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Review

# Advancing hydrogen storage: critical insights to potentials, challenges, and pathways to sustainability<sup>\*</sup> Nisha T Padmanabhan<sup>1</sup>, Laura Clarizia<sup>2</sup> and Priyanka Ganguly<sup>3</sup>



Research in green hydrogen production is advancing through photocatalysis and electrocatalysis, but storage remains a challenge. Promising hydrogen carriers, such as methanol, ammonia, formic acid, liquid organic hydrogen carriers, and metal hydrides, face issues like low hydrogen content and high energy demands. This review highlights innovations in hydrogen storage, focusing on carrier synthesis and photocatalytic hydrogen release for sustainable, energy-efficient solutions. Advancing catalysts, reactors, lifecycle assessments, and economic feasibility is crucial. Hybrid approaches and augmented intelligence are essential for developing cost-effective, high-efficiency storage systems, driving progress toward a sustainable hydrogen economy.

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### Introduction — the current state of hydrogen production and storage

Hydrogen plays a pivotal role in the global transition toward net-zero emissions, offering the highest gravimetric energy density among fuels at 33.3 kWh/kg (120 MJ/kg). Hydrogen is crucial for reducing fossil fuel dependence and meeting energy demands, but production remains energy intensive. Traditional methods like steam methane reforming and coal gasification produce gray hydrogen, while emerging green hydrogen technologies, including electrolysis, electrochemical, photocatalytic, and photoelectrochemical processes, focus on sustainability and reducing carbon emissions.

Global efforts to transition from gray to green hydrogen by leveraging renewable energy sources such as solar and offshore wind have been documented [1]. These initiatives often adopt public–private partnership models to address technological and economic barriers. Photocatalytic hydrogen production relies on solar energy and semiconductors with suitable band gaps. Despite promising advancements, challenges remain in catalyst stability, minimizing charge carrier recombination, and optimizing reactor designs for scalability. Large-scale reactors have been explored, but commercial viability remains elusive due to issues such as nanomaterial production, immobilization, and efficient extraction.

Recently, Sparc Hydrogen, a joint venture between Sparc Technologies, Fortescue, and the University of Adelaide, announced progress on a pilot plant utilizing photocatalytic water splitting technology. This cutting-edge method produces hydrogen directly from sunlight and water, eliminating the need for electrolyzers and electricity, thereby reducing costs and decoupling production from renewable power price fluctuations [2]. Like the photocatalytic approach, electrochemical hydrogen production faces challenges in designing efficient cathode and anode materials. Across all methods, scaling up remains a critical obstacle. However, in a recent

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breakthrough, UK-based startup Electrogenos introduced a revolutionary catalyst designed to enhance the efficiency and longevity of green hydrogen production [3]. The company's advanced disc-shaped stainlesssteel electrodes for alkaline electrolyzers are manufactured through electroplating, enabling high current densities at lower voltages. These electrodes exhibit a degradation rate of under 3% during prolonged testing, potentially lowering production costs and accelerating large-scale adoption, with commercial products expected by 2025.

Recent advancements in combining multiple techniques for water splitting show promise at an industrial scale. For instance, HGenium has announced plans to develop a pilot plant dedicated to green hydrogen production[4]. Unlike conventional methods reliant on electricity, this approach utilizes thermal or thermochemical processes to split water. The required heat can be sourced from industrial processes, concentrated solar power, or even nuclear energy, presenting a versatile and innovative pathway for sustainable hydrogen generation.

Hydrogen storage, a critical component of its adoption as an energy source, has not progressed as rapidly as production technologies. Since hydrogen is a gas at ambient temperature and pressure, it must be transported in compressed or liquefied forms, introducing substantial technical and economic obstacles. Storing hydrogen in these states poses safety risks, requires robust systems to prevent leaks, and demands efficient containment solutions. Hydrogen can be stored as compressed gas, liquefied hydrogen, or cryo-compressed gas. However, challenges related to weight, volume, and hydrogen embrittlement remain significant concerns.

Bridging the gap between hydrogen production and storage is essential to realizing its potential as a clean energy carrier. Research has increasingly focused on integrating hydrogen production with storage, particularly exploring the potential of photocatalytic hydrogen release from carriers. Instead of relying on a single approach, integrating multiple techniques for both production and storage offers a promising pathway toward commercial-scale applications. Figure 1 illustrates an artificially generated depiction of a hydrogen production and storage system that combines various techniques working in tandem.

### Potential hydrogen carriers and their underlying challenges

An optimal chemical hydrogen source must meet several criteria, including high gravimetric and volumetric energy densities, low toxicity, eco-friendly production, mild storage conditions, compatibility with existing infrastructure, and ease and safety in handling and

transport. Moreover, hydrogen storage and release processes should be energy-efficient and cost-effective.

Methanol (MeOH) and ammonia (NH<sub>3</sub>) are produced on an industrial scale and have high hydrogen content, but they are classified as toxic and flammable under the United Nations' Globally Harmonized System [6]. Urban and industrial wastewater often contains high levels of NH<sub>3</sub>. Developing technologies to remove NH<sub>3</sub> while producing hydrogen energy presents a sustainable solution for environmental remediation and green energy generation.

Formic acid (FA) offers favorable thermodynamics, dehydrogenation at ambient conditions, and direct synthesis from CO<sub>2</sub>. However, it is corrosive and has a low hydrogen content (<5 wt%). Liquid organic hydrogen carriers (LOHCs) are manageable and offer moderate hydrogen densities (5.8-7.3 wt%), yet they face challenges like restricted availability and toxicity.

The following discussion on MeOH, NH<sub>3</sub>, FA, LOHCs, and metal hydrides (MHs) highlights advancements in catalysts, reactor designs, and innovative materials, offering promising directions for efficient and scalable hydrogen storage solutions [7].

Hydrogen's low volumetric density (Table 1) necessitates the use of 700-bar compressed tanks for storage and transportation, which presents both significant cost and safety challenges. To facilitate the widespread adoption of hydrogen-powered fuel-cell vehicles, the United States Department of Energy has set specific targets for hydrogen storage systems: a gravimetric storage capacity of 6.5 wt% and a volumetric storage capacity of 50 gH<sub>2</sub>/1 [8]. The development of storage materials, such as LOHCs, that can surpass these system-level benchmarks is thus highly desirable. Significant advancements have been made in hydrogen storage, yet most materials still exhibit limited volumetric capacity. From an industrial perspective, volumetric capacity is often more critical than gravimetric capacity. This is primarily due to space constraints in automobiles, where the size of the storage tank is a limiting factor. Additionally, the volumetric capacity of a hydrogen storage system has a greater influence on the driving range of fuel-cell vehicles compared to its gravimetric counterpart. Consequently, the development of hydrogen storage materials with the highest possible volumetric capacity, while also maintaining excellent gravimetric performance, remains a key priority [9].

MeOH offers advantages such as low volatility, high hydrogen content (12.5 wt%, Table 1), and aligns with carbon neutrality when synthesized via CO2 capture and green hydrogen. Electrochemical CO<sub>2</sub> reduction faces solubility and efficiency challenges, but Cu-based

Figure 1



Artificially generated image of hydrogen production and storage solution combining different techniques simultaneously (generated through ChatGPT with the prompt; generate an image of a futuristic outlook of green hydrogen production and storage solutions working in tandem) [5].

electrocatalysts show promise [10]. Global MeOH production is projected to reach 190 Mt by 2030 [11].

Hydrogen release from MeOH typically requires catalytic steam reforming at 200-300°C. Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts are effective but face stability issues [21]. Nibased catalysts improve durability but require higher temperatures [22], while PdZn and Pd-Cu alloys offer stability with cost-performance trade-offs [23].

Solar-driven photocatalytic MeOH reforming has gained attention as an alternative to water splitting, producing hydrogen and valuable by-products like formaldehyde and FA. Enhancing yield requires innovation in photocatalysts, including carbon- and silver-based materials. Promising strategies involve exploring double perovskites, optimizing Z-scheme systems, and standardizing quantum yield metrics [24].

NH<sub>3</sub> contains 17.8 wt% hydrogen, but 96% is produced via Haber-Bosch, contributing 1.2% of global emissions [17]. To improve sustainability, research focuses on renewable-powered electrolysis for hydrogen, catalysts for NH<sub>3</sub> synthesis at lower pressures/temperatures, and alternative synthesis methods. Key catalysts include ironbased materials, Ru-supported systems, and Ni/Co catalysts with promoters like barium [25-27]. Electrochemical NH<sub>3</sub> production using solid-state electrolytes and low-temperature membranes is under study but needs refinement for scalability [28]. Hydrogen release from NH<sub>3</sub> is energy intensive due to high N-H bond activation. Advances include noble metal catalysts (Ru, Ir), optimized supports (Al<sub>2</sub>O<sub>3</sub>, carbon materials), and promoters like K and Ba [29-31]. Photocatalytic NH<sub>3</sub> splitting using TiO2, ZnO, and graphene in alkaline conditions is a promising room-temperature method [32,33]. Yuan et al. demonstrated Cu-Fe-AR effectiveness under laser illumination [34].

FA production from CO<sub>2</sub> benefits from Ru- and Ir-based catalysts, while FA dehydrogenation utilizes metal nanoparticles. Non-noble catalysts like CoP and FeP show promise, though FA adsorption mechanisms remain under study [35,36].

As shown in Figure 2, different approaches (i.e. the use of proper cocatalysts, the formation of heterojunctions, and Z-scheme photocatalysts) to improving photocatalysts would be beneficial for hydrogen release from MeOH, NH<sub>3</sub>, and FA by facilitating charge separation and enhancing reaction kinetics.

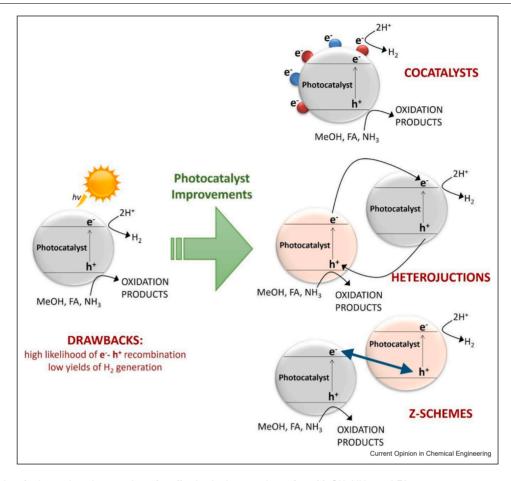
LOHCs enable efficient hydrogen storage via reversible hydrogenation-dehydrogenation. The benzene-cyclohexane system offers 7.2 wt% capacity but requires ~300°C for dehydrogenation [37]. The toluene-methylcyclohexane system (6.2 wt%) is cost-effective but relies on expensive Pt-based catalysts and ultra-pure hydrogen [38]. Advances in Fe-promoted Mo carbide and RuNi/TiO<sub>2</sub> catalysts enhance efficiency under mild conditions [39]. Electrochemical hydrogenation [40] and Ni/CeO<sub>2</sub> solar-assisted catalysts [41] lower energy costs.

Table 1						
Key physical and flammability properties of hydrogen and	rties of hydrogen		hydrogen carriers are discussed in this review [4,12-20].	[4,12–20]		
Carrier	H <sub>2</sub> capacity (wt%)	Volumetric energy density (MJ/I)	Gravimetric energy density Boiling (LHV) (MJ/kg) T (°C)	Boiling T (°C)	Flash point T, closed cup (°C)	Flammability limits in air (LFL- UFL, vol%)
H <sub>2</sub> MeOH	100 [12]	0.0108 (STP) [19] 17.3 (STP) [18]	120 [19] 19.9 [16]	-252.9 [12] 64.7 [12]	Flammable gas [12]	4-75 [12] 6.7-36.5 [17]
NH <sub>3</sub>	17.8 [12]	12.7 (10 bar, -34 °C)	18.6 [16]	-33.4 [12]		15–27 [17]
FA	4.4 [4]	6.4 (STP) [20]	5.3 [20]	100.8 [12]	48 (FA content=99 wt%)	12-38 (FA content = 99 wt%) [17]
Benzene/cyclohexane	7.2 [12]	6.7 [12]	40.170 [13]	80/81 [12]	-11/-18 [12]	1.2-8/1.3-8.4 [12]
i oluene/metnylcyclonexane Naphtalene/decalin	6.2 [12] 7.3 [12]	5.6 [12] 7.8 [12]	40.369 [13] /	218/185 [12]	4/-6 [12] 80/57 [12]	0.9–5.9/0.7–5.4 [12]
Dibenzyltoluene/ perhydrodibenzyltoluene	6.2 [12]	6.8 [12]	/	390/287 [12]		/
NaBH <sub>4</sub>	10.8 [12]	15.5 [12]	7.6 [14]	/	/	/
MgH <sub>2</sub>	7.6 [12]	15.8 [12]	29.2 [15]	_	/	

Naphthalene-decalin (7.3 wt%) faces by-product issues, while dibenzyltoluene (6.2 wt%) ensures safety [17]. Innovations in microchannel reactors drive scalable LOHC applications [42]. Hybrid solutions have been proposed to further enhance hydrogen storage and address technical issues observed at the industrial scale. For instance, when evaluating heating oils, the high viscosity of these hydrides plays a crucial role in determining their feasibility for real-world hydrogen storage applications. Some researchers suggest that combining different hydrides (e.g. benzyltoluene/dibenzyltoluene-based mixtures [43]) could provide a more effective solution by reducing viscosity and accelerating reaction times. MHs offer up to 18.5 wt% hydrogen storage but face kinetic challenges. Additives. nanostructuring, and alloying improve efficiency, while NaBH<sub>4</sub> regeneration and MgH<sub>2</sub> destabilization remain key research areas [44,45]. While MXenes (layered carbides or nitrides of transition metals) facilitate both chemical and physical hydrogen adsorption, notably through Kubas-type interactions, where hydrogen molecules bind to metal centers without dissociation, allowing reversible storage under ambient conditions [46]. In contrast, MOFs like MOF-177 utilize physisorption within their expansive surface areas and adjustable pores, achieving hydrogen uptakes of approximately 7.5 wt% at 77 K and 70-80 bar [47]. Carbonaceous materials, for instance, carbon nanotubes (CNTs), store hydrogen via physisorption on their surfaces, with storage capacities influenced by surface area, pore structure, and defects; however, significant storage at ambient conditions remains challenging, often requiring cryogenic temperatures and high pressures. The electrochemical hydrogen storage however can also show a flipin and kick-in insertion mechanisms into CNT walls, with activation barriers of approximately 1.5 eV and 2.0 eV [48].

The stability of these materials is critical for understanding the long-term usage in case of nanomaterials. Hydrogen storage materials, especially those that rely on adsorption, like MOFs, COFs, MXenes, porous carbons, and MHs, depend on their long-term stability. Prolonged exposure of H<sub>2</sub> in case of MOFs and COFs especially in high temperature and pressure can result in collapse of the pore structure and structural degradation. In an effort to mitigate this, researchers focus on developing air-stable materials. Using a mix of Cu and Zn precursors, Sengupta et al. reported synthesizing a Cu(I)based MOF called NU-2100 [49]. Zinc acts as a catalyst in this process, converting an intermediate MOF into NU-2100 without becoming part of the finished structure. Under ambient conditions, NU-2100 has a great capacity to store hydrogen (10.4 g/l, 233 K/100 bar to 296 K/5 bar), is air stable, and has one of the highest initial isosteric heats of adsorption (32 kJ/mol). Often open metal sites are good for bonding of H<sub>2</sub>, while these sites

Figure 2



Possible approaches for improving photocatalysts for effective hydrogen release from MeOH, NH<sub>3</sub>, and FA.

are susceptible to oxidation. Ligand oxidation commonly occurs at ambient temperatures and in moisture and could result in reduction of the adsorption and overall stability [50]. In case of MHs, these materials offer high volumetric density and ideal for small- and large-scale deployment. However, these materials come with their own challenges, such as the kinetic degradation, particle coarsening [51]. Frequent hydrogenation and dehydrogenation can lead to formation of passive layer on the surface and can lead to reduction of the kinetics over time. The use of catalysts can prevent in slowing down of the overall kinetics due to repeated cycles. Similarly, repeated cycles can also result in sintering on the surface of the MHs resulting in coarsening of the particles. Tuning the structure of the MHs to nano dimensions and its pore can also contribute toward improved kinetics and reduce the coarsening [52].

### Sustainability metrics and future directions of hydrogen storage

Sustainable hydrogen deployment depends on efficient, and environmentally friendly cost-effective, storage solutions. While promising hydrogen carriers exist, challenges such as high energy demands for hydrogen release and poor carrier recyclability limit widespread adoption. Photocatalytic and photoelectrocatalytic dehydrogenation offer low-carbon hydrogen release using sunlight and advanced catalysts, but by-product formation remains a key challenge. For instance, FA dehydrogenation often produces CO due to formate/bicarbonate interconversion. An optimized reaction system using trace Ru-5 complexes can enable CO-free hydrogen release with high stability in formate/bicarbonate-based storage [53].

Ammonia-based hydrogen storage presents toxicity concerns, including NOx and hydrazine by-products. While photocatalytic NH<sub>3</sub> decomposition operates under milder conditions than thermal or plasma-based methods, it suffers from low hydrogen yield and immature photoreactor designs (TRL=1-2) [54]. NH<sub>3</sub> electrolysis, however, achieves comparable energy efficiency (1.32 Wh/g) to thermal decomposition (3 Wh/g) while producing 25 kg/h of hydrogen and benefiting from phase separation for easier recovery. Future efforts should focus on developing advanced photo-electrocatalysts with enhanced kinetic activity and resistance to nitrogen adatom poisoning.

For MeOH photoreforming, rational catalyst design and advanced material integration can help overcome current limitations. Jiao et al. demonstrated that a flow membrane reactor at low temperatures and atmospheric pressure produces hydrogen 1.63 times more efficiently than batch reactors due to improved mass transfer [55]. Low-cost, durable catalysts and advanced membranes can enhance energy efficiency by reducing MeOH crossover and improving proton conductivity. Sustainable MeOH production via CO<sub>2</sub> electrochemical reduction or biomass conversion could further lower environmental impact.

FA has lower toxicity than NH<sub>3</sub> or MeOH and releases hydrogen efficiently at low temperatures. While NH<sub>3</sub> is ideal for large-scale hydrogen transport, its high energy demand for cracking, purification costs, and low energy recovery hinder efficiency [56]. Additionally, NH<sub>3</sub> hydrophilicity and corrosiveness necessitate leak-proof infrastructure, posing technical and societal challenges.

In LOHCs, an ideal candidate for electrochemical cycling should offer high hydrogen capacity, fast reaction rates, and high Faradaic efficiency to minimize side products. Inspired by photosynthesis, hydroquinones enable safer hydrogen storage, mimicking photosystems I and II through photocatalytic reduction and oxidation. Recent studies highlight hydroquinone/quinone fuel cells as a promising energy application [57].

The large-scale deployment of LOHCs in mobile applications should address energy-intensive hydrogen release processes, system integration complexities, and the need for efficient, durable catalysts. Umicore has initiated a breakthrough in long-term research focusing on LOHC technology, specifically targeting the development of advanced platinum group metal-based catalysts to optimize hydrogenation and dehydrogenation processes [58], aiming to enhance the practicality of LOHC systems in fuel-high entropy alloyscell electric vehicles. Whereas, Axens has partnered with Chiyoda Corporation to facilitate efficient hydrogen storage and transportation using methylcyclohexane and toluene as carriers [59].

Beyond FA, MeOH, NH<sub>3</sub>, and LOHCs, nanomaterial-based hydrogen storage faces stability challenges, as materials degrade under environmental fluctuations or lose structural integrity after repeated cycling [60]. CNTs, MOFs, and graphene struggle with volumetric hydrogen density, pressure and temperature limitations, slow kinetics, and long-term stability. MOFs require improved dehydrogenation, high-pressure stability, and

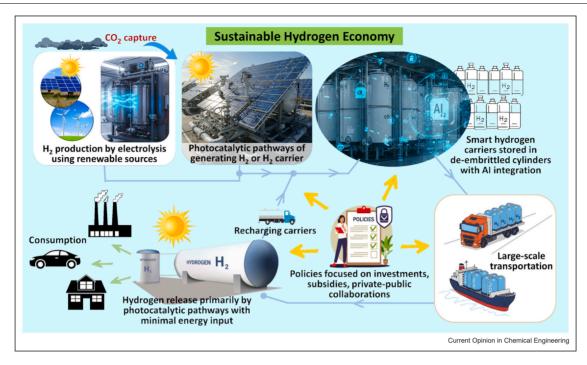
lower energy demands for reconstruction. Enhancing adsorption enthalpies and pore volumes could improve storage capacity.

MHs offer high volumetric density, stability, and reversibility at ambient conditions. Nanoporous Mg(BH<sub>4</sub>)<sub>2</sub> structures achieve 144 g/l hydrogen storage, surpassing conventional methods [61]. High-entropy alloys like TiV<sub>2</sub>ZrCrMnFeNi demonstrate 1.6 wt% hydrogen absorption with rapid kinetics [62]. Coupling hydrides with photocatalytic systems enhances hydrogen dissociation and diffusion during cycling [63]. Further research should focus on improving metal alanates and MOFs by addressing slow kinetics and stability issues while integrating carbon-based materials like graphene to optimize thermodynamics and kinetics for practical hydrogen storage applications.

Beyond the development of hydrogen carriers, hydrogen embrittlement is a major challenge in metal-based systems like steel, where the small size and high mobility of hydrogen weaken materials, especially high-strength steels, over time. Meda et al. emphasize that hydrogen embrittlement is exacerbated by a combination of critical hydrogen concentration, applied stress levels, and the material's intrinsic properties, which together accelerate the weakening and failure of metal structure [64]. To address large-scale storage challenges, innovative solutions like Vallourec's 'Delphy' system offer scalable underground hydrogen storage, using steel tubes to reduce surface footprint 30-fold, with capacities from 1 to 100 metric tons for safe, durable solutions [65]. Similarly, high-entropy alloys (HEA) such as FeMnCo-CrAl or TiVCrMnMoCe made of multi-element exhibit less susceptibility to hydrogen embrittlement as they introduce lattice distortions, preventing the diffusion of H<sub>2</sub> molecules to cause any early fractures [66]. The BCC phase has been the subject of recent research, allowing for changes to improve storage characteristics. The development of the Ti-V-Cr-Mn-Mo-Ce alloy, which was created by vacuum arc melting with Ce doping, represents a major advancement in this research [67]. This alloy offers a remarkable 3.6 wt percentage hydrogen storage capacity, fast absorption (40 s for 1% Ce doping), and a -17.96 kJ/mol H<sub>2</sub> desorption enthalpy.

Integrating photocatalytic hydrogen storage with power electronics and energy management is feasible but requires cost reduction for commercial viability [68]. Aldriven systems optimize hydrogen production, storage, and utilization, enabling predictive maintenance and adaptive control [69]. Machine learning (ML) enhances infrastructure design, refining efficiency, and operational strategies for sustainable hydrogen energy solutions [70]. Density functional theory (DFT) integrated with ML could be used to predict the hydrogen adsorption behavior of the nanomaterials. In a recent such effort, the

Figure 3



Envisioning a sustainable hydrogen economy through electrocatalytic and photocatalytic pathways for H<sub>2</sub> and H<sub>2</sub> carrier production, coupled with simultaneous CO2 capture, effective storage and large-scale transport, photocatalytic hydrogen release, together with enhanced AI and policy support. Al, artificial intelligence.

authors reported the use of DFT + ML to predict the activation energy of an efficient amorphous NiFeP catalyst for chlorine evolution [71]. Similarly, Jia et al. reported the use of DFT + ML to predict the bilayermodified graphene doped with B atoms and modified with Li and Ti atoms to improve the hydrogen storage ability [72]. Such calculations with the aid of artificial intelligence (AI) enable in shortening the material prediction time. Larger institutions such as Google's DeepMind have AlphaFold prediction tool that is presently serving to find novel protein structures. Such amino acid analysis serves to understand the fundamentals of life and the importance of smaller molecules in it. Such prediction tools could be used to provide insights about nanomaterials for different applications. AI enhances hydrogen storage by improving performance, reducing waste, minimizing energy loss, and extending system lifespan. By spotting deviations from regular operations, anomaly detection techniques like Autoencoders and Isolation Forest are essential for maintaining safety and efficiency in hydrogen storage facilities. These ML methods identify anomalies by analyzing common patterns. By learning a compressed representation of typical data and detecting deviations through reconstruction errors, autoencoders are able to identify anomalies. Isolation Forest, on the other hand, effectively identifies outliers by isolating anomalies and randomly dividing the data [73]. Figure 3 outlines a sustainable hydrogen economy enabled by catalytic pathways, CO<sub>2</sub> management, and AI- and policy-driven support.

Global hydrogen initiatives target decarbonization but face infrastructure challenges. Projects like Germany's Energiepark Mainz and the UK's NH3 exploration offer scalable solutions [74]. Power-to-gas integrates hydrogen into gas grids, while underground storage advances sustainability [75]. Strategies like the U.S. 'hydrogen shot' and EU's hydrogen plan drive market adoption. Various optimization strategies have been explored [76,77] to integrate hydrogen storage with intermittent renewable energy sources like wind and solar, improving grid stability and reducing operational costs. Combining hydrogen and battery storage systems captures surplus energy during peak production and releases it during high demand [77]. Advanced control strategies, such as deep reinforcement learning [78], optimize real-time scheduling, while particle swarm algorithm models [79] determine optimal sizing and placement of hydrogen storage, considering demand fluctuations, renewable variability, and economic constraints to balance the grid effectively.

Lifecycle assessments on hydrogen storage technologies are contingent upon the factors such as energy consumption during storage, material selection for storage, and indeed on integrating renewable sources. Using wind/solar energy for hydrogen production and subsequent storage in salt caverns will provide lowest cumulative environmental impact, rather than relying on systems based on grid electricity. Projects like HySHIP advance hydrogen shipping, but economic feasibility remains underexplored [80]. Policymakers must support investments, safety regulations, and global trade planning while leveraging subsidies and advanced tools for scalable, cost-effective commercialization.

## Techno-economic considerations for hydrogen carriers

The integration of hydrogen carriers into the energy sector depends on production methods, transport logistics, infrastructure, and policy support. Economic feasibility requires linking hydrogen carrier production to renewable energy sources. Ammonia-based systems emit less carbon than LOHCs, with the toluene/methylcyclohexane supply chain being the most cost-effective. However, costs remain highly sensitive to electricity prices and electrolyzer expenses. LOHC applications face economic challenges due to the high cost of dehydrogenation, which could be mitigated by integrating industrial waste heat. Additionally, the recyclability of carbon-based carriers depends on effective CO<sub>2</sub> capture and LOHC recovery.

The maritime sector faces decarbonization challenges due to strict weight and energy constraints. Hydrogen proton exchange membrane fuel cells are ideal for voyages under a week, while methanol steam reforming and ammonia with solid-oxide fuel cells are options for longer trips. Rail transport favors ammonia and compressed hydrogen over MHs and LOHCs. Infrastructure development is crucial, particularly for port refueling stations and hydrogen distribution networks. Logistics significantly impact hydrogen costs, with LOHCs preferred for long-distance transport and CH2 for shorter routes. Policy measures, including incentives and carbon taxation, could accelerate adoption, while a global logistics framework is essential for an efficient hydrogen supply chain.

### **Conclusions and perspectives**

Optimizing adsorption/desorption kinetics, thermal stability, storage density, and economic scalability are key challenges in commercial hydrogen storage. Advanced materials like HEAs, MOFs, and MXenes show promise but have limitations. MXenes offer tunable chemistry and fast kinetics but require structural modifications to enhance hydrogen binding and prevent degradation. MOFs excel in adsorption due to their high surface area but suffer from low volumetric density and require cryogenic conditions for efficient desorption. HEAs provide stable, high-density storage but face challenges with hydrogen diffusion and energy-intensive desorption. Addressing these issues requires innovative strategies such as catalyst integration, hybrid materials, and nanostructuring. Enhancing thermal stability with protective

coatings and alloy tuning is crucial. Green, scalable synthesis methods, like solvent-free MOF fabrication or alternative metal HEAs, will boost commercial viability. Infrastructure development, energy integration, policy support, and investments are essential for large-scale adoption, making hydrogen a key player in achieving net-zero goals.

### **Data Availability**

No data were used for the research described in the article.

### **Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

### Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the author(s) used ChatGPT in the writing process to generate an image. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the published article. The credits for the image used according to the LLM source are mentioned in Figure 1.

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This review thoroughly examines the key attributes of different hydrogen carriers, focusing on their production, transport, and hydrogen release, while highlighting the challenges hindering broader adoption. The final section presents a thermo-economic comparison from the literature, outlining critical factors for choosing the most appropriate technology.

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