reaction             |
| IFC                             | international fire code                 |
| ImIP                            | imidazolium-based ionic polymer         |
| IR spectroscopy                 | infrared spectroscopy                   |
| MCH                             | methylcyclohexane                       |
| Mo <sub>2</sub> N               | molybdenum nitride                      |
| MOFs                            | metal-organic frameworks                |
| MWCNTs                          | multiwalled carbon nanotubes            |
| NaBH <sub>4</sub>               | sodium borohydride                      |
| NFPA                            | National Fire Protection Association    |
| NH <sub>3</sub> BH <sub>3</sub> | ammonia borane                          |
| NiS                             | nickel sulfide                          |
| NMR                             | nuclear magnetic resonance              |
| NPC                             | nitrogen- and phosphorus-codoped carbon |
| OER                             | oxygen evolution reaction               |
| PDA                             | polydopamine                            |
| SEM                             | scanning electron microscopy            |

|                                       |  |
|---------------------------------------|--|
| TGA                                   | thermogravimetric analysis                 |
| TiN                                   | titanium nitride                           |
| TRLs                                  | technology readiness levels                |
| WC                                    | tungsten carbide                           |
| XAS                                   | X-ray absorption spectroscopy              |
| XPS                                   | X-ray photoelectron spectroscopy           |
| XRD                                   | X-ray diffraction                          |
| (MgH <sub>2</sub> ) TiCl <sub>3</sub> | magnesium hydride and titanium trichloride |

## AUTHOR CONTRIBUTIONS

**Conceptualization:** Feras Alasali, Amr M. Obeidat, and Mohammed I. Abuashour. **Methodology:** William Holderbaum, Waleed Hammad, Derar Almomani, and Mohammed I. Abuashour. **Formal analysis:** Feras Alasali, Mohammed I. Abuashour, Amr M. Obeidat, and William Holderbaum. **Investigation:** Feras Alasali, Mohammed I. Abuashour, Derar Almomani, and Waleed Hammad. **Resources:** All authors. **Data curation:** All authors. **Writing—original draft preparation:** Mohammed I. Abuashour, William Holderbaum, Derar Almomani, and Feras Alasali. **Writing—review and editing:** All authors. **Visualization:** All authors. **Supervision:** All authors. **Project administration:** Mohammed I. Abuashour. All authors have read and agreed to the published version of the manuscript.

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## CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

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