Advances in hydrogen storage materials: harnessing innovative technology, from machine learning to computational chemistry, for energy storage solutions

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ABSTRACT

The demand for clean and sustainable energy solutions is escalating as the global population grows and economies develop. Fossil fuels, which currently dominate the energy sector, contribute to greenhouse gas emissions and environmental degradation. In response to these challenges, hydrogen storage technologies have emerged as a promising avenue for achieving energy sustainability. This review provides an overview of recent advancements in hydrogen storage materials and technologies, emphasizing the importance of efficient storage for maximizing hydrogen's potential. The review highlights physical storage methods such as compressed hydrogen (reaching pressures of up to 70 MPa) and material-based approaches utilizing metal hydrides and carbon-containing substances. It also explores design considerations, computational chemistry, high-throughput screening, and machine-learning techniques employed in developing efficient hydrogen storage materials. This comprehensive analysis showcases the potential of hydrogen storage in addressing energy demands, reducing greenhouse gas emissions, and driving clean energy innovation.

1. Introduction

Global energy demand has been steadily increasing due to factors like population growth, economic development, and urbanization. Predictions suggest the world population will reach around 9.7 billion by 2050, consequently continuing the rise in energy demand. Presently, fossil fuels, encompassing coal, oil, and natural gas, account for approximately 80% of the world's energy consumption [1,2]. The combustion of these fuels results in substantial greenhouse gas emissions, primarily carbon dioxide (CO_2), which contribute significantly to global warming, climate change, and adverse environmental effects such as severe weather events, rising sea levels, and loss of biodiversity [3–6]. Moreover, these fuels release pollutants like nitrogen oxides (NOx), sulfur oxides (SOx), and particulate matter (PM), leading to air pollution

and detrimental impacts on human health. Geopolitical tensions and concerns about energy security have arisen due to the uneven distribution of fossil fuel resources [7].

In response to environmental concerns and energy security issues, many nations are investing in renewable energy sources like solar [8], wind [9], and hydroelectric power [10]. These sources produce minimal to no greenhouse gas emissions, thereby reducing the carbon footprint of the energy sector [11,12]. Hydrogen, touted as a game-changer in the global energy landscape, plays a pivotal role in achieving sustainability. It is a clean, renewable, and versatile energy carrier with potential applications across transportation, power generation, industrial processes, and more [13]. The reasons for hydrogens importance include its clean energy credentials, renewability, role in energy storage, versatility in applications, the potential for domestic production enhancing energy

security, and the innovation and technological advancements it necessitates, driving economic growth and job creation [14].

For balancing the variable energy generation from renewables with demand and avoiding curtailment, energy storage systems such as batteries, compressed air, pumped storage hydropower, flywheels, and thermal energy storage have been proposed. However, these systems come with technical challenges, varying efficiencies, risks, and higher upfront costs compared to conventional methods. Hydrogen storage offers a promising solution by converting surplus electricity into hydrogen or producing it from low-carbon processes, which can be utilized as fuel in combustion engines or fuel cells. Hydrogen boasts the highest energy per mass among fuels and holds the potential for significant contributions to decarbonizing the global energy mix [15].

The pursuit of efficient hydrogen storage materials stands as a crucial aspect in the quest for sustainable energy solutions amid the global shift toward cleaner options. However, the challenge of secure and efficient storage inhibits its widespread adoption. Designing materials proficient in the storage and controlled release of hydrogen is pivotal for maximizing its potential in the energy landscape. These endeavors involve meticulous considerations, encompassing the material's structural attributes, porosity, surface area, capacity, stability, and safety. Addressing these design considerations is fundamental to the advancement of hydrogen storage technology and its pivotal role in clean energy applications [16].

Hydrogen storage technologies can be broadly classified into two categories: physical-based and material-based approaches. Physical storage methods encompass compressed gas, liquid, and cryo-compressed forms, wherein storage conditions, such as pressure or temperature, are manipulated. Contrastingly, material-based or solid-state storage relies on materials like metal hydrides, complex hydrides, and carbon-containing substances such as activated carbon, graphene, and carbon nanotubes. These materials utilize absorption or adsorption techniques, with the release of molecular hydrogen typically achieved through thermal or catalytic decomposition. This avenue of hydrogen storage has spurred extensive research into designing both homogeneous and heterogeneous catalysts to enhance hydrogen generation [17–20].

Despite significant advancements in computational frameworks and theoretical methodologies, progress has been constrained by the empirical and sequential nature of experimental work. However, recent strides in theoretical tools such as density functional theory (DFT), high-throughput screening, crystal structure prediction, and nascent machine learning approaches are reshaping the landscape. These innovations in computational chemistry, data informatics, and machine learning are catalysts, potentially accelerating the kinetics in the development of energy-related industries [21].

The objective of this review is to provide an overview of recent advancements in hydrogen storage materials and technologies. It aims to emphasize the importance of efficient storage for maximizing the potential of hydrogen as a clean and sustainable energy source. The review discusses various physical and material-based hydrogen storage technologies, explores the design considerations for hydrogen storage materials, and highlights the role of computational chemistry, high-throughput screening, and machine learning techniques in developing efficient storage materials. The ultimate goal is to showcase the potential of hydrogen storage in addressing energy demands, reducing greenhouse gas emissions, and driving clean energy innovation.

2. Hydrogen storage technologies

2.1. Physical storage technologies

Hydrogen has garnered significant attention as a promising energy carrier with the potential to drive a sustainable future, owing to its high energy density on a weight basis. However, its low volumetric energy density presents a formidable challenge for efficient and safe storage. To tackle this issue, various physical storage technologies for hydrogen have been developed. These methods, which include compression and liquefaction technologies, either individually or in combination, offer innovative solutions for storing hydrogen in dense and stable forms. Such technologies play a pivotal role in overcoming the limitations associated with hydrogen's lightweight and gaseous nature, enabling its efficient transportation and utilization across various applications [22]. They serve as a gateway to unlock hydrogen's potential as a clean energy carrier [23], with applications spanning fuel cell vehicles [24] and industrial processes [25]. Fig. 1 Provides a concise overview of various hydrogen storage technologies.

In light of this, it becomes evident that physical storage technologies for hydrogen are integral to the widespread adoption and utilization of hydrogen in achieving a clean and sustainable energy future. They enable the harnessing of hydrogen's high energy density and its potential to generate emission-free energy. In this exploration, we will delve into the world of physical storage technologies for hydrogen, examining the principles, advantages, and limitations of these innovative solutions that play a pivotal role in harnessing the potential of hydrogen as a clean energy source.

2.1.1. Compressed hydrogen technique

The compressed hydrogen technique, a well-established method for hydrogen gas storage, is a critical aspect of transportation applications, particularly in the context of fuel cell cars [26]. This approach involves physically compressing hydrogen gas into pressure containers or tanks, and these tanks are engineered with the specific purpose of withstanding high pressures, often reaching up to 35 MPa (350 bar) and even 70 MPa (700 bar) while ensuring safety. While higher pressures offer the advantage of increased energy density, they also introduce design and material challenges for these tanks, necessitating a balanced consideration of both their positive aspects and challenges. On the positive side, this technique is marked by its maturity, with hydrogen gas compression technology being well-established and comprehensively understood. Additionally, it offers the prospect of fast refueling, potentially matching the speed of gasoline refueling with the development of appropriate infrastructure. Furthermore, compressed hydrogen has a solid safety track record, having proven itself reliable in various applications under existing laws and technologies.

However, the method is not without its challenges. Firstly, it demands significant energy for the compression process, which in turn reduces the overall efficiency of hydrogen as an energy carrier. Secondly, despite the light nature of the hydrogen stored, the tanks themselves, especially those designed for higher pressures, can be quite heavy. In terms of volumetric storage capacity, the technique provides around 24 g/L and 40 g/L at 350 and 700 bar, respectively, at room temperature [27], which can be a limiting factor. Additionally, establishing a robust infrastructure for compressed hydrogen storage and distribution is a significant challenge. It requires the development of a widespread network of refueling stations, pipelines, and storage facilities to support the demand for compressed hydrogen. The cost and complexity of building this infrastructure pose barriers to its widespread adoption [28]. Lastly, the cost of tanks, especially those constructed with materials like carbon fiber, can be notably high. In the realm of hydrogen storage, there are various types of vessels categorized into four distinct categories.

Type I cylinders are made from seamless steel, which allows them to store hydrogen at high pressures. However, they tend to be heavy and have a lower energy storage density than other cylinder types [29]. Their maximum pressure is 20 MPa, and their gravimetric storage capacity is only 1 wt%. Type II cylinders have a steel liner reinforced with a composite wrap, which makes them lighter and more efficient than Type I. However, they are more expensive to produce [30]. Type II cylinders can be used at pressures up to 30 MPa and are suitable for industrial applications rather than onboard applications, such as automobiles.
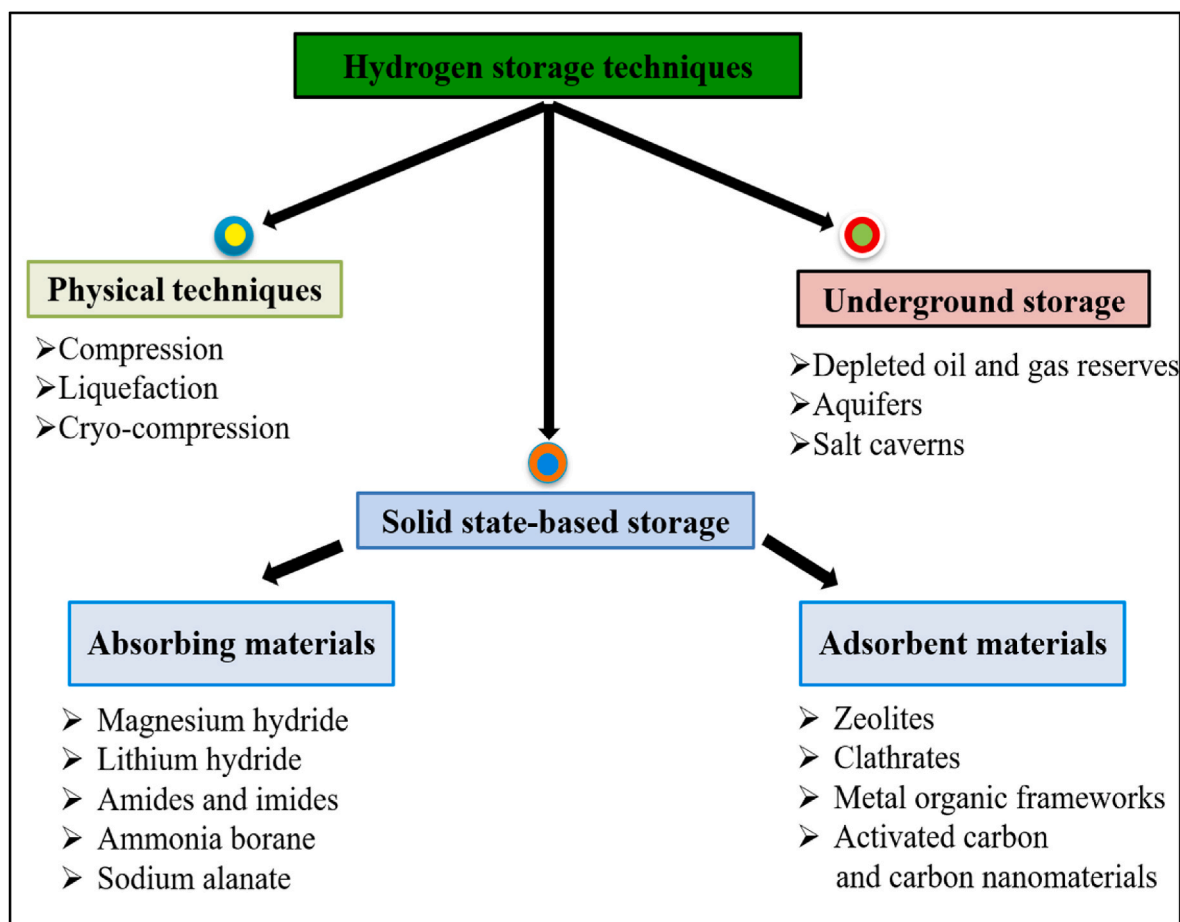
Fig. 1. Classification of hydrogen storage technologies into three major categories.

Type III vessels are high-pressure containers with a seamless aluminum liner fully enveloped by layers of composite materials. This design reduces their weight compared to Type I and Type II cylinders while maintaining high-pressure capabilities. However, they have low thermal conductivity, which may not be ideal for applications requiring efficient heat dissipation during hydrogen compression [31]. Type III cylinders can store hydrogen at pressures up to 70 MPa. Finally, Type IV cylinders have a plastic liner fully wrapped with composite materials, making them the lightest among all high-pressure hydrogen storage cylinders. However, their comprehensive wrapping leads to higher production costs [32]. Type IV cylinders can store hydrogen at pressures up to 70 MPa. Each cylinder type has its own set of advantages and limitations, making them suitable for various applications based on specific requirements and considerations.

2.1.2. Liquefied hydrogen storage

Liquefied hydrogen storage entails the cryogenic preservation of hydrogen gas in its liquid state, a procedure imperative for mitigating the inherent low energy density limitation associated with gaseous hydrogen storage [33]. To liquefy hydrogen, it must subjected to cryogenic temperatures, typically maintained below 20 K (−253 °C), a temperature significantly lower than its critical point of 33 K [26]. This intricate process mandates successive compression and expansion stages, wherein equipment such as compressors, heat exchangers, and expansion turbines is employed to attain and sustain the requisite cryogenic conditions. Subsequently, the liquefied hydrogen is securely contained within cryogenic tanks that are meticulously designed to withstand extreme cold and inhibit boil-off, a phenomenon marked by the gradual evaporation of stored liquid hydrogen, leading to pressure escalation within the storage vessel. The transportation of liquefied hydrogen can be facilitated through dedicated cryogenic pipelines or specialized road tankers equipped with cryogenic storage systems. Moreover, an emerging global trend encompasses the maritime transportation of liquefied hydrogen within dedicated containers on ships [34].

In a comprehensive analysis, we can delineate the notable advantages and drawbacks of liquefied hydrogen storage. On the advantageous front, liquefied hydrogen offers a substantially elevated energy density compared to gaseous hydrogen, rendering it eminently suitable for the protracted storage and long-distance transportation of hydrogen [35]. Furthermore, the technology underpinning hydrogen liquefaction and storage is deeply entrenched and bears a long-standing history of practical application, particularly within the aerospace domain [36]. Conversely, the pronounced energy intensity of the hydrogen liquefaction process entails a formidable energy demand, necessitating a substantial input of energy resources to realize and sustain the requisite cryogenic conditions [37]. In addition, the establishment of the requisite infrastructure for the widespread adoption of liquefied hydrogen storage poses a formidable challenge [38], stemming from the exacting specifications governing storage and transportation, which mandate the deployment of specialized facilities and equipment to meet these stringent requirements.

2.1.3. Cryo-compressed hydrogen storage

Cryo-compressed hydrogen storage is an innovative paradigm that synergistically integrates the principles of cryogenic storage and high-pressure gas storage, with a primary objective of ameliorating the intrinsic challenges posed by both methodologies when employed in isolation. These challenges encompass aspects such as the voluminous storage requirements and heightened pressure prerequisites of

conventional high-pressure gas storage, along with the inescapable boil-off losses encountered in the cryogenic hydrogen storage paradigm [32]. The focal aim of this approach is to optimize hydrogen storage solutions across diverse applications, with a pronounced emphasis on the automotive sector.

Cryo-compressed hydrogen storage operates by conserving hydrogen at cryogenic temperatures, albeit at pressures exceeding those encountered in conventional liquid hydrogen storage systems. The operational temperature regime typically ranges between 20 and 70 K, and the pressures can scale up to 35 MPa [39]. Notably, this approach offers an enhanced volumetric storage capacity, reaching up to 80 g/L, as opposed to the approximately 70 g/L attainable in the case of liquefied hydrogen storage [26]. The storage vessels integral to this technique are intricate constructs that necessitate materials endowed with the capacity to endure the extremities of high pressures and exceedingly low temperatures. Typically, these storage tanks are fashioned from composite materials fortified with carbon fibers to ensure structural robustness [29]. Cryo-compressed hydrogen storage is an innovative solution addressing key challenges in the hydrogen storage field.

Analogous to the two antecedent hydrogen storage methodologies, cryo-compressed hydrogen storage exhibits a spectrum of affirmative and negative attributes. On the affirmative front, it endows higher energy density in both gravimetric and volumetric terms when juxtaposed with the discrete cryogenic and high-pressure storage systems. The safety aspect is another positive facet, as the operation occurs at temperatures where hydrogen is rendered less reactive.

Nonetheless, the cryo-compressed hydrogen storage paradigm is not devoid of challenges. Technological complexity is a prominent concern, as the development of a system capable of safe and efficient hydrogen storage under the demanding conditions of high pressure and low temperatures necessitates intricate engineering solutions. Furthermore, the requisite infrastructure for cryo-compressed storage remains an ongoing development, replete with a multitude of challenges that encompass the quest for materials capable of withstanding extreme operating conditions and the formulation of efficient cooling systems.

It is important to note that the cost of each storage technology depends on various factors, including the scale of the system, materials used, manufacturing processes, and market demand. Generally, compressed hydrogen storage incurs lower capital costs compared to other methods, while liquefied hydrogen storage can be more expensive due to the need for cryogenic infrastructure. Cryo-compressed hydrogen storage, positioned between the two in terms of cost, offers an intermediate solution. Ongoing research and development efforts aim to reduce costs and improve the efficiency of all storage technologies, thereby enhancing the economic viability of hydrogen as an energy carrier.

To summarize, these three distinctive hydrogen storage approaches each hold a pivotal role within the sphere of hydrogen technology, each endowed with varying degrees of efficiency, safety considerations, and technological readiness. Ongoing research endeavors are indispensable to grapple with and resolve the inherent challenges intrinsic to each method, thereby advancing the frontiers of hydrogen storage and transportation technologies.

2.2. Material-based hydrogen storage

The chemical mode also referred to as material-based hydrogen storage, represents a more organized approach to hydrogen storage. In this technology, hydrogen is either chemisorbed or physisorbed onto a host material and subsequently released as needed. The interaction between the surface of the host material (adsorbent) and the hydrogen gas (adsorbate) is governed by field forces, which are instrumental in retaining the hydrogen in proximity to the host [40]. This method addresses certain limitations of physical storage techniques, eliminating the need for complex and heavy-pressure vessels [41]. It also allows for controlled hydrogen release at specific temperatures, enhancing safety.

A range of materials, including metal hydrides [42], complex hydrides [43], ammonia-based compounds [44], carbon materials, metal-organic frameworks [45], covalent organic frameworks [46], clathrates [47], and other bio-waste and porous materials [48], has been explored for chemical hydrogen storage. For instance, metal hydrides form robust metal-hydrogen bonds, enabling hydrogen absorption and release through heating or catalysis [49]. Complex hydrides, on the other hand, are multi-element compounds known for their substantial storage capacities via chemical processes [50]. Each material has its unique strengths and limitations based on various factors [51]. There is no universally ideal hydrogen storage material; the choice depends on hydrogen storage capacity, operating conditions, thermodynamics, kinetics, stability, reversibility, availability, cost, and environmental impact. Subsequent sections will delve into advancements in selected materials for chemical hydrogen storage.

In addition, liquid organic hydrogen carriers (LOHCs) present an alternative option for hydrogen storage. In LOHC systems, hydrogen is bonded with H_2-lean ions, and a catalytic dehydrogenation process is employed for release. These systems offer simplicity in operation, environmental friendliness during storage and release, and the potential for reusing the liquid carrier, which is non-corrosive and non-toxic and stored at low pressure. However, LOHCs have limited hydrogen storage potential, with the maximum recorded value being 7.2 wt%, which restricts their widespread use [52].

2.2.1. Chemical sorbents

Chemical sorption involves the covalent binding of hydrogen to a host material, resulting in the breaking down of hydrogen molecules into atomic form due to strong binding enthalpy [53]. Compounds containing hydrogen are disintegrated into atoms and incorporated into the molecular structure of the catalyst substance during chemical sorption [30]. Metal hydrides are a prominent category among materials suitable for chemical sorption. Despite its advantages, such as the ability to store hydrogen under normal conditions and eco-friendly operations, chemical sorption faces challenges such as high expense, weight, and operational temperature, along with the need to enhance charge-discharge kinetics and manage the production of undesirable gases during desorption [54].

2.2.1.1. Metal hydrides. Metal hydrides, a category of materials composed of metal and hydrogen, have garnered considerable attention recently due to their substantial hydrogen-storage capacities, rendering them promising for hydrogen-based energy systems. Their attributes, including high energy density, relatively low cost, and environmental friendliness, render them attractive for applications spanning portable electronics, electric vehicles, and renewable energy systems. However, their advancement for hydrogen storage encounters significant hurdles, notably the identification of materials with high hydrogen-storage capacity while maintaining stability, safety, and economic viability [55].

Various metal hydrides, such as those derived from magnesium, aluminum, and titanium, are under scrutiny by researchers aiming to fulfill the requisites mentioned above. The performance of metal hydrides hinges on several factors, including the metal selection, size and morphology of hydride particles, material purity, and the presence of impurities. These materials form via reversible chemical reactions as certain metals or alloys absorb hydrogen, leading to high volumetric hydrogen density and storage capabilities [56]. Ongoing research endeavors focus on crafting efficient metal hydrides for hydrogen storage, capable of securely and densely storing hydrogen by expanding the metal lattice during absorption and contracting it during release. However, achieving optimal hydrogen absorption and desorption capacities at suitable temperatures and pressures poses a challenge.

Metal hydrides generally have a hydrogen storage capacity of approximately 1%–2% of their weight, which can increase to 5%–7% with active heating for hydrogen removal. While metal hydride tanks can repeatedly store and release hydrogen, their storage capacity is

limited by the accumulation of impurities within the tanks, which clog the spaces where hydrogen would typically be stored, reducing the tank's capacity. The amount of heat transferred, hydrogen absorbed, and hydrogen desorbed in a reversible metal hydride operating at room temperature and atmospheric pressure is generally dependent on the metal alloy used for hydrogen storage [22]. A simplified model illustrating how hydrogen is stored and absorbed in a metal hydride is depicted in Fig. 2.

2.2.1.1.1. Magnesium hydride (MgH$_2$). Magnesium hydride (MgH$_2$) showcases remarkable gravimetric (7.6 wt%) and volumetric (110 kg H$_2$ m^{-3}) hydrogen densities owing to its inexhaustible, cost-effective nature, lightweight, and high chemical stability [57]. However, a major obstacle associated with MgH$_2$ pertains to its robust thermal stability, particularly the formidable Mg–H bond ($\Delta H = 75$ kJ/mol), which impedes hydrogen release. Consequently, achieving effective hydrogen adsorption/desorption with MgH$_2$ at ambient pressure necessitates moderately high temperatures (>300 °C) [58]. Despite the benefits mentioned above, there are challenges associated with its practical use, including high thermodynamic stability, slow kinetics, and high operating temperatures [59]. Modification strategies, such as catalyst addition and nanostructuring by reducing the particle size [60], have been explored to improve its kinetics and reduce operating temperatures. To further clarify the nanostructuring effect, the low surface area of bulk Mg results in a low rate of hydrogen dissociation on the magnesium surface [61]. Consequently, small particle sizes and large specific surface areas of nanostructures made using mechanical ball milling, and nanoconfinement can shorten hydrogen diffusion paths and increase the kinetics of hydrogen desorption and absorption.

In line with the abovementioned ball milling technique, a recent study [62] indicated that about 6.28 wt% of hydrogen at 523 K required absorption and desorption over periods of 20 min and 50 min under pressures of one and zero MPa, respectively, using reactive ball milling of magnesium powder under high pressure of hydrogen gas for 25 h. However, the aggregation of ball-milled nanoparticles during the successive cycles of hydrogen release and uptake could deteriorate the reversible hydrogen storage capacity [63]. Therefore, the application of nano scaffolds is considered a good strategy for avoiding nanoparticle agglomeration. This strategy was employed in a recent investigation [64], in which a porous three-dimensional activated carbon nanostructure modified with Ni and Fe was used to impregnate MgH$_2$ to attain a high hydrogen storage capacity of approximately 6.63 wt% at 453 K and 1 MPa in just 5 min with a high degree of stability.

Generally, the dehydrogenation of magnesium hydride is an endothermic process, indicating that it involves an input of energy to cause bond breakage and release the stored hydrogen. The energy barrier of this process can be described by the activation energy needed to start the dehydrogenation reaction. This activation energy is commonly ranging from 150 to 200 kJ/mol for the dehydrogenation of magnesium hydride. In a recent trial by Meng et al. [65], the activation energy dropped to 78 kJ/mol by catalyzing the reaction using V$_4$Nb$_{18}$O$_{55}$ microspheres at room temperature with a stable reversible capacity of 6.0 wt% for magnesium hydride for ten cycles. Concomitantly with improving the performance and stability of magnesium hydride, Wang et al. [59] found that 6.5 wt% H$_2$ was released in 10 min at 573 K and started to absorb H$_2$ at 313 K using an alloy of different metals, including Cr, Mn, Fe, Co, and Ni. Additionally, 97% hydrogen storage volume was maintained in the same study after twenty cycles at 573 K.

2.2.1.1.2. Lithium hydride (LiH). Lithium hydride (LiH), which is considered one of the lightest metal hydrides ever, has a high gravimetric hydrogen storage capacity of up to around 12.6 wt% [66] but requires high temperatures (673–973 K) and pressures for both hydrogen absorption and desorption. Practical applications of lithium hydride face persistent challenges in terms of kinetics and reversibility. One of the primary obstacles is its high formation energy (−90.5 kJ/mol) and the requirement of a high desorption temperature (700–1000 K). Moreover, LiH readily reacts with humidity, resulting in the irreversible formation of surface corrosion layers, such as lithium oxide and lithium hydroxide. Despite these challenges, controlled hydrolysis of LiH under low relative humidity is recognized as an efficient method for generating hydrogen, particularly for mobility [67,68].

Various strategies have been explored to mitigate the thermodynamic issues associated with LiH. For instance, mechanical milling has been employed to reduce the thermodynamic stability of the lithium hydride-silicon mixture, enabling the storage of 5 wt% hydrogen at 763
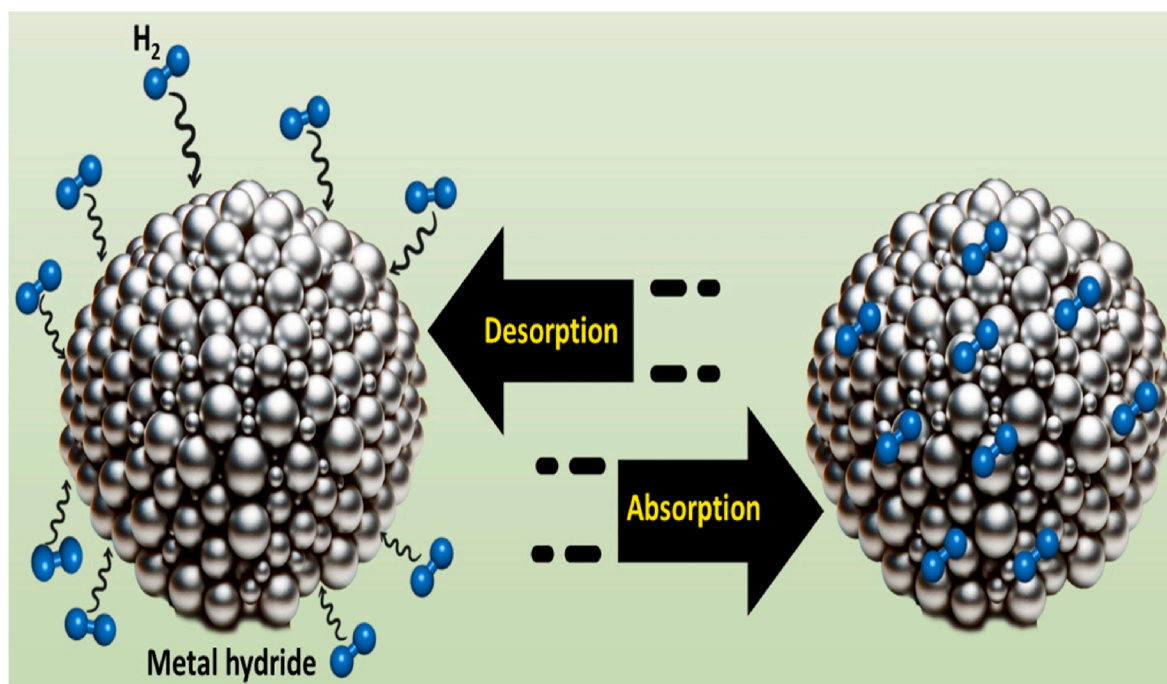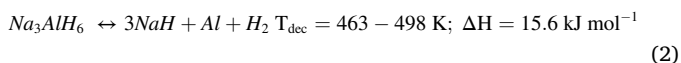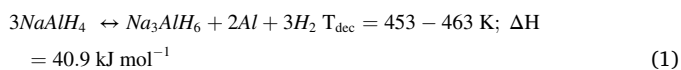

Fig. 2. Illustration of a simplified model depicting metal hydride storage, showcasing the process of hydrogen absorption and desorption within the hydride structure.

K [69]. Similarly, blending LiH with germanium has demonstrated the ability to decrease system stability and store 3 wt% hydrogen at 673 K [70,71]. In another study, Lei Wang and colleagues [72] synthesized LiH nanoparticles via the catalytic hydrogenation of Li, revealing that these nanoparticles, once coated with Ni, can release hydrogen from 373 K. Moreover, Pluengphon et al. [73] investigated Na–Li–H compositions by mixing Na and Li cations under high pressure, utilizing ab initio random structure searching and cluster expansion techniques. Their findings indicated that high pressure enhances the structural stability of Na_3LiH_{12}, $Na_2Li_2H_{12}$, and $NaLi_3H_{12}$ compounds, as confirmed by phonon and elastic constant calculations.

Carbon is a common additive that was previously used to enhance the adsorption/desorption of hydrogen at a temperature less than 473 K [74]. Moreover, a new strategy of inducing vacancy defects in the structure of LiH by varying the concentration of these vacancies from 1 to 25% was very recently investigated by Bahou et al. [68] in 2023. Consequently, they found that gravimetric hydrogen storage capacity increased from 12.6 wt% to 14.6 wt% upon using 16% lithium vacancies.

2.2.1.1.3. Sodium alanate (NaAlH₄). Sodium alanate is a complex metal hydride that can store hydrogen reversibly. It has a relatively high gravimetric capacity (up to 5.5 wt%). However, it requires high temperatures for hydrogen release and often suffers from limited reversibility and stability. Sodium alanate undergoes decomposition to liberate hydrogen via a series of three sequential steps, as depicted by the following reactions [75]:

$$3NaAlH_4 \leftrightarrow Na_3AlH_6 + 2Al + 3H_2 \text{ T}_{dec} = 453 - 463 \text{ K}; \Delta H$$
$$= 40.9 \text{ kJ mol}^{-1} \quad (1)$$

$$Na_3AlH_6 \leftrightarrow 3NaH + Al + H_2 \text{ T}_{dec} = 463 - 498 \text{ K}; \Delta H = 15.6 \text{ kJ mol}^{-1} \quad (2)$$

$$NaH \leftrightarrow Na + {}^1\!/_2 \ H_2 \text{ T}_{dec} \geq 673 \text{ K}; \Delta H = 120 \text{ kJ mol}^{-1} \quad (3)$$

Notably, the final step takes place at temperatures exceeding 673 K. Consequently; the practical hydrogen content is achieved primarily through the initial two reactions, transpiring at temperatures below 498 K, affording a hydrogen storage capacity of 5.6 wt%. However, the elevated desorption temperature and constrained reversibility curtail its practical utility [75].

It has been observed that doping transition metal compounds can lower reaction temperatures, facilitating hydrogen release at reduced temperatures, enhancing reaction kinetics, and improving reversibility [67,76]. In this regard, Ren et al. [77] produced titanium hydride as nanoplates supported on graphene to result in a complete dehydrogenation of sodium alanate at 353 K and rehydrogenation at 303 K under 10 MPa H₂ with a reversible hydrogen capacity of 5 wt%. Additionally, other materials, such as carbon nanomaterials, have been investigated as potential dopants [78,79].

2.2.1.1.4. Ammonia borane (AB, H₃NBH₃). Ammonia borane, a chemical compound synthesized under mild operational conditions, boasts a notable theoretical hydrogen content of 19.6 wt% [80]. This compound serves as a hydrogen source through thermal or chemical processes, rendering it well-suited for portable applications. Ammonia borane is a subject of extensive research due to its impressive stability and non-toxic properties. Various methodologies have conventionally been employed to liberate the stored hydrogen from ammonia borane, with thermal dehydrogenation being a prominent option.

Thermal dehydrogenation entails the application of elevated temperatures to initiate the release of hydrogen, often requiring temperatures exceeding 373 K, thereby cleaving the B–H and N–H bonds within the compound and liberating hydrogen gas [81]. While this approach is conceptually straightforward, it frequently necessitates the use of relatively high temperatures and may exhibit slow kinetics.

An alternative, potentially more efficient method for hydrogen release from ammonia borane involves hydrolysis. Ammonia borane exhibits a notable resistance to hydrolysis in aqueous solutions, thus demanding the presence of an efficient catalyst to induce hydrolytic dehydrogenation at ambient temperatures. Metal-catalyzed hydrolysis emerges as a viable choice, affording the release of a substantial quantity (7–8%) of hydrogen under mild conditions [82]. Thermodynamically unstable metal nanoparticles offer another avenue, which can be kinetically stabilized against agglomeration either through solid support materials characterized by extensive surface areas or via the use of ligands in solution. While the dispersion of metal nanoparticles maintained in the liquid phase by anions or polymers exhibits enhanced hydrogen release efficiency due to more active sites, it's important to note that metal nanoparticles supported on solid materials tend to be less susceptible to aggregation, thus ensuring prolonged lifetimes in comparison to those dispersed in solutions [83]. In light of these considerations, it becomes apparent that there is no universally optimal material for hydrogen storage, as each material presents a unique spectrum of advantages and limitations.

2.2.1.1.5. Metal nitrides including amides (M(NH₂)x) and imides (M (NH)x). Metal amides and imides, such as lithium and magnesium amides and imides constitute a type of complex hydrides that can exhibit gravimetric hydrogen storage capacities in the range of approximately 4–10 wt%, and even higher in some cases [84]. The formulas of these metal amides and imides are represented by the letters M(NH₂)x and M (NH)x, respectively. The specific capacity depends on the metal, the composition of the compound, and the conditions under which hydrogen absorption occurs. Reports indicate metal amides and imides have a hydrogen release efficiency ranging from 50% to 90%. However, it must be noted that obtaining high hydrogen storage content and high release efficiency at low temperatures necessitates the presence of a catalytic material [26]. In addition, amides and imides undergo a dehydrogenation reaction in which ammonia is produced [31]. Consequently, this ammonia production consumes hydrogen, poisons the catalyst, and causes damage to the fuel cell.

A recently published article conducted by Che et al. [85] investigated the catalytic effect of $Li_3VO_4@LiVO_2$ in enhancing the hydrogen absorption and desorption efficiency of lithium-magnesium imide (Li–Mg–N–H) system using three different catalyst ratios (5, 10, and 15 wt%). Among the three ratios, the 10 wt% exhibited the best performance by increasing the hydrogen absorption efficiency from 4.1 wt% using the pristine hydride to 4.7 wt%, and the desorption efficiency approximately from 4.2 wt% to 4.8 wt% at 523 K and zero MPa. Furthermore, the activation energy of the hydrogen desorption was reduced from 117.86 kJ/mol to 99.44 kJ/mol upon using 10 wt% $Li_3VO_4@LiVO_2$.

2.2.2. Physical sorbents

Physisorption entails the physical attachment of hydrogen molecules onto the surface of an adsorbent through weak van der Waals forces, typically characterized by a binding energy ranging from 10 to 100 meV [86,87]. This process occurs rapidly at lower operating temperatures and does not involve any chemical reactions. Materials conducive to physisorption include those with large surface areas and porous structures, such as activated carbon, highly porous metal-organic frameworks (MOFs), covalent organic frameworks (COFs), porous aromatic frameworks (PAFs), and porous organic polymers.

The utilization of porous adsorbent materials facilitates the volumetric densification of hydrogen without imposing significant alterations to the thermodynamic or kinetic properties of storage at elevated pressures. This effect is particularly pronounced at low temperatures, with numerous traditional and innovative adsorbents demonstrating considerable densification of hydrogen at 77 K, corresponding to the normal boiling point of liquid nitrogen, a readily accessible coolant. Initially, emphasis was placed on assessing the gravimetric hydrogen storage capacities of adsorbents for comparison with alternative storage concepts in liquid and solid states; however, recent attention has shifted

towards optimizing volumetric properties [88].

2.2.2.1. Activated carbon and carbon nanomaterials. The hydrogen storage capacity of activated carbon is typically around 1–2 wt% at room temperature and moderate pressures, which is lower than that of advanced materials like metal hydrides. Further, the desorption efficiency of hydrogen from activated carbon can also be limited as it often requires low temperatures ranging from 70 to 398 K for desorption, making the process energy-intensive. However, the wide availability, low cost, and high surface area of activated carbon materials attract researchers' interest to further investigate these materials in storing hydrogen. Further, activated carbon can be utilized in the context of adsorption-based hydrogen purification and gas separation processes, where it can selectively adsorb impurities like carbon dioxide and moisture from hydrogen gas streams.

One of the classic techniques used for improving the hydrogen adsorption efficiency of various materials, such as activated carbon, is ball milling since it helps to increase the surface area. This technique was used 20 years ago by Shindo et al. [89], who recorded a hydrogen storage capacity of almost 3 wt% after milling a commercial sample of activated carbon for 80 h. Applying cryogenic temperatures is another common practice to enhance the hydrogen adsorption efficiency of activated carbon. In this regard, Jemma et al. [90] reported a hydrogen uptake efficacy of 1.8 wt% using activated carbon prepared by the pyrolysis of lignin material of eucalyptus chips at 0.1 MPa and 77 K. Upon using the same temperature, Wróbel-Iwaniec et al. [91] reported storage capacities of 2.95 wt% and 5.61 wt% at 0.1 MPa and 4 MPa, respectively, using chitosan-based activated carbon. Also, Akasaka et al. [92] recorded an improving storage efficiency from 0.6 wt% to 4 wt% after decreasing the temperature from 298 K to 77 K using a coffee bean-based carbon material. Such a study confirmed the efficient use of cryogenic temperatures to improve hydrogen storage capacity.

Carbon nanotubes have been explored as potential materials for hydrogen storage due to their unique structure and properties. The hydrogen storage capacity of carbon nanotubes can vary depending on different factors, such as their diameter, length, functionalization, and operating conditions. The hydrogen storage capacity of single-walled carbon nanotubes can be high, theoretically up to 5 to 10 wt% at room temperature [93]. Experimentally achieving this storage capacity has proven challenging due to optimizing nanotube structure, enhancing hydrogen adsorption and desorption kinetics, and ensuring safe and efficient cycling. Thus, using carbon nanotubes is not practically viable for widespread commercial use in on-board transportation applications [94]. The hydrogen storage capacity achieved at room temperature and standard pressure in various carbon nanotube variants falls significantly short of the goal established by the United States Department of Energy for on-board hydrogen storage systems. However, when the temperature is lowered to 77 K, certain carbon nanotube samples do meet or surpass the United States Department of Energy's target for hydrogen storage.

Certain carbon nanotubes and their hybrid counterparts using metal and oxide nanoparticles can surpass the final objective established by the United States Department of Energy for on-board transportation purposes regarding hydrogen storage capacity. In this regard, Akbarzadeh et al. [95] achieved a 10.94 wt% hydrogen storage capacity using a nanocomposite of iron-silver/titania/carbon nanotube. Another composite of carbon nanotubes and magnesium hydride catalyzed by a vanadium catalyst was used by Kadri et al. [96] by which they observed a hydrogen storage capacity of 6.50 wt% in just a minute and a hydrogen release of 6.50 wt% in 10 min at 473 K and 573 K, respectively. In addition, nitrogen-doped carbon nanotubes were proven to be highly efficient hydrogen storage materials, such as the composite of nitrogen-doped carbon nanotubes mixed with lanthanum oxide that was very recently prepared by Liang et al. [97] and showed a gravimetric capacity of 7.4 wt% at 373 K and 1.8 MPa. So, it is a fact that various materials are being investigated continually to enhance the storage

capacity of carbon nanotubes.

2.2.2.2. Metal-organic frameworks (MOFs). A class of porous materials made up of metal ions or metal clusters coupled to organic ligands. These materials have a large surface area and adjustable pore diameters. Due to their high porosity and substantial surface area, MOFs have demonstrated a strong potential for storing hydrogen through physisorption. Some MOFs have demonstrated hydrogen capacities exceeding 10 wt%, higher than conventional materials. However, achieving such high capacities at ambient conditions is still challenging while maintaining a reversible storage/release cycle. While MOFs have high gravimetric capacities, their volumetric densities are often lower due to the large void spaces between the porous structures [98]. The slow kinetics of both hydrogen adsorption and desorption and the structural changes or degradation upon repeated cycles of hydrogen uptake and release are also two main issues limiting the applicability of MOFs. Therefore, optimizing the metal-organic linker combination, pore sizes, and understanding the interactions between the MOF structure and hydrogen molecules are still a growing era for researchers to enhance the efficiency of metal-organic frameworks.

The spill-over mechanism presents a promising solution for addressing the weak interaction of hydrogen adsorption by utilizing porous carbon materials. This approach, facilitated by metal-based catalysts, operates effectively at room temperature, enhancing hydrogen storage capabilities. In the spill-over mechanism, hydrogen molecules migrate from the catalyst to the surface of porous carbon materials, improving hydrogen storage properties. This process involves several key steps: chemisorption of hydrogen on the surface, dissociation on the metal catalyst, migration of hydrogen from the catalyst to the porous carbon materials surface, and diffusion and desorption at the substrate surface. Achieving hydrogen chemisorption requires a catalyst with significant hydrogen adsorption capacity, typically within an energy range of 0.8–1.8 eV. Subsequently, hydrogen atoms must overcome a substantial energy barrier, ranging from 2.45 to 3.2 eV, for migration to the substrate. Techniques such as hole doping can reduce this energy barrier. Diffusion of hydrogen atoms within the substrate, particularly in MOFs, poses challenges due to the strong C–H bond, resulting in an energy barrier of 1.05–2.16 eV on the MOFs' surface [99,100]. Fig. 3. illustrates the hydrogen migration process across MOFs.

Bambalaza et al. [101] investigated the hydroxylation effect on the hydrogen storage capacity of the University of Oslo Framework 66 (UIO-66), and the positive effect was confirmed by the increased capacity from 3.8 wt% to 4.6 wt% at 77 K and 10 MPa. In addition, metal-organic framework 5 (MOF-5), which is also called isoreticular metal-organic framework 1 (IRMOF-1), was mainly used by Omar Yaghi's research group in hydrogen storage [102], and it exhibited 7.1 wt% at 77 K and 4 MPa that went up to 11.5 wt% at 17 MPa with a volumetric storage capacity of 77 g/L. To increase the interaction of hydrogen molecules with the structure of the MOF and to achieve hydrogen storage under benign conditions, several approaches should be considered, such as the addition of different types of metals to provide extra-framework sites [103]. In line with this approach, Orcajo et al. [104] investigated the effect of lithium ions by introducing a lithium-crown ether complex within the structure of two mesoporous MOFs; Chromium (III) terephthalate Materials of Institute Lavoisier (Cr-MIL-101) and Iron (III) carboxylate Materials of Institute Lavoisier (Fe-MIL-100). The volumetric capacity of Cr-MIL-101 and Fe-MIL-100 increased from 10.89 to 10.82 g/L to 12.27 and 11.21 g/L, respectively, at 298 K and 17 MPa.

2.2.2.3. Covalent organic frameworks (COFs). Covalent organic frameworks (COFs) are a class of materials that resemble MOFs but do not contain heavy-metal ions. They are constructed using organic building blocks through dynamic covalent formation methods. COFs have extended crystalline structures with high surface areas and low
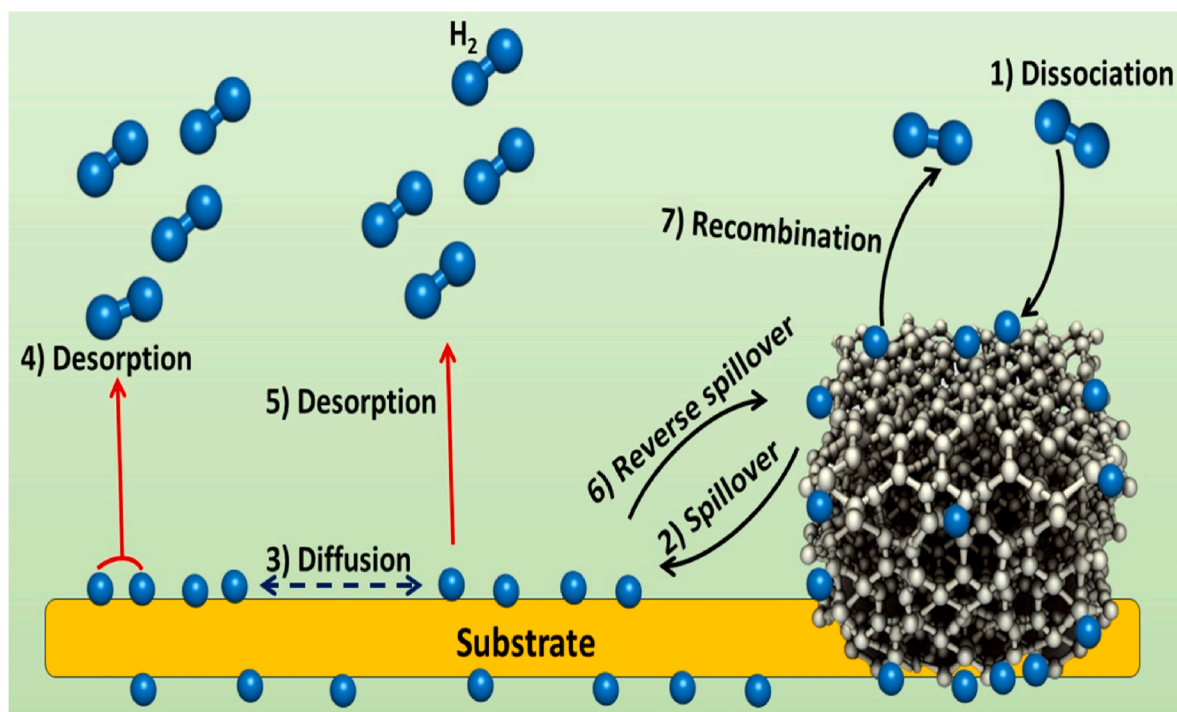
Fig. 3. Visual representation of the hydrogen mobilization pathways in hydrogen storage facilitated by the spill-over mechanism.

densities, similar to MOFs. The absence of heavy-metal ions in COFs provides an advantage in gravimetric hydrogen storage capacity due to their lower density. Depending on the dimensional array of the hypothetical unit cell used to depict the crystalline framework, COFs are categorized as 2D or 3D [105].

Yaghi's team pioneered the use of reticular chemistry to craft both 2D and 3D COFs, incorporating organic components interconnected by boronate ester and/or boroxine units [106,107]. These frameworks exhibit extensive ordered structures, forming a poly-crystalline network due to the partially reversible nature of covalent bond formation during the condensation reaction, known as dynamic covalent chemistry. In addition, Yaghi and his colleagues conducted studies on the hydrogen storage properties of 2D and 3D COFs and found that COF-102 outperforms other COFs, capable of storing close to 7 wt% of hydrogen at 77 K and 35 bar [108,109].

The hydrogen storage capacities of COFs (both 2D and 3D) under high pressure are excellent. However, they fall far short of the standard set by the United States Department of Energy (DOE), which requires a capacity of 4.5 wt% at temperatures ranging from 233 to 333 K by 2020 [110,111]. To address this limitation, researchers have explored the decoration of COFs with metal atoms, which has significantly improved their hydrogen adsorption ability. Zhao et al. [111] discovered that COF-1, when lithium-decorated at 300 K under standard atmospheric pressure, could adsorb three hydrogen molecules around the lithium atom, resulting in a hydrogen adsorption performance of 5.26 wt% at room temperature. Shangguan et al. [112] focused on the hydrogen storage capacity of scandium (Sc)-modified semiconductor COF-1. The modified COF-1 structure demonstrated enhanced hydrogen storage, with each Sc atom stably adsorbing up to four H_2 molecules. The hydrogen storage performance of 6Sc–COF–1 was found to be 5.23 wt% at 300 K, surpassing other materials. At 400 K, all adsorbed hydrogen molecules were released, confirming the material's excellent reversibility. Choi et al. [113] investigated the use of metal-decorated COFs for hydrogen storage. Li and Mg ion-decorated COFs demonstrated hydrogen adsorption energies of 0.28 and 0.30 eV, respectively, exceeding the United States Department of Energy target of 6.5 wt%. The study also explored the effect of counterions on hydrogen storage.

Kalidindi et al. [114] focused on using COFs as templates for Pd nanoparticles and studying their hydrogen storage properties. The Pd@COF-102 hybrid material exhibited a narrow size distribution of Pd nanoparticles, even at high loadings (30 wt%). The hydrogen storage capacity of Pd@COF-102 was enhanced by a factor of 2–3 compared to similar systems, with close to 7 wt% of hydrogen stored at 77 K and 35 bar.

2.2.2.4. Porous organic polymers (POPs). Amorphous porous organic polymers (POPs) have emerged as promising contenders for hydrogen storage due to their convenient processability and robust mechanical properties. POPs can be classified into four main categories: (i) porous aromatic frameworks (PAFs), (ii) conjugated microporous polymers (CMPs), (iii) hyper-*cross*-linked polymers (HCPs) and (iv) polymers of intrinsic microporosity (PIMs) [115].

PAFs represent a category of porous substances primarily comprising light elements like carbon (C), hydrogen (H), oxygen (O), and nitrogen (N). They demonstrate notable adjustability during synthesis, yielding reproducible outcomes. PAFs offer numerous beneficial attributes, including elevated specific surface area, notable porosity, robust chemical and thermal stability, strong π-π conjugation, and extensive versatility. Consequently, PAFs have diverse applications, particularly in fields such as gas storage [116]. Ben et al. [117] focused on synthesizing a porous aromatic framework called PAF-1 with high stability and exceptional surface area. PAF-1 demonstrated a Langmuir surface area of 7100 m²/g, outperforming highly porous MOFs. It also exhibited high thermal and hydrothermal stabilities. Additionally, PAF-1 showed significant uptake capacities for hydrogen (10.7 wt% at 77 K, 4.8 MP). Yuan and colleagues [118] synthesized a range of PAF-1 derivatives by substituting the central carbon atom of the tetrahedral monomers with adamantane (PPN-3), silicon (PPN-4), and germanium (PPN-5), specifically for hydrogen storage. The authors found that PPN-4 exhibited a high surface area of 6461 m²/g (BET) and 10063 m²/g (Langmuir). PPN-4 demonstrated impressive hydrogen storage capacities, with an excess uptake of 8.34 wt% at 77 K and 5.5 MP, reaching a total uptake of 13.6 wt% at 8 MP. These results make PPN-4 one of the highest-performing materials for hydrogen storage, surpassing many

other porous materials and even comparable to the best values reported in MOFs.

CMP compounds represent noteworthy examples of adsorption materials that have recently witnessed significant advancements. The majority of measured adsorption capacities were typically determined at 77 K, a temperature significantly lower than the typical operational temperatures required for practical applications [119]. In his context, Qiao et al. [120] focused on the design and synthesis of two novel conjugated microporous networks, P-1 and P-2, for gas storage and separation applications. The networks were prepared through $FeCl_3$ oxidative coupling polymerization. The results showed that P-2 had a higher BET surface area (1222 m^2/g) compared to P-1 (611 m^2/g), indicating improved porosity. The hydrogen storage capacity of P-1 was found to be 1.05 wt% at 77 K and 1.1 bar, while P-2 exhibited a higher capacity of 1.66 wt%. The isosteric heat for hydrogen adsorption was 9.89 kJ/mol for P-1 and 10.86 kJ/mol for P-2. These findings suggest that P-2 has promising potential for hydrogen storage applications [121]. The CMPs, named CMP-G1 and CMP-G2, were synthesized through a tandem oxidative reaction in one-pot. The CMPs exhibited large surface areas and micropore sizes ranging from 0.5 to 1.5 nm. The hydrogen adsorption capacity was determined to be 2.69 wt% for CMP-G1 and 2.14 wt% for CMP-G2 at 20 bar and 77 K, respectively. These findings indicate the potential application of CMP-Gs in hydrogen storage, highlighting their significance in the development of clean energy sources.

HCPs are essentially highly interconnected porous polymers. Their inception dates back to the early 1970s when Davankov and colleagues first introduced them [122]. HCPs were synthesized through the extensive post-crosslinking of linear polystyrene (PS) chains, achieved via Friedel–Crafts reactions. This process involves the formation of structural bridges between adjacent aromatic rings and other chains while in a highly swollen state. The resulting porous materials offer numerous advantages over non-porous counterparts due to their high porosity [123]. For hydrogen storage, Lee et al. [124] investigated the hydrogen adsorption properties of microporous HCPs synthesized from polystyrene. The polymer exhibited a high apparent BET surface area of 1466 m^2/g and a nitrogen Langmuir surface area of 2138 m^2/g. At 77 K and 1.5 MP, the polymer adsorbed 3.04 wt% hydrogen, which represents the highest level of hydrogen adsorption observed for an organic polymer. The study aimed to address the challenge of hydrogen storage for fuel applications. Compared to other materials, such as carbon and MOFs, the HCPs showed promising hydrogen sorption capacities, particularly at pressures above 0.5 MP. The results demonstrate the potential of organic polymers as attractive candidates for hydrogen storage due to their light elemental composition, synthetic versatility, and high surface areas. Another research conducted by Wood and his team [125] focused on hydrogen storage in microporous HCPs networks. They synthesized a series of networks using bischloromethyl monomers and found that the materials exhibited high microporosity with BET surface areas up to 1904 m^2/g. Among the networks, those based on 4, 4′-bis(chloromethyl)-1,1′-biphenyl (BCMBP) showed the highest gravimetric storage capacity for hydrogen, reaching 3.68 wt% at 1.5 MP and 77.3 K. The isosteric heat of sorption for hydrogen on these materials was determined to be in the range of 6–7.5 kJ/mol.

PIMs represent a widely researched polymer class characterized by rigid ladder-like backbones interspersed with sites of contortion, hindering efficient packing in the solid state and resulting in substantial free volume [126]. Consequently, PIMs demonstrate relatively high surface areas ranging from 560 to 1760 m^2/g and micropores smaller than 2 nm, as defined by the International Union of Pure and Applied Chemistry (IUPAC) [127–129]. Despite their appealing intrinsic properties and processability, PIM-1 exhibits relatively low hydrogen storage capabilities (<2 wt%) [127]. This limitation is attributed to its constrained surface area and pore volume, posing challenges for enhancement. Previous efforts to improve the surface area and gas storage properties of PIM-1 involved incorporating high-surface-area powders such as MOFs

or activated carbon. For testing the stability of PIM for hydrogen storage, Rochat et al. [130] investigated the long-term stability of the PIM-1 for hydrogen storage applications. Over a period of 400 days, the mechanical and surface properties of PIM-1 were examined. The results showed that most mechanical and surface properties remained stable over time, including mechanical strength, elasticity, and surface area. However, there was a small but statistically significant decrease in the hydrogen storage capacity of PIM-1, particularly in the initial stages of aging. This decrease was attributed to the slow rearrangement of the polymer scaffold. Overall, the study demonstrated that PIM-1 possesses the necessary long-term stability for realistic hydrogen storage applications.

2.2.2.5. Zeolites. Zeolites are crystalline aluminosilicates with well-defined porous structures. Due to their unique microporous nature and large surface area, zeolites have been investigated as potential materials for hydrogen storage [131]. Zeolites store hydrogen mainly through physisorption, which is a type of physical adsorption resulting from weak Van der Waals forces between the hydrogen molecules and the surface of the zeolite. The adsorption process is reversible, so hydrogen can easily be released when needed.

The utility of zeolites for hydrogen storage is contingent upon several factors, with their significant surface area being a pivotal consideration, often ranging from several hundred to well over a thousand square meters per gram [132]. This large surface area offers hydrogen molecules a large number of adsorption sites, increasing their storage capacity. Zeolites' pore sizes and topologies can be customized during the synthesis process, enabling optimization for optimal hydrogen uptake. Moreover, zeolites are thermally stable, which is advantageous for storing hydrogen at high temperatures. Also, there is interest in the phenomenon known as "hydrogen spillover", where metal-loaded zeolites can dissociate molecular hydrogen on the metal and then spill the atomic hydrogen onto the adjacent zeolite support, potentially increasing storage capacity [133]. However, this mechanism is still a subject of research and debate.

Another main factor is the ionic exchange characteristic within the zeolite structures that improve their storage capacity [134]. Further, zeolites are valuable because their ion-exchange property allows the modification of the valence state and size of the exchangeable cations, which in turn controls the diameter of the cages and channels, making it possible to manipulate the zeolite's accessible space [135]. One of the early-conducted studies to investigate zeolites is the one done by Langmi et al. [135], in which the storage capacity trend improved for the first time by increasing the cation size followed by a capacity drop upon further increasing the cation size using alkali and alkaline earth metal ions. This trend was observed by the enhanced capacity from 1.79 wt% using sodium-based-zeolite X to 1.96 wt% by potassium-based-zeolite X, followed by a drop to 1.46 wt% and 1.32 wt% using rubidium and cesium-based-zeolite X, respectively.

Similarly, the alkaline earth metal cations increased the storage capacity from 1.62 wt% to 2.19 wt% by shifting from magnesium to calcium-based-zeolite X, followed by a drop to 1.68 wt% using strontium-based-zeolite X at 77 K and 1.5 MPa. Such a result was attributed to the zeolite's pore blocking by the large size of cations. Other types of zeolites were used in hydrogen storage, such as ultra-stable Y zeolite that attained 0.4 wt% at 303 K and 5 MPa [136], and zeolite socony mobil-5 that reached 2.89 wt% at 77 K and 1.2 MPa [137]. On the other hand, some limitations influence the efficiency of zeolites in storing hydrogen, such as their low hydrogen storage capacity at ambient temperatures and pressures that still fall short of the standards specified for realistic automotive applications. In addition, the energy required to desorb hydrogen (release it from the storage material) is sometimes higher than ideal for some applications.

2.2.2.6. Clathrates. Clathrates, scientifically termed gas hydrates, are

intricate crystalline formations arising from the structural arrangement of water molecules. These formations assume a cage-like architecture, adept at encapsulating guest molecules devoid of any chemical bonding. Typically, these guest molecules manifest as gases. Given the heightened demand for safe and efficient materials conducive to hydrogen storage, clathrates have emerged as an encouraging category of substances for potential application. The containment of hydrogen within water cages, as facilitated by clathrates, serves to substantially reduce the associated hazards related to sudden gas release or explosive occurrences [138].

Clathrates can be broadly categorized into two principal types: clathrate hydrates and semi-clathrate hydrates. This categorization is contingent upon the nature of the interactions between the guest species and the host framework. Semi-clathrate hydrates exhibit a combination of partial hydrogen bonding and van der Waal's forces in the interactions between guest and host entities, as elucidated in recent research by Gupta et al. [139]. In contrast, clathrate hydrates primarily rely on weak van der Waal forces governing the interaction between host and guest molecules.

Recent studies, such as the work by Veluswamy et al. [140], underscore a growing interest in investigating clathrate hydrates for hydrogen storage. This interest is attributed primarily to several positive attributes, which encompass (i) the utilization of minimal promoters in conjunction with water to enhance operational conditions, (ii) the ability to store hydrogen in its molecular form, allowing for immediate utilization with minimal thermal or depressurization requirements; (iii) the capacity to store hydrogen at moderate temperatures and pressures, particularly in cases involving low promoter content; and (iv) the promise of substantial gravimetric and volumetric storage capacities. It is crucial, however, to acknowledge that, as noted by Zhang et al. [138], certain challenges must be surmounted, including (i) the notable volume requirement for the supporting medium, (ii) the substantial energy input necessary for ice production; (iii) concerns related to the efficiency of hydrogen uptake; and (iv) limitations tied to mass transfer. The classification of clathrate structures primarily revolves around their crystallographic characteristics, as visually represented in Table 1.

The difficulty in forming clathrates under typical ambient conditions primarily arises from hydrogen's small molecular size, presenting a significant obstacle. Therefore, scientists have initiated investigations into diverse techniques to improve storage capacity. One of these approaches involves the utilization of assisting gases like tetrahydrofuran and methane, which have demonstrated the ability to catalyze the formation of hydrogen clathrates [141]. As depicted in Tables 1 and it is evident that pure hydrogen does not readily give rise to a stable structure I. Therefore, various promoters are employed to facilitate the

formation and stabilization of such clathrates. Among these promoters, methane, as utilized by Matsumoto et al. [142], yields a modest hydrogen content of only 0.02 wt% at 263 K and 70 MPa. In another study, propane was utilized to promote the formation of hydrogen hydrates, and the storage capacity was just 0.17 wt% at 270 K and 12 MPa [143]. A better result was reported by Belosludov et al. [144] when the storage capacity reached 2.5 wt% at 250 K upon using ethane as a promoter, yet a very high pressure of 300 MPa. Therefore, researchers are trying to investigate other types of hydrogen hydrates, such as structure II.

The use of promoter molecules, such as tetrahydrofuran, has shown promising outcomes in enhancing the hydrate structures of type II for hydrogen storage. The presence of these promoter molecules aids in stabilizing the hydrate structure and significantly augments the hydrogen storage capacity. One of the early studies [145] that used tetrahydrofuran in 2004 to reduce the pressure required to store hydrogen in a structure II binary clathrate hydrate to 5 MPa at 279.6 K resulted in just 1 wt% of hydrogen storage. Such a result could be attributed to the exclusive presence of hydrogen molecules within the small cages, with their complete absence in the larger cages, which were occupied by tetrahydrofuran.

A year later, an investigation by Lee et al. [146] was conducted to improve the hydrogen storage capacity of structure II binary clathrate hydrate by reducing the concentration of tetrahydrofuran from 5.56 to 0.7, 0.5, and 0.15 mol%. Consequently, the capacity increased from 2.1 to 2.4, 2.7, and 4.03 wt%, respectively, at 12 MPa and 270 K. In 2009, Sugahara et al. [147] could not produce pure hydrogen hydrates at 70 MPa and 255 K, but they successfully synthesized hydrogen-tetrahydrofuran binary hydrates at the same conditions, showing 3.4 wt% of hydrogen storage. In 2017, a study carried out by Liu et al. [148] demonstrated that the gravimetric capacity of hydrogen was about 4.4 wt% using pure hydrogen hydrates. Consequently, this capacity diminished to a range of 1.6–3.8 wt% upon using binary hydrates of hydrogen and tetrahydrofuran at 140 K.

Other promoters were also used to produce binary structure II clathrate hydrates, such as methane, as employed by Belosludov et al. [149] to obtain a gravimetric capacity of 2.6 wt% at 250 K and 70 MPa. Furthermore, a recent study in 2023 was undertaken by Liu et al. [150] in which they attained a storage capacity of 3.43 wt% at 270 K and 20 MPa. Another promoter, nitrogen gas, was utilized by Liu et al. [151] to replace hydrogen in both small and large cages of binary hydrates to increase the hydrogen storage capacity to 4.4 wt% at 243 K and 15 MPa. Epoxycyclopentane is another promoter used very recently by Chen et al. [152] to produce a binary hydrate with a hydrogen storage capacity of 0.63 wt% at 262 K and 18.2 MPa. Thus, various promoters could be used to produce these binary hydrate structures.

The Solid-HyStore technology has numerous advantages that make it stand out as a potential replacement for traditional hydrogen storage techniques like compressed hydrogen and liquid hydrogen. Methylcyclohexane, methyl *tert*-butyl ether, and 1,1-dimethylcyclohexane are the most common promoters used in producing binary hydrates of Solid-HyStore [138]. In this regard, Papadimitriou et al. [153] reported that the storage capacity was 1.4 wt%. This storage capacity was achieved by introducing methylcyclohexane as a promoter to facilitate the formation of a binary Solid-HyStore hydrate at 274 K and 500 MPa.

Recently, semi-clathrates hydrates have received a great deal of interest because of their extraordinary capacity to store low molecular weight-gas molecules such as carbon dioxide, methane, and hydrogen even at temperatures and pressures that are close to ambient conditions by combining water molecules with quaternary ammonium salts. Additionally, the quaternary ammonium salt solution has a lower vapor pressure than volatile organic solutions like tetrahydrofuran solution, minimizing the possibility of contaminants being introduced to the hydrogen gas generated during the dissociation of hydrates [138]. Tetrabutylammonium bromide, tetrabutylammonium chloride, and tetrabutylphosphonium bromide are some of the common quaternary salts

Table 1
Classification of clathrates based on crystallographic attributes.

Structure I (sI)	Structure II (sII)	Structure H (sH)
• A cubic structure, and is one of the most common types of clathrates. • It consists of small dodecahedral (12-faced) and larger tetrakaidecahedral (14-faced) cages. • Common gases that form sI hydrates include methane, ethylene, and others, but pure hydrogen typically doesn't form stable sI hydrates. • Mixtures of hydrogen with other gases can, however, stabilize the formation of sI hydrates.	• A cubic structure. • It consists of small dodecahedral and larger hexakaidecahedral (16-faced) cages. • Larger gases, like ethane, propane, and carbon dioxide, form sII hydrates. • sII hydrates are more accommodating to hydrogen, especially in the presence of suitable promoter gases. For instance, hydrogen can form sII hydrates in the presence of tetrahydrofuran or certain other organic molecules.	• A hexagonal structure. • It has small dodecahedral, medium-sized hexakaidecahedral, and large icosakaioctahedral (24-faced) cages. • Gases like krypton, xenon, and some larger hydrocarbons form sH hydrates. • Hydrogen can also form sH hydrates under certain conditions, especially when other larger guest molecules are present to occupy the large cages.

used in the formation of semiclathrates hydrates. The feasibility of utilizing tetrabutylammonium chloride and tetrabutylphosphonium bromide-based semi-clathrates for hydrogen storage was explored by Deschamps and Dalmazzone [154]. They determined that these materials exhibited hydrogen storage capacities of 0.12 wt% (at 288.9 K) and 0.14 wt% (at 285 K), respectively, under a pressure of 15 MPa. Another study by Strobel et al. [155] revealed a slightly higher storage capacity (0.21 wt%) compared to the study mentioned above using tetra-*n*-butylammonium bromide at 279.5 K and 13.8 MPa. Based on the above-mentioned information, a comparison between clathrates and semi-clathrates is presented in Fig. 4 to clarify the main differences between these types. Comprehensive tabulated comparison of hydrogen storage materials was summarized in Table 2.

2.3. Underground storage of hydrogen

Underground hydrogen storage emerges as a highly promising approach for effectively managing substantial hydrogen volumes while offering notable advantages in terms of safety and spatial efficiency. Subsurface formations, including aquifers, depleted oil and gas reservoirs, and salt caverns, are considered suitable options for hydrogen storage [159]. Salt caverns, in particular, are highly favored due to their advantageous attributes, encompassing low permeability and expansive storage capacity, which bestow significant buffering capacity, making

them suitable for accommodating intermittent energy sources [160]. An underground gas storage facility involves the artificial accumulation of gas in the natural environment, typically at a considerable depth, often exceeding several hundred meters. The stored gas consists of two components: the working gas, which is injected into and extracted from the storage, and the cushion gas, which remains within the facility throughout its operational lifespan. The purpose of the cushion gas is twofold: to maintain a minimum pressure level that prevents the ingress of water into the storage space and to ensure optimal conditions for gas injection [161,162].

Advantages of underground gas storage facilities include [161].

I. Enhanced safety: Underground facilities are less vulnerable to risks such as fires, terrorist attacks, or military actions compared to surface storage tanks.
II. Efficient space management: Underground facilities can store significant amounts of gas while occupying relatively small surface areas. In contrast, surface tanks would require extensive space to achieve the same storage capacity. The compact nature of underground facilities allows for easier integration with the landscape and existing infrastructure.
III. Cost-effectiveness: Constructing underground gas storage facilities is generally more economical compared to surface facilities

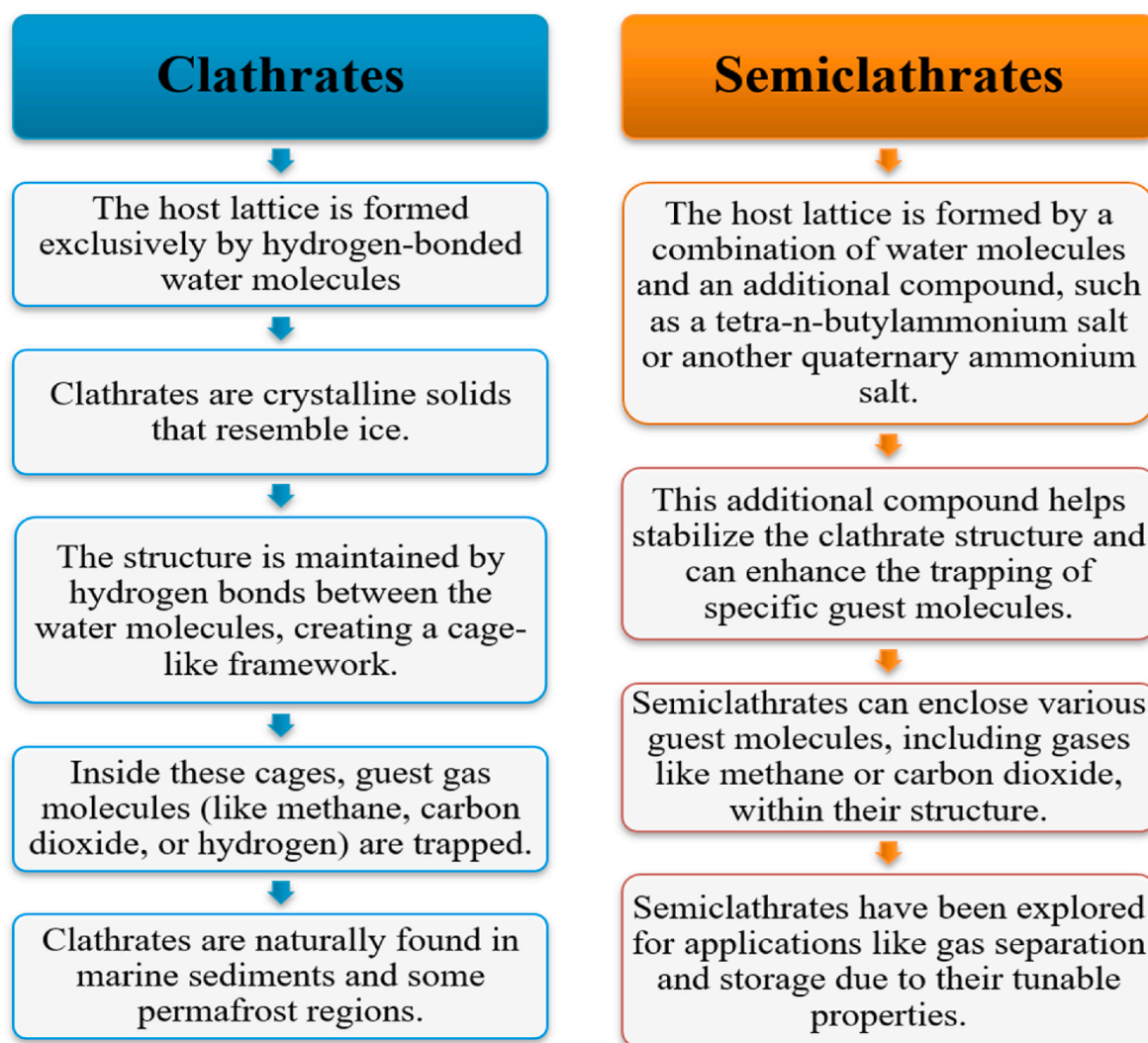

Fig. 4. Comparative insight on distinguishing clathrates from semi-clathrates. Clathrates are composed solely of water molecules, while semi-clathrates necessitate the presence of quaternary ammonium salts in their formation.

Table 2

Comprehensive tabulated comparison of hydrogen storage materials.

Storage material	Gravimetric hydrogen storage capacity (wt%)	Temperature (K)	Pressure (MPa)	Reference
Ball-milled magnesium hydride	6.28	523	1	[62]
Magnesium hydride impregnated with a porous 3D activated carbon nanostructure modified with nickel and iron	6.63	453	1	[64]
Sodium alanate with titanium hydride as nanoplates supported on graphene	5	353	10	[77]
Lithium-magnesium imide	4.1	523	0	[85]
Lithium-magnesium imide enhanced by 10% lithium vanadate@lithium vanadium oxide	4.7			
Activated carbon from pyrolyzed lignin material based-eucalyptus chips	1.8	77	0.1	[90]
Chitosan-based activated carbon	2.95	77	0.1	[91]
	5.61		4	
Coffee bean-based carbon material	0.6	298	12	[92]
	4	77		
Nitrogen-doped carbon nanotubes mixed with lanthanum oxide	7.4	373	1.8	[97]
University of Oslo Framework 66 (UIO-66)	3.8	77	10	[101]
Hydroxylated University of Oslo Framework 66 (UIO-66)	4.6			
Isoreticular metal-organic framework 1 (IRMOF-1)	7.1	77	4	[102]
	11.5		17	
2,2-bipyridine-5,5′-dicarboxylate (bpdc)-based University of Oslo framework	5.7	77	2	[156]
Magnesium hydride	6.91	648	1	[157]
Magnesium@cobalt (II)-based metal-organic framework	5.19			
Magnesium@iron (II)-based metal-organic framework	5.37			
Magnesium hydride promoted by vanadium-based metal-organic framework	6.4	573	3.2	[158]
Structure I of clathrates promoted by methane	0.02	273	70	[142]
Structure I of clathrates promoted by propane	0.17	270	12	[143]
Structure I of clathrates promoted by ethane	2.5	250	300	[144]
Structure II of clathrates promoted by tetrahydrofuran (binary hydrates)	1	279.6	5	[145]
Structure II of clathrates promoted by tetrahydrofuran (binary hydrates)	4.03	270	12	[146]
Structure II of clathrates promoted by tetrahydrofuran (binary hydrates)	3.4	255	70	[147]
Pure hydrogen hydrates	4.4	140	0.1	[148]
Binary hydrates of hydrogen and tetrahydrofuran	1.6–3.8			
Structure II of clathrates promoted by methane (binary hydrates)	2.6	250	70	[149]
Structure II of clathrates promoted by methane (binary hydrates)	3.43	270	20	[150]
Structure II of clathrates promoted by nitrogen (binary hydrates)	4.4	243	15	[151]
Structure II of clathrates promoted by epoxycyclopentane (binary hydrates)	0.63	262	18.2	[152]
Solid-HyStore hydrate promoted by methylcyclohexane (binary hydrates)	1.4	274	500	[153]
Tetrabutylammonium chloride-based semiclathrates	0.12	288.9	15	[154]
Tetrabutylphosphonium bromide-based semiclathrates	0.14	285		
Tetra-*n*-butylammonium bromide-based semiclathrates	0.21	279.5	13.8	[155]
Sodium based-zeolite X	1.79	77	1.5	[135]
Potassium based-zeolite X	1.96			
Rubidium based-zeolite X	1.46			
Cesium based-zeolite X	1.32			
Magnesium based-zeolite X	1.62			
Calcium based-zeolite X	2.19			
Strontium based-zeolite X	1.68			
Ultra-stable Y zeolite	0.4	303	5	[136]
Zeolite socony mobil-5	2.89	77	1.2	[137]

of similar capacity. The lower construction costs contribute to the overall cost efficiency of underground storage.

IV. Abundance of suitable geological structures: Many countries and large areas possess suitable geological formations for underground gas storage. These structures provide favorable conditions for the establishment and operation of underground facilities.

To ensure the secure and efficient storage of hydrogen underground, a comprehensive understanding of the structural and geochemical characteristics of these subterranean formations is essential throughout the process of geological hydrogen sequestration [163]. Despite the challenges, underground storage remains a viable and pivotal component in the realization of a hydrogen-based economy, demanding ongoing research and development endeavors [164]. Readers seeking a more comprehensive exploration of underground hydrogen storage are encouraged to delve into the detailed article by Ref. [165].

2.3.1. Salt cavern

Salt caverns, primarily cylindrical in shape, are artificial excavations within thick underground salt deposits constructed through solution mining, a process involving controlled water injection into a well drilled into the salt rock. This method facilitates the dissolution of salt, forming

caverns with specific dimensions [166,167]. These caverns, typically built up to 2000 m deep with volumes reaching 1,000,000 cubic meters, are well-suited for storing various substances, particularly gases, under high pressures [167]. The pressure range during operation usually falls between 30% and 80% of lithostatic pressure [168]. Geological factors such as salt tightness, mechanical properties, and resistance to chemical reactions render salt caverns an attractive option for hydrogen storage, bolstered by the sealing capabilities conferred by the viscoplastic attributes of evaporitic rocks [169,170].

Salt deposits suitable for cavern construction can be categorized as salt domes, bedded formations, or salt cushions, with bedded salt requiring a minimum thickness of 200 m and depth ranging from 500 to 1400 m [166,167,171]. However, maintaining structural stability becomes challenging beyond a certain depth due to salt deformation [172, 173]. Despite being globally distributed, suitable rock salt formations are geographically constrained compared to porous geological formations [174]. Salt caverns offer versatility through the ability to modify their geometry, dependent on factors such as solution mining method, cavern depth, and salt deposit type. This adaptability allows for customization of shape, dimensions, and volume to meet specific storage requirements [171,175].

In both the United Kingdom and the United States, only a limited

number of sites currently accommodate hydrogen storage within salt caverns. Notable examples include Teesside in the UK and Clemens Dome, Spindletop, and Moss Bluff in the US [161,176]. The Teesside facility, operational since the 1970s, utilizes elliptically shaped salt caverns situated at depths ranging from 350 to 450 m, boasting a collective volume of 210,000 cubic meters. Conversely, the salt caverns at Clemens Dome and Moss Bluff, located at a depth of 800 m from the cavern's top, have larger capacities of approximately 580,000 cubic meters each. Clemens Dome has been in operation since 1983, while Moss Bluff commenced operations in 2007. These longstanding projects serve as compelling evidence of the technical viability of underground hydrogen storage over extended periods [176,177].

Caglayan et al. [177] focused on the technical potential of salt caverns for hydrogen storage in Europe. The study estimated the storage capacity and suitability of European subsurface salt structures for hydrogen storage. The results indicated that salt cavern storage is a promising technology due to its large capacity, low investment cost, high sealing potential, and low cushion gas requirement. The total technical storage potential for hydrogen across Europe was estimated at 84.8 PWh_{H2} (petawatt-hours of hydrogen), with onshore salt caverns within 50 km of the coast constituting approximately 30% (7.3 PWh_{H2}) of the total potential. Germany had the highest storage potential among European countries, with 9.4 PWh_{H2}. Norway also showed significant potential for offshore caverns with 7.5 PWh_{H2}. These findings highlight the significant role of salt caverns in facilitating hydrogen storage in Europe. A recent study conducted by Dias et al. [178] focused on the hydrogen storage process in salt caverns, specifically in the Brazilian pre-salt fields. The study analyzed the integrity of the caverns, considering thermomechanical effects, such as temperature and pressure variations. A simulation approach was used, coupling thermomechanical finite element analysis with thermodynamics gas simulation. The results highlighted the importance of thermal effects in maintaining the integrity of the salt rock. Significant temperature amplitudes were found to compromise rock integrity by inducing tensile stresses and affecting permeability. The study emphasized the suitability of salt caverns for underground hydrogen storage due to their low porosity, low permeability, relevant creep, and self-healing properties.

In China, Liu et al. [179] evaluated the feasibility of large-scale underground hydrogen storage in bedded salt rocks, using Jiangsu province as a case study. The Jintan salt mine in Jiangsu was identified as a potential site for underground hydrogen storage. The study analyzed the geological conditions and stability of the salt caverns for underground hydrogen storage, as well as their tightness. The results showed that the gas tightness of the underground hydrogen storage salt caverns could be as low as 18 m^2 or lower. It was estimated that salt caverns could provide favorable conditions for a 36.9 TWh-scale underground hydrogen storage in Jiangsu. The study concluded that underground hydrogen storage in bedded salt rocks offers a feasible and economical solution for large-scale hydrogen storage, particularly in regions abundant in renewable energy and salt resources.

2.3.2. Aquifers

Aquifers, characterized by their porous and permeable rock formations filled with fresh or saline water, present a potential alternative for underground hydrogen storage, particularly in areas lacking depleted hydrocarbon deposits or salt caverns. Unlike the latter options, aquifers are widely distributed in sedimentary basins worldwide, often situated near major energy consumers and urban centers. Aquifers have a history of safe use for natural gas storage, making them a viable option for hydrogen storage [161].

The process of hydrogen storage in deep aquifers mirrors that in depleted oil and gas deposits, necessitating specific geological conditions. The selected rocks for injection must exhibit favorable reservoir characteristics and be overlain by impermeable roof rocks to prevent gas migration. Creating storage space in aquifers involves displacing the water-filled pore space downward and sideways, leading to an increase

in pressure. During injection, gas displaces water, creating a dynamic gas/water boundary that shifts during the storage facility's operation. However, a drawback is that some gas remains unrecoverable in the aquifer [161,169,170].

Despite the potential of aquifers, various hazards are associated with hydrogen migration, such as leakage along undetected faults and biochemical reactions. The tightness of aquifers is initially unknown, necessitating costly tests to determine overall site tightness and the sealing properties of overlying rocks. The risk of hydrogen leakage to the surface is considered low, and potential eruptions can be prevented by subsurface safety valves. Aquifers offer an advantage in that stored hydrogen cannot ignite due to the lack of oxygen, eliminating the risk of flammable mixture formation [170].

While aquifers are globally distributed, suitable rock formations for cavern construction are geographically constrained compared to porous geological formations. Despite these challenges, aquifers provide versatility in modifying cavern geometry to meet specific storage needs. However, the creation of aquifer storage facilities tends to be costlier due to the need for extensive drilling and testing to ensure tightness.

To date, literature lacks reports of pure hydrogen storage in aquifers, but town gas storage projects, comprising around 50% hydrogen and 50% methane, have been undertaken in Europe [170,180,181]. Saline aquifers, with their widespread distribution and high storage capacities, present a cost-effective option for long-term hydrogen storage. They offer greater storage capacities compared to depleted oil and gas reservoirs, making them a valuable resource for large-scale geological hydrogen storage worldwide. The environmentally friendly nature of aquifer storage, with no freshwater injection or brine disposal, makes it an attractive option for contributing to the global clean energy transition. Extensive research and field experience with natural gas storage and carbon capture and storage operations in saline aquifers provide valuable hydrogeological and geological information. Saline aquifers have hosted the most current natural gas storage operations globally, making them well-suited for large-scale hydrogen storage. However, aquifers pose economic challenges, requiring higher infrastructural investments compared to depleted reservoirs and salt caverns [174].

In regions where depleted reservoirs are absent, aquifers have become a viable option for underground hydrogen storage. These porous rock formations must exhibit high porosity, permeability, and capacity for comparable efficiency to depleted reservoirs. However, economic considerations pose challenges, as aquifers demand higher infrastructure investments, including above-ground facilities like wells, pipelines, and injection techniques. The economic viability of aquifer storage is further compromised by excessive hydrogen-water production and changes in the liquid-gas interface during injection and withdrawal cycles. The challenges shared with depleted reservoirs, such as the need for hydrodynamic assessments and favorable reservoir characteristics, underscore the need for a thorough evaluation of aquifers as a viable option for large-scale underground hydrogen storage [182].

2.3.3. Depleted oil and gas reservoirs

Natural gas and petroleum deposits, found in geological traps like porous rocks such as carbonates or sandstones, constitute reservoirs where hydrocarbons accumulate. These reservoirs are commonly sealed by rocks to prevent hydrocarbon migration. Over a century of successful natural gas operations has established depleted reservoirs as economically feasible options for underground hydrogen storage. Criteria for successful long-term underground hydrogen storage in such reservoirs include safety, integrity, and economic feasibility evaluations. Utilizing remnants of native gases in these reservoirs as cushion gas ensures tightness and sustains pressure. However, challenges such as bacterial hydrogen loss, biological reactions, cushion gas mixing, and hydrogen purity during withdrawal need addressing [166,170,182,183].

Depleted gas reservoirs are currently the most promising option for large-scale hydrogen storage due to their proven capacities and existing infrastructure. Yet, knowledge gained from storing other gases like

methane and carbon dioxide does not guarantee suitability for hydrogen due to its different characteristics. Hydrogen's reactivity with reservoir rocks can alter pore structures, affecting injectivity and storage capacity. While hydrogen loss during storage is minimal, significant losses occur through residual trapping, geochemical reactions, and caprock leakage. Understanding fluid migration through reservoirs is crucial, considering mineralogical changes induced by hydrogen interaction [184].

Comprehensive datasets on reservoir rocks and their changes with hydrogen interaction are essential. However, significant gaps exist in understanding mineralogical, chemical, and petrophysical changes upon hydrogen interaction. Microbial activity in reservoirs can lead to hydrogen conversion to other gases, impacting storage capacity and safety. Depleted oil and gas reservoirs, with known trapping capacities and operational pressure ranges, are feasible for medium-term hydrogen storage and production. Despite being an attractive option, technology for underground hydrogen storage in porous reservoirs is still under-developed, with uncertainties remaining [184–186].

Storing hydrogen in depleted oil and gas fields offers advantages such as available residual gas for cushioning and potential long-term gas retention. Medium-term commercial timeframes for hydrogen storage are shorter than those for long-term carbon dioxide sequestration, reducing the risk of hydrogen leakage. Existing infrastructure, geological data, and wellbores in depleted fields enhance their attractiveness for underground hydrogen storage compared to untested aquifers. Efficient space management, lower storage costs, and readily available geological information further bolster the case for utilizing depleted oil and gas fields for hydrogen storage [187,188].

In conclusion, physical hydrogen storage methods involve compressing or liquefying hydrogen gas, making it suitable for transportation but requiring significant energy. Solid-state-based methods, like metal hydrides or metal-organic frameworks, chemically bind hydrogen within a solid matrix, providing moderate storage capacities at near-ambient conditions but often necessitating high temperatures for release. Underground storage, using geological formations like salt caverns or depleted reservoirs, offers vast storage capacities and can accommodate large-scale needs for hydrogen but involves complex infrastructure and potential safety concerns. Each method has its advantages and limitations, making them suitable for different applications based on factors like energy density, safety, and infrastructure requirements. The choice of storage technology depends on the specific use case and the desired balance between factors like efficiency, cost, and safety.

3. Designing materials for hydrogen storage

The design and optimization of chemical hydrogen storage materials consider thermodynamic feasibility, ensuring energy-efficient hydrogen uptake and release. Kinetics impact the efficiency of hydrogen storage systems by dictating the rate of hydrogen absorption and release. Material stability is vital for enduring repeated hydrogen absorption and desorption cycles without degradation, while reversibility enables the material's repeated use.

3.1. Design considerations and strategies for hydrogen storage material

The limitation in utilizing hydrogen as an energy carrier often stems from the challenge of effectively storing it. Hydrogen possesses a notably low volumetric energy density, measuring around 0.7 kJ L^{-1} at 25 °C under atmospheric pressure. Currently, the established method for hydrogen storage involves compression at 70 MPa, yielding an increased volumetric energy density of $\approx$3 MJ L^{-1} at the system level with composite tanks. These high-pressure hydrogen tanks have already found practical applications in the initial commercialization of hydrogen vehicles. However, for stationary applications, the utilization of compressed tanks becomes less viable due to their considerable cost, estimated at approximately AUD $685 per kg H$_2$ at the system level

[189].

Utilizing appropriate and sustainable materials stands as a crucial requirement in fostering the development of a hydrogen-based economy. Both theoretical and experimental studies have extensively explored various facets of hydrogen storage. The principal phenomena pivotal in hydrogen storage encompass physisorption, involving the storage of molecular hydrogen, and chemisorption, focusing on the storage of atomic hydrogen [190]. The effectiveness of these storage materials relies significantly on two vital aspects: gravimetric and volumetric density, demanding materials that are lightweight and compact. Gravimetric density is gauged by dividing the weight of stored hydrogen by the weight of the entire system (hydrogen + container), whereas volumetric density is determined by dividing the mass of stored hydrogen by the system's unit volume [191,192].

Within the ambit of advanced storage materials, several key avenues have emerged, each offering unique advantages and prospects for augmenting hydrogen storage capacity. Metal hydrides, known for their potential to harbor high amounts of hydrogen, have garnered substantial attention. Research endeavors are fervently seeking novel metal hydrides, employing alloying strategies and nanostructuring techniques to boost their storage capabilities while improving hydrogen absorption and desorption kinetics.

Metal hydrides serve as chemical storage systems that securely retain hydrogen in a solid state via an absorption process. Specific materials like metals, intermetallic compounds, or alloys possess the capability to absorb hydrogen under moderate pressure at low temperatures, leading to the formation of reversible solid compounds known as metal hydrides [193]. This absorption mechanism enables the potential storage of hydrogen at high density and low pressure within metal hydrides, offering a safer alternative in comparison to other storage methods [51, 194,195].

When evaluating various storage methods, the initial crucial metrics often considered are the gravimetric storage capacity and volumetric energy density. When assessing metal hydrides, the gravimetric capacity is determined by dividing the maximum mass of absorbed hydrogen by the mass of the hydride material, typically measured in weight percent (wt%). Broadly, metal hydride materials falling within the interstitial hydrides category generally exhibit gravimetric storage capacities spanning from 1 to 2 wt% [196].

The selection standards for metal hydride materials intended for hydrogen storage and compression applications rely on various essential factors. Firstly, the reversibility of both hydride formation and decomposition processes is crucial within the specified operating temperatures and hydrogen pressures pertinent to the application at hand. Additionally, the material must exhibit a notable and reversible hydrogen storage capacity under these operational conditions. These characteristics are discerned through pressure-composition-temperature traits observed in hydrogen gas and hydride-forming materials systems. The reversible capacity is linked to the plateau width on the pressure-composition isotherm, where the direction of the process (hydrogenation/H$_2$ uptake or dehydrogenation/H$_2$ release) hinges on the relationship between the actual hydrogen pressure and the plateau pressure at the given temperature. Moreover, other pivotal properties of metal hydride materials for efficient hydrogen storage and compression encompass rapid hydrogen absorption and desorption kinetics, resilience against impurity-induced poisoning in the supplied hydrogen, facile activation, sustained cyclic stability, affordability, and ease of manufacturing. These attributes collectively contribute to the suitability of the metal hydride materials for practical implementation in hydrogen-related applications [197,198].

Solid-state hydrogen storage employing metal hydrides presents numerous advantages over conventional and alternative methods. Notably, metal hydrides exhibit the capability to store significant volumes of hydrogen, showcasing high volumetric hydrogen storage densities, and inherently boast safer attributes compared to mechanical storage methods. Their safety profile arises from their operability at

relatively low temperatures and pressures akin to those found in fuel cell vehicles, and the release of hydrogen from metal hydrides occurs via an endothermic process. Hydrogen liberation from metal hydrides can occur either through an increase in temperature or a reduction in external pressure [51].

Alloying different metals has emerged as a promising strategy to bolster the storage capacity of metal hydrides. Alloying, the process of combining different metals to form a new material, holds significant potential in modifying the properties of metal hydrides for improved hydrogen storage. This technique leverages the synergy between metals to achieve enhanced storage capacities through tailored compositions and structural modifications [199].

In recent years, complex hydrides, a category of hydrides consisting of compounds involving light elements such as Li, Na, and/or Mg, have gained considerable attention. Within these compounds, hydrogen forms (non)covalent bonds with another metal or non-metal element (X), typically represented as $M[XH_m]_n$. These complex hydrides stand out due to their remarkably high hydrogen contents, which have sparked significant interest and research focus in hydrogen storage applications [200]. The substantial interest in complex hydrides stems from their high hydrogen density and the capability for de/rehydrogenation processes to occur without necessitating high pressures or low temperatures. This heightened attention arises due to the impressive hydrogen storage potential and the favorable conditions required for the release and uptake of hydrogen within these materials.

Complex hydrides exhibit diverse chemical compositions and bonding, stemming from a broad spectrum of complex anions derived from the amalgamation of hydrogen with elements such as boron, nitrogen, carbon, oxygen, aluminum, transition metals, and more. This diverse nature allows for a wide range of substances with adjustable functionalities, providing ample room for property optimization. In terms of hydrogen storage over complex hydrides, the process involves the dihydrogen dissociation into surface H atoms, followed by the diffusion of H into the bulk phase. The mechanisms underlying this phenomenon, including the homolytic or heterolytic splitting of hydrogen on the surface of complex hydrides, exhibit similarities to the activation and conversion of hydrogen over transition metal surfaces. Furthermore, certain complex hydrides possess a reductive and electron-rich nature, enabling them to supply electrons that facilitate chemical conversion processes. This characteristic adds to the versatility and potential applications of complex hydrides in mediating various chemical reactions involving hydrogen [201].

Complex hydrides like alanates and borohydrides have emerged as promising hydrogen storage materials, attracting significant attention in recent times [202]. Despite their potential, their thermodynamics and kinetics are not suitable for cycling under moderate pressure or temperature conditions. However, nanoscale hydrides, characterized by their substantial surface areas, abundant grain boundaries, and shorter diffusion distances, exhibit faster hydrogen desorption and absorption at lower temperatures compared to bulk hydrides [203]. The conventional method for preparing nanoscale hydrides involves high-energy ball milling, which mechanically reduces particle size. Nonetheless, this top-down approach often results in a wide particle size distribution, with the smallest attainable size around 100 nm, albeit crystallite size reduction to a few nanometers. Such particles often lack significant size effect, necessitating alternative methods [204].

In contrast, nanoconfinement, a more recent bottom-up strategy, generates smaller and more uniform nanoscale hydrides by infiltrating scaffolds with hydrides. This innovative approach has successfully produced nanoconfined alanates [205,206], ammonia borane [207–209], borohydrides [210], and magnesium hydrides within mesoporous silicas [211,212], nanostructured carbons [213], and MOFs [214].

Extensive research has focused on alanates, a subset of complex hydrides characterized by a metal cation and $[AlH_4]^-/[AlH_6]^{3-}$ anion. The exploration of alanates for reversible hydrogen storage, notably catalyzed by Ti in $NaAlH_4$, has garnered immense attention in hydrogen storage research [201]. $NaAlH_4$ stands out among the studied alanates, being the most extensively researched material due to several favorable attributes. It boasts moderate reaction heat during de/rehydrogenation, relatively high gravimetric and volumetric hydrogen densities (7.4 wt% and 59 kg m^{-3}, respectively) [215], and economical raw materials (Al and NaH). Nonetheless, the practical application of $NaAlH_4$ faces challenges due to its sluggish reaction kinetics. To address this limitation, various approaches have been employed, such as incorporating additives and catalysts like transition metals (Ti, Sc, Nb), rare-earth metals (Ce, Sm, etc.), and carbon-based materials. These substances are introduced to $NaAlH_4$ through methods like wet doping, ball milling, or direct synthesis [201,216].

Moreover, nanoconfinement techniques involving the encapsulation of $NaAlH_4$ within porous materials have demonstrated effectiveness in enhancing its hydrogen storage properties. This innovative approach has shown promise in overcoming the kinetic limitations of $NaAlH_4$, opening avenues for optimizing its practical utility in hydrogen storage applications [217,218].

Alanates have garnered significant attention due to their appropriate dehydrogenation enthalpies and high hydrogen capacities; however, they face challenges with inadequate reversible capacities. Similarly, amide-hydride composites display favorable thermodynamics and hydrogen capacities but encounter issues like slow kinetics and the production of ammonia as a side-product. Borohydrides, despite possessing high gravimetric hydrogen contents, suffer from sluggish kinetics, generation of side-products, and irreversibility. Over time, the scientific community has actively pursued solutions to overcome these drawbacks, leading to the development of various strategic approaches. Numerous successful strategies have been devised to address these limitations, including the optimization of compositional alterations by substituting anions and/or cations, forming composites with other hydrides or compounds, or coordinating neutral molecules to the cation of complex hydrides. Another approach involves catalytic modification by introducing catalysts or additives capable of enhancing hydrogen sorption and desorption kinetics. Additionally, nanoconfinement techniques, incorporating complex hydrides into nanoporous hosts, have been utilized to modify kinetics and/or thermodynamics.

Moreover, new candidate materials are emerging in the realm of hydrogen storage. For instance, metalorganic hydrides, which amalgamate inorganic and organic components, possess versatile chemistry, potentially expanding the scope of materials design and development. Similarly, organic complex hydrides, with their diverse range of organic compounds and versatile chemistry, exhibit potential and warrant further investigation. The accumulation of experimental and theoretical data continually augments our understanding of the physical and chemical properties of complex hydrides. This evolving knowledge has spurred the exploration of new research avenues, aiming to equip complex hydrides with enhanced capabilities to address challenges in clean energy production, storage, and conversion. These strategies involve compositional alterations, catalytic modifications, and nanoconfinement, each offering unique pathways to enhance the performance of complex hydrides in hydrogen storage and related applications [201].

Porous materials, characterized by their intricate network of pores and high specific surface areas, have drawn attention to their ability to adsorb and store significant amounts of hydrogen [115]. Among these materials, MOFs have gained significant attention as highly researched hydrogen adsorbents due to their distinctive structures comprising metal ions or clusters linked by organic ligands. These frameworks offer immense structural diversity and tunability, enabling the creation of custom-designed frameworks with precisely defined pore sizes and functionalities. This exceptional characteristic positions MOFs as promising candidates for hydrogen storage, granting meticulous control over surface area and pore volume to enhance hydrogen adsorption [219].

The formation of microporous crystalline MOFs occurs through the

self-assembly of inorganic metal clusters and organic linkers. This unique assembly process offers numerous variations in building blocks, contributing to the vast spectrum of properties exhibited by MOFs, particularly in terms of surface area, which often surpasses that of other materials. However, while this design flexibility enables the customization of MOF properties, it presents challenges in identifying optimal compositions due to the extensive parameter space that needs exploration [220,221].

In recent years, extensive endeavors have focused on enhancing MOFs performance by integrating them with a diverse array of functional materials, including polymers [222], graphene [223], metal nanoparticles (NPs) [224], enzymes [225], and carbons [226]. The strategies employed in creating composite materials serve to enhance not only the intrinsic abilities of each constituent but also generate new physicochemical attributes through synergistic effects. The integration of MOFs with functional materials presents significant potential in propelling advancements in energy technologies, particularly in the realm of hydrogen storage [227].

A notable avenue for enhancing MOF functionality involves the pyrolysis of MOFs, a process that transforms their organic ligands and metal nodes into various materials vital for energy applications, including porous carbons, metal oxides, metal sulfides, and multicomponent hybrids. The conditions of these pyrolysis processes, such as temperature, duration, and gas composition, enable precise control over product structures and component proportions, facilitating the integration of diverse functionalities. Capitalizing on the benefits inherited from MOFs, such as well-ordered pore structures and high surface areas, these derivatives showcase significantly enhanced performance compared to conventionally synthesized materials [227–229].

The introduction of oxygen, nitrogen, or any other electron-rich group into the structure of MOFs represents another strategy for improving hydrogen storage capacity [230]. These materials offer increased active sites due to modified electronic and geometric structures, thus demonstrating enhanced properties that result from the alteration of the materials' fundamental composition and structure [227]. This strategy has been reported by Li et al. [156], who used nitrogen-heterocyclic carboxylate ligand; 2,2-bipyridine-5,5′-dicarboxylate (bpdc) with a zirconium-based metal salt to produce UiO(bud). Obtained storage capacity of this material was found to be 5.7 wt% at 77 K and 2 MPa compared to 4.5 wt% obtained by the University of Oslo Framework 67 (UIO-67) [231] due to the anchoring of Lewis basic sites (bpdc) onto the surface of pores without losing the original high porosity. In addition, there are other strategies in which MOFs could be used in hydrogen storage.

In line with the above strategies, Ma et al. [157] investigated the efficiency of two composites using magnesium hydride with cobalt (II) and iron (II)-based MOFs prepared by ball milling. The gravimetric storage capacity decreased from 6.91 wt% using magnesium hydride to 5.19 wt% and 5.37 wt% using the composites of cobalt-based MOF and that of the iron-based MOF, respectively, at 648 K and 1 MPa. However, the activation energy dropped from almost 100 kJ/mol using magnesium hydride to 67 kJ/mol and 74 kJ/mol by the iron-based MOF and cobalt-based MOF, respectively. Also, the dehydrogenation temperatures of magnesium hydride-cobalt MOF and magnesium hydride-iron MOF composites are 151 kJ/mol and 142 kJ/mol compared to 181 kJ/mol using pure magnesium hydride. Lu et al. [158] synthesized a composite of vanadium-based MOF and magnesium hydride that achieved a hydrogen release of 6.4 wt% in just 5 min at 573 K and 3.2 MPa with an obvious reduction in both absorption and release activation energies from 157 to 78 kJ/mol and from 98 to 30 kJ/mol, respectively. So, the ability of these MOFs to improve the hydrogen release kinetics from other storage materials was verified.

In the realm of porous materials, carbon-based materials comprising activated carbons, carbon nanotubes, and graphene constitute a significant category. Renowned for their exceptional properties, including high surface area, remarkable mechanical strength, and superior

thermal conductivity, these materials have garnered attention for their potential in hydrogen storage applications. Notably, graphene and carbon nanotubes demonstrate impressive hydrogen adsorption capacities attributed to their expansive, accessible surface areas and porous architectures.

Various carbon materials, encompassing activated carbon, carbon aerogel, templated carbon, carbon nanotubes, carbon fibers, and graphene, have been extensively researched as potential hydrogen storage media. These materials can be derived from synthetic carbon precursors or natural sources like wood, coal, agricultural by-products, and biomass, employing diverse synthesis methods. The physicochemical properties, such as specific surface area, micropore surface area, total pore volume, and pore size, can be precisely tailored by selecting appropriate synthesis methods and relevant experimental parameters, thereby optimizing hydrogen uptake capacity within these porous carbons.

Enhancing the performance of porous carbon materials in physically adsorbing hydrogen involves strategies to improve the thermodynamics of hydrogen binding. Two fundamental approaches have been pursued for this purpose. The first method involves augmenting the specific surface area of carbon materials while creating engineered pore spaces at the nanometer scale to increase adsorption sites and potential wells. The second method focuses on functionalizing porous carbon materials by doping them with lightweight elements, inducing electron deficiency and enhancing the polarity of the carbon framework, thereby strengthening hydrogen interaction with the substrate. Developing porous carbon materials with high surface area and intermediate hydrogen adsorption enthalpies is identified as pivotal for reversible hydrogen storage at ambient conditions, signifying their indispensable role in future hydrogen-based economies [232].

3.2. High-throughput computational screening and machine learning

In recent decades, scientific computing has made remarkable strides in discovering and advancing novel materials, playing a pivotal role in supporting experimental endeavors. With advancements across various disciplines such as physics, chemistry, materials science, and computer science, computational techniques have become an indispensable branch within the realm of materials science and technology. This involvement has directly or indirectly contributed to the creation of various new materials, including low-dimensional nanomaterials [233], Li-ion battery materials [234], and topological insulators [235]. Initially limited by algorithms, software capabilities, and computational power, early computational approaches were primarily confined to analyzing and interpreting experimental results. However, their applications have significantly broadened over time [236].

In contemporary scientific research, computational methods are extensively employed to explore the underlying principles governing the physical and chemical properties of materials. They help establish comprehensive quantitative relationships between composition, structure, and material properties. In the domain of technology development, computation plays a crucial role in screening new material compositions and structures while optimizing the parameters for their virtual fabrication and processing [237]. Furthermore, computational methods are integral in material deployment. They facilitate the rapid enhancement of new materials, optimizing their performance characteristics, diagnosing accumulated damages, and predicting their overall service life. The evolving complexity of materials presents considerable challenges in their design and development. These challenges stem from their multifaceted components, diverse structures, intricate processes, and varied service environments [238].

The second-generation materials discovery method, high-throughput screening, involves computing the properties of numerous structures to identify those meeting specific criteria and having low energies, subsequently selected for synthesis. Typically, a computational high-throughput screening process involves four key steps: identification of

target properties, definition of screening spaces, property prediction, and selection of candidate materials. Identifying target properties stands out as one of the most crucial and challenging steps in these processes. For materials scientists, naming the desired macroscopic properties of functional materials in energy conversion or storage devices is generally feasible [21].

Consequently, designing new materials involves a multifaceted process encompassing numerous parameters, procedures, and pathways. The vast array of variables and their potential combinations in material design results in an expansive design space far beyond the scope of traditional trial-and-error experimentation. Thus, efficient virtual screening techniques have become imperative for narrowing down the space, allowing for a more focused and strategic experimental search [238].

In materials modeling, interactions between atoms are typically described using energy-force methods categorized as semiempirical, and first-principles approaches. Semiempirical methods rely on force fields or classical potentials, customized with specific parameters to mirror experimental or quantum-chemistry outcomes. These approaches enable extensive studies of hydrogen-storage materials across diverse thermodynamic ranges, maintaining a reasonable level of complexity. Their unique capability even encompasses modeling chemical reactions, encompassing bond formations and breakages through dedicated reactive force fields. Nevertheless, their applicability might falter when extrapolated to conditions differing from their initial design. These methods, due to their cost-effectiveness, allow for explicit modelling of thermal and structural disorder effects, which are pivotal in the simulation of hydrogen-storage materials. For instance, quantum nuclear effects (QNE) significantly influence gas adsorption in these materials at room temperature. In-depth analysis employing semiempirical potentials and quantum simulation techniques, such as path-integral Monte Carlo methods, has elucidated the role of QNE in processes like the adsorption of hydrogen and deuterium molecules onto carbon-based nanotubes [189].

On the other hand, first-principles methods, such as quantum Monte Carlo, provide atomic interaction details directly from quantum mechanics, ensuring higher accuracy in computational studies. Among these methods, Density Functional Theory (DFT) stands out due to its balanced precision and computational efficiency, making it extensively utilized in hydrogen-storage material research [189,239].

In the domain of MOFs, computational investigations predominantly rely on the Grand Canonical Monte Carlo (GCMC) simulation technique to assess H_2 adsorption within these structures. GCMC has proven instrumental in accurately predicting gas adsorption in porous materials, serving as a valuable complement to experimental gas adsorption isotherms. For GCMC simulations, essential inputs encompass the crystallographic information file (CIF) of the MOF. These CIFs can be sourced from publications detailing MOF synthesis, computation-ready databases like CoRE-MOF offering CIFs for molecular simulations, or the Cambridge Structural Database cataloging deposited MOF CIFs. Alongside CIFs, GCMC simulations necessitate potentials for H_2 molecules (e.g., Buch's, Darkrim and Levesque's potentials) and MOFs (like Universal Force Field and Dreiding), as well as information on temperature and pressure during the adsorption process [240].

A typical approach involves comparing gas uptakes from GCMC simulations with experimentally measured gas uptakes under identical temperature and pressure conditions to determine and validate the input parameters for GCMC simulations. These simulations yield data on the amount of adsorbed H_2 within a MOF under specified conditions and provide insights into the heat of adsorption, which reflects adsorbent-gas interactions at lower loads. The quantified amount of adsorbed H_2 serves as a basis for calculating the deliverable H_2 capacity of a material, representing the quantity of hydrogen released between adsorption and desorption pressures. The escalating number of experimentally synthesized and theoretically designed MOFs, coupled with advancements in computational tools and increased computing power, has expedited efforts in high-throughput computational screening (HTCS) of materials for H_2 storage. HTCS enables the rapid evaluation of numerous materials, allowing the identification of the most promising candidates tailored for specific applications based on predefined performance metrics [241].

The interaction between MOFs and H_2 significantly influences the deliverable H_2 capacity, impacting both the material's saturation capacity at adsorption pressure and the quantity of gas released at desorption pressure. Achieving high deliverable H_2 capacities relies on optimizing this interaction to strike a balance that is neither excessively strong nor too weak. Efforts have been made to enhance adsorbent-H_2 interactions at room temperature by implementing modifications. Specifically, magnesium alkoxide functionalization was employed on MOFs and porous aromatic frameworks, resulting in the creation and evaluation of 18,383 hypothetical materials. These newly generated materials underwent scrutiny via GCMC simulations to assess their potential to improve adsorbent-H_2 interactions [242].

Ahmed et al. [243] conducted computational screening of 5309 MOFs and identified promising candidates with high gravimetric and volumetric hydrogen densities. Experimental evaluations were carried out, and the MOF called IRMOF-20 demonstrated an uncommon combination of high useable volumetric and gravimetric capacities. The measured capacities of IRMOF-20 exceeded those of the benchmark compound MOF-5, which is considered a standard for combined volumetric and gravimetric performance. The computational predictions were found to be most accurate when using pseudo-Feynman-Hibbs-based grand canonical Monte Carlo calculations. These calculations allowed for the estimation of hydrogen capacities in MOFs. The study highlights the importance of computational screening in identifying materials that optimize overall storage performance. It addresses the challenge of balancing gravimetric and volumetric hydrogen densities in MOFs, which is crucial for maximizing the driving range of fuel cell vehicles.

Subsequently, the same research team presents a systematic assessment of hydrogen storage capacities in MOFs. The authors computationally screened a database of nearly 500,000 real and hypothetical MOFs and experimentally evaluated the most promising materials. They identified three MOFs, namely SNU-70, UMCM-9, and PCN-610/NU-100, with useable capacities surpassing that of the benchmark MOF-20, which had the highest combined volumetric and gravimetric performance previously. The analysis of trends across the database revealed a volumetric ceiling at approximately 40 g-H_2 L^{-1}, indicating the need for the development of adsorbents with larger volumetric capacities. Contrary to earlier studies, the useable capacities in the highest-performing MOFs were found to be negatively correlated with density and volumetric surface area but maximized by increasing gravimetric surface area and porosity. This suggests that property-performance trends identified for total capacities may not apply to useable capacities. The computed results showed that volumetric capacities increased with increasing gravimetric capacity up to around 10 wt%, beyond which the volumetric performance plateaued. The study identified 102 compounds that exhibited useable capacities greater than that of MOF-20 on both volumetric and gravimetric bases [221].

Deniz et al. [244] focused on the computational study of Li-doped fullerene pillared graphene nanocomposites (Li-FPGNs) for enhancing hydrogen storage. The study utilized GCMC simulations to examine the hydrogen physisorption in Li-FPGNs under different temperature and pressure conditions. The GCMC simulations demonstrated that the hydrogen adsorption performances of undoped FPGNs could be significantly improved by Li doping and the selection of different types of fullerenes. The researchers optimized the gravimetric, volumetric, and deliverable hydrogen adsorption performances of FPGNs by considering various doping ratios and types of fullerenes. The results showed that Li-FPGNs with a doping ratio of Li: C = 15:100 exhibited promising hydrogen storage capabilities. At 77 K and 1 bar, the total gravimetric adsorption capacity of Li-FPGNs reached 9.1 wt%, which represents

approximately a two-fold increase compared to undoped FPGNs.

Additionally, Li doping enhanced the excess hydrogen storage capacity of FPGNs up to three times at ambient temperature. These findings suggest that Li-FPGNs hold potential as effective materials for hydrogen storage applications. By utilizing computational methods such as GCMC simulations, the research provides valuable insights into the optimization of Li-FPGNs' performance for hydrogen adsorption. Numerical values, such as the gravimetric adsorption capacity and the improvement ratios, highlight the significant enhancements achieved through Li doping in the studied nanocomposites.

To study the hydrogen storage properties of COFs, Bian et al. [245] investigated the structural characteristics and hydrogen storage properties of five boron-phosphorus cube-based covalent organic frameworks (BP-COFs) using DFT and molecular simulations. The study focuses on computational chemistry aspects related to hydrogen storage. The researchers characterized the structures of the five BP-COFs and studied their hydrogen adsorption properties through GCMC simulations. The simulations were conducted at temperatures of 77 K and 298 K under a pressure of 0.1–100 bar. The results indicated that BP-COF-4 and BP-COF-5 exhibited higher hydrogen adsorption capacities compared to BP-COF-1 to BP-COF-3 at both temperatures. In the field of computational chemistry, the authors employed DFT calculations and molecular simulations to gain insights into the hydrogen storage capabilities of the BP-COFs. This approach allows for the exploration and evaluation of various materials and their structural properties, aiding in the design and development of efficient hydrogen storage materials.

Regarding metal hydrides, Li et al. [246] explored the use of graphene as a catalyst to improve the dehydrogenation kinetics of MgH_2 for hydrogen storage. The study employs computational chemistry methods, specifically spin-polarized first-principles calculations based on DFT. The researchers investigated the effect of graphene dopants on hydrogen release from MgH_2. It was demonstrated that graphene dopants, particularly B/P codoped graphene (BP@graphene), can enhance the dehydrogenation process by reducing both the reaction barrier and reaction energy. The computational results predicted that the MgH_2/BP@graphene heterojunction exhibits excellent dehydrogenation thermodynamics and kinetics.

In a recently published article, Rana et al. [247] presented a computational approach for analyzing and predicting thermodynamic properties of metal hydrides, with a focus on hydrogen storage applications. The authors develop a framework based on the lattice reverse Monte Carlo (RMC) method and apply it to the nickel hydride (NiHx) system. Using their approach, the authors were able to accurately construct the phase diagram of NiHx in a matter of minutes, considering less than 10 configurations. This is significantly faster compared to the popular technique of GCMC, which would require sampling millions of configurations. The computational workflow presented in the paper offers a promising solution for rapidly analyzing and predicting thermodynamic properties of metal hydrides, facilitating materials discovery in the field of hydrogen storage. The results demonstrate the efficiency of the RMC approach in incorporating configurational terms and accurately constructing phase diagrams. The computational overhead of the RMC method is negligible compared to traditional methods, making it suitable for systems with a large number of atoms. The study also highlights the importance of computational techniques in accelerating the discovery and optimization of materials for hydrogen storage.

Jing et al. [248] focused on the development of metalorganic hydrides for hydrogen storage through a combination of theoretical predictions and experimental validation. The aim is to identify materials with high hydrogen capacities and suitable thermodynamics for efficient hydrogen uptake and release. The study screened more than 90 metalorganic hydrides theoretically, considering the substitution of reactive hydrogen (H) in organic compounds with light alkali metals such as lithium (Li) and sodium (Na). Among the screened compounds, 20 pairs were identified that exhibited both high hydrogen capacities ($\geq$5 wt %) and suitable thermodynamics (heat of H_2 desorption: 25–35 kJ/mol-H_2)

for hydrogen storage. Four specific metalorganic hydrides were selected for further investigation and synthesis. Theoretical predictions indicated that lithium indolide and lithium octahydroindolide pairs had a theoretical hydrogen capacity of 6.1 wt% and an ideal heat of hydrogen absorption (ΔHd) of 33.7 kJ/mol-H_2. Experimental validation confirmed the theoretical predictions, demonstrating partially reversible hydrogen uptake and release at a low temperature of 100 °C. The computational study involved the calculation of hydrogenation enthalpy change (ΔHh) for the metalorganic hydrides. Metal substitution was found to efficiently reduce the ΔHd of the organic compounds, indicating improved hydrogen storage properties upon metalation. The stabilization of both H-lean and H-rich compounds through metalation contributed to the reduction in ΔHd. Overall, the research showcases the potential of metalorganic hydrides for addressing the challenges of hydrogen storage. The combination of theoretical predictions and experimental validation proved effective in identifying promising materials and guiding their synthesis. The computational study provided valuable insights into the thermodynamic properties of the metalorganic hydrides, facilitating the rational design of materials for hydrogen storage.

In today's digital era, the data-driven approach has seen significant advancements and growth, particularly in the domain of machine learning (ML). Widely embraced by researchers, ML has garnered substantial attention across scientific research and business sectors, finding applications in diverse fields such as natural language processing [249, 250], computer vision [251,252], biomedicine [253,254], robotics [255,256], data classification, and mining [257]. Researchers have extensively used ML models to analyze specific material attributes in databases. These models, particularly effective for high-dimensional and complex systems, accurately predict material performance, uncover hidden material trends, and swiftly aid in the design of new materials. Consequently, this approach reduces both time and costs while offering precise guidance for researchers.

The application of ML techniques has extended to the study of various materials, encompassing carbon materials [258], MOFs [259], lithium-ion battery materials [260], and catalytic materials [261]. ML not only optimizes material performance but also establishes relationships between material composition, structure, and performance. Additionally, it improves theoretical computational methods, optimizes parameters, and automates setting parameters for different systems, replacing conventional semiempirical parameters.

ML techniques broadly fall into four categories: supervised learning, unsupervised learning, semi-supervised learning, and reinforcement learning. Supervised learning involves training algorithms using labeled data sets (x, y), allowing computers to classify or regress unknown data based on the learned mapping from input to output. Common supervised learning models include neural networks (NN), decision trees (DT), support vector machines (SVM), k-nearest neighbors (KNN), and Naive Bayesian models. In contrast, unsupervised learning lacks labeled data, requiring classification based on similarities among input samples. Clustering and association rules are commonly employed for this purpose, aiming to minimize intra-class gaps and maximize inter-class gaps. Principal component analysis (PCA), self-encoding algorithms, and deep learning are among the prevalent unsupervised learning approaches. Semi-supervised learning combines aspects of both supervised and unsupervised learning, utilizing a dataset containing labeled and unlabeled data for pattern recognition. Transductive learning and inductive learning are two prominent methods within semi-supervised learning, differing in their treatment of unlabeled data during testing. Finally, reinforcement learning involves computers learning through trial and error to maximize rewards and performance within an environment, guided by rewarding and punishing signals obtained from interacting with the environment. Temporal differential learning and Q-learning represent two prevalent methods within the domain of reinforcement learning [262].

First-principles methods accurately compute crucial physical

quantities relevant to hydrogen storage materials, such as the free energy of hydrogen storage/release reactions and materials decomposition processes. Yet, determining the most favorable reaction pathways, adsorption sites, and chemical structures necessitates guessing from various candidate processes and configurations, primarily reliant on chemical intuition. This approach might be incomplete or prone to errors, especially when addressing intricate problems. To tackle these "open" challenges, the aspiration is for theoretical frameworks capable of automatically predicting the thermodynamically optimal reaction paths, states, and configurations based solely on the system's chemical composition or similar information. ML techniques offer a solution, focusing on computational affordability and objectiveness over chemical intuition [189].

In the realm of hydrogen storage materials, ML employs algorithms and statistical models to enhance computational performance for specific tasks. These tasks include predicting lowest-energy configurations and decomposition reaction pathways. However, ML models require training on comprehensive sets of data, often generated through first-principles methods, a process that can be challenging to complete. Theoretical studies in hydrogen storage materials utilizing ML techniques are emerging, and it's expected that their prevalence will grow steadily. These studies offer vast versatility, enabling the screening of numerous systems and processes. Examples include analyzing the catalytic activity of the hydrogen evolution reaction on nanoclusters, generating thousands of new alloy combinations with favorable enthalpies of formation for high-pressure hydrogen compressor materials, and identifying the performance limits of physical hydrogen storage in a wide range of nanoporous materials [263,264].

In this context, a recently published article conducted by Nations et al. [265] aimed to explore the use of machine learning techniques for predicting the energy of formation and hydrogen storage capacity of metal hydrides. The study utilized various machine-learning models, including ridge regression, decision trees, random forest ensembles, and gradient-boosting ensembles. The researchers collected data from public databases, such as Materials Project and HydPark, which provided information on metal hydrides. They performed feature engineering to extract relevant parameters, including electronegativity, density, atomic density, d-character, f-character, band gap, hydrogen weight fraction, magnetization, temperature, and pressure. The models were benchmarked, and the random forest ensemble yielded the lowest test set error, indicating its superior performance. This ensemble method was then used to fill in missing entries of energy of formation in the dataset. The materials were further evaluated based on hydrogen storage capacity and energy of formation suitability. The study found that readily available features, including those derived solely from the chemical formula, were highly predictive and promising for high-throughput screening of novel hydride formulations. The machine learning techniques employed in this research provided a means to build relationships between properties that may not be evident through traditional condensed matter theory.

Kim et al. [266] conducted a study to forecast the pressure-composition-temperature (PCT) curves of AB_2-type hydrogen storage alloys by applying machine learning techniques. The research involved the use of three distinct machine learning models: random forest, K-nearest neighbor, and deep neural network (DNN) for predictive purposes. To bolster the dataset, two different data generation methods were utilized, alongside proposing an innovative form of PCT curve functions aimed at enhancing the accuracy of predictions. The results indicated that the DNN model outperformed the other two models, showing a high average correlation value (R2 = 0.93070), indicating a strong linear relationship between the predicted and measured values. The prediction accuracy was evaluated using mean absolute error (MAE) and root mean squared error (RMSE), which were not specified in the provided content. However, the article mentioned that these evaluation metrics were employed. The study focused on predicting the hydrogen absorption behavior of AB_2 alloys at a fixed temperature (303 K) using machine learning models. The input features for the models included temperature, pressure, and nine alloy compositions. The prediction accuracy was assessed by comparing the predicted values with the measured values, and higher correlation values indicated better prediction performance. Overall, the research demonstrated the effectiveness of machine learning in predicting PCT curves of hydrogen storage alloys. By utilizing machine learning models, the study provided insights into the behavior of AB_2-type alloys, which can aid in the selection and design of hydrogen storage materials for various applications.

For carbon-based materials, Thanh et al. [267] focused on predicting hydrogen storage using ML models, specifically the random forest model, combined with nature-inspired algorithms. The study aimed to develop a predictive model for hydrogen storage on porous carbon adsorbents. Various input variables, including carbon-based adsorbents, chemical activating agents, ratios, micro-structural features, and operational parameters, were used in the ML model. The results showed that the RF model combined with particle swarm and gray wolf optimizations (PSO and GWO) achieved high accuracy in both the train and test phases, with R^2 values of approximately 0.98 and 0.91, respectively. Sensitivity analysis revealed that temperature, total pore volume, specific surface area, and micropore volume were the most relevant factors for hydrogen uptake. The relevance scores for these factors were 1 and 0.48, respectively. The feasibility of the algorithms was evaluated using different training sizes, ranging from 80% to 60%. The RMSE and MAE values ranged from 0.6 to 1 and 0.38 to 0.52, respectively. These metrics indicate the accuracy of the predictive model. Overall, the study contributes to the development of sustainable energy sources by providing insights into the design of porous carbon adsorbents for hydrogen storage. The use of nature-inspired algorithms in the ML model development process is a novel approach that can be applied to other areas of materials science and engineering. The research demonstrates the potential of ML techniques in predicting the performance of porous carbon materials and optimizing their hydrogen adsorption capabilities.

Shekhar and Chowdhury [268] focused on predicting hydrogen storage in MOFs using machine-learning techniques. The authors aimed to overcome the limitations of high-throughput computational research by utilizing machine learning as an alternative to traditional methods like experiments and simulations. The study employed a feed-forward neural network (FNN) as well as the extremely randomised tree (ERT) model to predict the hydrogen delivery capacity of a large number of MOFs. The FNN model demonstrated superior performance in forecasting the gravimetric capacity, while the ERT model was more effective in predicting the volumetric capacity. The dataset used for training and evaluation consisted of 918,734 MOFs from various databases. Additionally, the authors performed GCMC simulations to validate the predictions made by their machine-learning models. The results of the research indicated that machine learning, particularly the FNN and ERT models, showed promising capabilities in accurately evaluating the hydrogen storage capacities of MOFs. These predictions were achieved with a significantly shorter computational time compared to traditional molecular simulations. The authors highlighted the potential of machine learning in accelerating the discovery of optimum MOFs, minimizing input data requirements, and efficiently screening large MOF databases for high-capacity materials. Overall, the research demonstrated the successful application of machine learning in predicting hydrogen storage capacities in MOFs, offering a promising avenue for future advancements in clean and sustainable fuel technologies.

Similarly, Ahmed et al. [269] discussed the development and application of machine learning models to predict hydrogen storage capacities in MOFs. The study aims to accelerate the discovery of high-capacity hydrogen adsorbents by accurately predicting hydrogen uptake across a diverse set of MOFs. The authors trained machine learning models using a dataset of 918,734 MOFs sourced from 19 databases. With only seven structural features as input, the models were able to identify 8282 MOFs with the potential to exceed the capacities of

state-of-the-art materials. The identified MOFs were characterized by low densities (<0.31 g/cm^3), high surface areas (>5300 m^2/g), large void fractions (>0.90), and significant pore volumes (>3.3 cm^3/g). The study quantified the relative importance of the input features and examined the dependencies on the machine learning algorithm and training set size. It was found that pore volume played a crucial role in predicting gravimetric capacity, while void fraction was important for volumetric capacity. The developed machine learning models are available online, enabling rapid and accurate predictions of hydrogen capacities for new MOFs based on limited structural data. The use of machine learning in this context offers a promising approach to overcome the challenges associated with the vast number of MOFs and limited experimental data, facilitating the discovery of efficient hydrogen storage materials.

Another recent study conducted by Salehi et al. [270] utilized various ML approaches to predict hydrogen storage capacities in MOFs, including Multi-layer Perceptron (MLP), SVM, Random Forest (RF), CatBoost, LightGBM, XGBoost, and Committee Machine Intelligence System (CMIS). These models were trained on experimental data collected from different studies. The results showed that the CMIS model outperformed other models, achieving an R^2 value of 0.982 and an RMSE value of 0.088. The Leverage approach was employed to identify and eliminate suspected data points, leading to improved predictability. Only 2.04% of the data points were identified as suspected. Sensitivity analysis revealed that surface area, pore volume, pressure, and temperature had nearly equal contributions to hydrogen storage in MOFs. This finding suggests that these parameters play crucial roles in designing storage systems for hydrogen.

Borja et al. [271] explored the application of ML models in predicting hydrogen storage capacities in MOFs. The study aimed to identify top-performing MOF structures that can meet target hydrogen uptakes efficiently. The researchers evaluated the performance of 13 ML models in predicting the gravimetric and volumetric hydrogen uptake of real MOF structures. Among the models studied, 12 models achieved an R2 value greater than 0.95 for both gravimetric and volumetric uptakes in MOFs. This indicates a strong correlation between the predicted and simulated/experimental results. Additionally, the study introduced a 4-20-1 ANN model that predicts the bulk, shear, and Young's moduli for MOFs. The ML models with high R2 values can be used to select MOFs for hydrogen storage applications.

The application of machine learning models in predicting hydrogen storage capacities in MOFs offers significant benefits. It allows researchers to identify and select the most promising MOFs for experiments, reducing the time and cost associated with conducting experiments on a vast number of potential MOFs. By accurately predicting the storage capacities, the models aid in optimizing operational conditions for hydrogen storage processes that utilize MOFs.

4. Conclusion

In conclusion, this review underscores the pivotal advancements in hydrogen storage technologies and materials, crucial for enabling the widespread adoption of hydrogen as a clean energy source. With global energy demand set to soar to 9.7 billion by 2050, the imperative for sustainable energy solutions is urgent. Despite increasing investments in renewable sources like solar, wind, and hydroelectric power, efficient energy storage systems are essential to mitigate fluctuations in energy generation, especially given the environmental impacts of fossil fuel. Hydrogen storage emerges as a promising solution due to its high energy density and potential for decarbonizing the global energy mix. Physical storage technologies, including compressed hydrogen and liquefaction techniques, offer innovative solutions for storing hydrogen in dense and stable forms. Compressed hydrogen, widely used in transportation applications, particularly in fuel cell cars, is well-established. Liquefied hydrogen storage enables higher energy density but presents challenges in terms of safety and infrastructure due to its cryogenic requirements.

Material-based hydrogen storage approaches, utilizing metal hydrides, complex hydrides, and carbon-containing substances, provide alternatives to physical storage. These materials employ absorption or adsorption techniques, with the release of molecular hydrogen achieved through thermal or catalytic decomposition. Research efforts focus on designing efficient catalysts to enhance hydrogen generation. Considerations such as structural attributes, porosity, surface area, capacity, stability, and safety are vital in the development of efficient hydrogen storage materials. Computational chemistry, high-throughput screening, and machine learning have emerged as powerful tools in accelerating material design, contributing to progress in energy-related industries. To achieve a sustainable energy future, overcoming challenges associated with hydrogen storage, such as low volumetric energy density, safety concerns, and infrastructure requirements, is crucial. Developing efficient and secure hydrogen storage materials is essential for maximizing hydrogen's potential as a clean energy carrier in transportation, power generation, and industrial processes.

Future research in hydrogen storage materials and technologies may focus on advanced material design, nanotechnology, integrated storage systems, advanced characterization techniques, sustainable hydrogen production, safety considerations, and computational approaches. These efforts aim to improve storage efficiency, safety, and practicality while exploring renewable production methods and addressing infrastructure challenges. Enhanced materials, nanoscale engineering, and data-driven approaches will contribute to the widespread adoption of hydrogen as a clean energy source.

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.

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