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Hydrogen Storage Technologies: A Comprehensive Review of Physical, Chemical and Materials-Based Approaches

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Abstract

This review provides a systematic analysis of the hydrogen storage methods, classifying them into three main categories: physical, chemical, and materials-based approaches. Physical methods include compressed gas and cryogenic liquid storage, offering mature yet infrastructure-intensive solutions. Chemical methods involve metal hydrides and liquid organic hydrogen carriers (LOHCs), which enable high volumetric densities and stable, long-term storage through reversible reactions. Materials-based strategies including carbon nanomaterials, metal–organic frameworks (MOFs), and doped graphene derivatives offer advanced pathways for hydrogen adsorption through physisorption and chemisorption, with promising gravimetric and volumetric capacities. Special attention is given to the influence of physical and chemical activation on carbon-based materials, as well as the role of doping, structural modification, and functionalization in enhancing hydrogen uptake. Emerging technologies such as nitrogen- and boron-doped carbon nanotubes and LOHC systems are discussed in terms of their advantages, limitations, and potential for integration into future hydrogen infrastructure. Through critical evaluation of current materials, performance metrics, and engineering challenges, this review highlights the importance of interdisciplinary innovation in storage technologies. The findings underscore the urgent need for continued research and investment to overcome thermodynamic limitations, improve kinetics, and reduce system costs. Ultimately, advanced hydrogen storage solutions are essential for achieving global net-zero targets and mitigating the environmental and health crises linked to conventional energy systems.

Keywords: Hydrogen storage; Liquid organic hydrogen carriers (LOHCs); Metal–organic frameworks (MOFs); Chemical storage; Physical storage.
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1. Introduction

Over the past hundred years, humans have been burning large amounts of fuels such as coal, oil, and gas. During combustion, a significant amount of carbon dioxide (CO_2) is released into the atmosphere. This gas remains in the atmosphere for a long time approximately 100 years and contributes to global warming.[1-3] As scientists have proven, the more CO_2 in the air, the higher the Earth's surface temperature rises. This is not just a prediction; it is based on solid scientific research. For example, air bubbles trapped in ancient ice cores from Antarctica allow scientists to determine the atmospheric CO_2 concentration over the past 800,000 years. These long-term data help us better understand changes in the Earth's weather and climate.[4-6]

Today, the amount of carbon released into the atmosphere from fuel combustion has reached billions of tons. Each increase of 1 ppm (part per million) of CO_2 corresponds to 2.12 billion tons of carbon, which translates to 7.77 billion tons of CO_2. This is a huge amount CO_2 is a greenhouse gas that traps heat from the sun. As its concentration increases, more heat accumulates on Earth, changing the climate. Scientists study ancient air bubbles and ice core layers to determine past CO_2 levels and corresponding temperatures. However, since the air gets trapped in the ice slightly later than the ice forms, there is a small time mismatch in the data.[7,8]

Energy consumption (for electricity, heating, and transportation) on Earth increases every year, and this is the main reason for the rise in harmful gas emissions. For 420,000

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years, the CO_2 level on Earth never exceeded 300 ppm. Today, it has reached approximately 425 ppm. Based on the above data, you can calculate how many billions of tons this increase represents. This is a very dangerous situation an unprecedented level. These numbers clearly indicate that human activity is altering the Earth's atmosphere and climate. If we do not reduce the emission of harmful gases, climate-related disasters may occur in the future.[9]

According to 2025 research, up to 40 percent of global glacial ice including critical Himalayan glaciers, one of the world's most important freshwater sources is locked in to melt by the end of this century, even with aggressive climate action. If the world continues at its current pace, losses could reach 50-90 percent under higher warming scenarios, causing widespread freshwater shortages and affecting billions of people. Arctic sea ice has also been steadily declining over the last 50 years. Satellite observations since 1979 show that ice volume has decreased by approximately 13% per decade. If greenhouse gas emissions continue to rise, the Arctic could be completely ice-free in the summer by mid-century. This would intensify heat absorption from the sun and accelerate global warming.[10-12]

Another alarming issue is the thawing of permafrost soil in the Arctic. This soil contains roughly twice as much carbon as is currently in the atmosphere, equivalent to about 1,700 billion tons. As it thaws, it releases this carbon, further contributing to global warming.[13,14] In 2015, forest fires burned 9 million hectares in Alaska and northern Canada, releasing more carbon than ever before. In 2018, around 60 wildfires were recorded in Arctic Sweden. Fires are also increasing in Greenland, Siberia, Ukraine, and Canada. Even Antarctica, located at the South Pole, is under threat.[15,16] Over the past 25 years, this region has lost approximately 3.4 trillion tons of ice. The rate of ice loss has accelerated, with an average of about 136 billion tons per year. In the 1980s, 40 billion tons of ice melted annually, but after 2009, this number rose to 219 – 252 billion tons per year. This phenomenon contributes to rising sea levels, posing serious risks to coastal countries. Greenland's ice mass is also rapidly declining. NASA satellite data show that ice in Greenland is melting at an average rate of 267-270 billion tons per year, faster than in Antarctica. This affects ocean currents in the Atlantic and may cause abrupt weather changes in Northern Europe. In recent years, rainfall in Greenland has increased doubling in summer and tripling in winter accelerating ice melt even more.[17-20]

Although carbon dioxide (CO_2) is not considered toxic at low concentrations (400–600 ppm), elevated levels can pose significant health risks. Short-term exposure to concentrations above 1,000 ppm may cause symptoms such as headaches, dizziness, shortness of breath, and cognitive impairment. At levels between 2,000 and 5,000 ppm, CO_2 can lead to confusion, unconsciousness, or even death due to hypercapnia (excess CO_2 in the blood) or oxygen deficiency.[21-23]

The human body reacts to increased CO_2 levels primarily through the respiratory system. As CO_2 concentration rises, the body increases the breathing rate to expel the excess gas. This hyperventilation may result in a condition known as respiratory alkalosis, where blood pH rises, potentially causing muscle twitching, hand tremors, and dizziness. Prolonged exposure to high CO_2 concentrations especially in poorly ventilated indoor environments can lead to chronic health problems. Studies have indicated that long-term exposure to levels above 3,000 ppm significantly declines cognitive performance in workplace environments. For example, recent studies demonstrate that exposure to concentrations between 1,000–3,000 ppm leads to decreased attention and slower reaction times, leading to safety hazards in fields such as aviation and construction.[24-28]

Moreover, chronic hypercapnia weakens the immune system, increasing vulnerability to respiratory infections and cardiovascular complications particularly dangerous for people with existing health conditions or the elderly. High carbon dioxide concentrations are closely linked to poor air quality, which exacerbates respiratory disorders such as asthma and chronic obstructive pulmonary disease (COPD). Studies have shown that indoor carbon dioxide levels above 1,500 ppm increase the frequency of respiratory symptoms. High carbon dioxide concentration also weakness normal lung function and increases inflammation in the airways.[29-31]

The cardiovascular system is also affected by elevated CO_2 levels. During hypercapnia, the heart compensates for oxygen-deprived tissues by increasing the heartbeat. Prolonged exposure to CO_2 can aggravate heart conditions, potentially causing arrhythmias and other complications, especially in individuals with preexisting vulnerabilities. Recent studies have also focused on CO_2's impact on the nervous system, showing that it impairs cognitive performance, mood regulation, decision-making, and motor coordination. Even at 1,000 ppm, a decline in mental performance has been observed, with higher levels significantly reducing attention span, memory, and problem-solving ability. Some individuals also experience diminished social interaction.[32-34]

Controlled laboratory studies have shown that CO_2 concentrations around 2,500 ppm lead to notable cognitive dysfunction. These findings are especially concerning in industrial and office environments, where they can threaten employee productivity and safety. Although CO_2 is a natural and essential component of the atmosphere, its excessive accumulation especially in enclosed spaces can seriously harm respiratory, cardiovascular, and nervous systems. Preventive measures such as proper ventilation, installation of CO_2 monitoring systems, and the implementation of green technologies are crucial.[35-38]

Certain vulnerable populations are more susceptible to the

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harmful effects of elevated CO_2. These include children, the elderly, and individuals with respiratory or cardiovascular conditions. In children, high indoor CO_2 levels can worsen asthma and reduce lung function, potentially increasing school absences and leading to long-term health issues. For elderly individuals especially those with weakened respiratory or cardiovascular systems even short-term CO_2 spikes can be dangerous. Aging reduces physiological resilience, making the elderly more sensitive to CO_2 exposure. Pregnant women are also considered vulnerable; studies suggest that high CO_2 levels during pregnancy may impact fetal development and birth outcomes, potentially affecting long-term child health.[39-41]

The physiological and biochemical effects of CO_2 exposure include disruption of the body's acid-base balance, resulting in hypercapnic respiratory acidosis, a condition where blood becomes more acidic due to increased CO_2. The body responds by increasing breathing rate and cardiac output. Prolonged exposure can activate inflammatory responses, contributing to chronic respiratory conditions, reduced resistance to infections, and weakened immunity. Oxidative stress, increased production of reactive oxygen species (ROS), and altered immune responses are among the primary mechanisms triggered by CO_2 exposure. Further research is required to fully understand the entire spectrum of these effects.[42-45]

These escalating environmental and health challenges underscore the urgent need for a global transition away from fossil fuels toward sustainable, low-carbon energy systems. Hydrogen emerges as a pivotal clean energy carrier, capable of decarbonizing sectors such as heavy transportation, industrial processes, and power generation where electrification alone is insufficient. Unlike fossil fuels, hydrogen combustion produces only water vapor, and when generated from renewable sources via electrolysis, it offers a zero-emission pathway that can also mitigate indoor and atmospheric CO_2 buildup. However, the realization of a hydrogen economy faces significant hurdles, chief among them the efficient and safe storage of hydrogen. Hydrogen's low volumetric energy density necessitates advanced storage solutions to enable its practical use in vehicles, stationary power systems, and grid-scale applications (Fig. 1).

This review paper examines the state-of-the-art in hydrogen storage technologies, categorizing them into physical methods (*e.g.*, compressed gas and cryogenic liquid storage), chemical methods (*e.g.*, metal hydrides and chemical hydrogen carriers), and materials-based approaches (*e.g.*, nanomaterials and metal-organic frameworks). We evaluate their performance metrics, including gravimetric and volumetric capacities, reversibility, cost, and safety considerations, while highlighting recent advancements and remaining challenges. By synthesizing current research and projecting future trends, this review aims to guide the development of viable hydrogen storage solutions essential for achieving net-zero emissions and mitigating the climate and health crises outlined above.

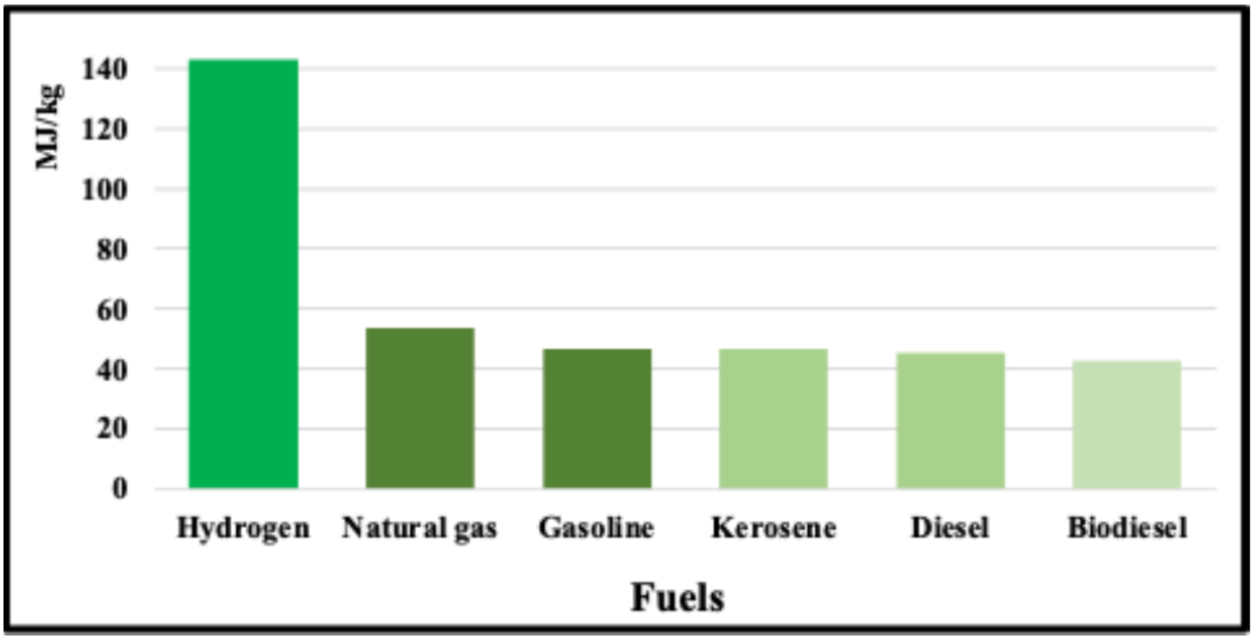

Fig. 1: Comparison of Energy Density of Various Energy Carriers.

2. Basics of hydrogen storage

Hydrogen storage is one of the most challenging and critical issues in the development of hydrogen energy. This is because the physical and chemical properties of hydrogen make its efficient, safe, and cost-effective storage and transportation difficult. In Fig. 2, the main areas of hydrogen storage are illustrated. To effectively develop hydrogen storage technologies, it is first necessary to deeply understand its storage mechanisms. In this section, we will examine in detail the physical, chemical, and adsorption storage methods, revealing their theoretical foundations and practical application features.

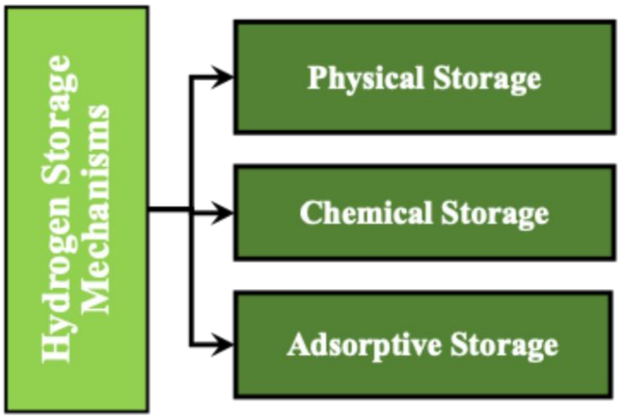

Fig. 2: Diagram of the main mechanisms of hydrogen storage: physical (gas and liquid), chemical (hydrides, LOHC), and adsorption (CNT, MOF, carbon).

2.1 Physical storage

Storing hydrogen in gaseous form requires specialized high-pressure tanks. Standard pressure levels are typically 350 bar and 700 bar. These tanks are commonly made from steel, aluminum, or materials reinforced with carbon fiber composites. The reservoirs used for gas storage are constructed from steel, aluminum, or carbon fiber-coated composite materials. However, this method has its drawbacks.[46-48] Firstly, operating under high pressure necessitates stringent safety measures. Secondly, the weight and volume of the tanks pose challenges for transportation (Department of Energy (DOE). (2022).)[48-50] Evaluating the energy efficiency of hydrogen storage technologies involves considering several key parameters. Firstly, gravimetric density (wt%) describes the proportion of hydrogen mass relative to the total system mass. A high gravimetric density indicates the ability to store a large amount of hydrogen in lightweight materials, which is critical for transportation and aerospace applications. Secondly, energy density (MJ/kg) measures the amount of energy released from 1 kilogram of hydrogen. Theoretically, 1 kg of hydrogen can yield approximately 120 MJ of energy, a figure twice that of gasoline, highlighting hydrogen's potential as a future energy carrier. Thirdly, storage volume and pressure indicators are essential specialized tanks are required to store hydrogen under high pressure. For instance, a 150-liter tank at 70 MPa can hold approximately 5.4 kg of hydrogen, sufficient to power a small vehicle for 500–600 km. Additionally, the durability, weight, and temperature resistance of the tank material significantly influence the overall system efficiency. Fourthly, the speed and reversibility of the hydrogen storage and release process are also crucial. In pressure- or temperature-controlled systems, the ability to quickly charge and release hydrogen as needed enhances the system's practical utility. The tank's own mass also impacts energy efficiency, as reservoirs made from lightweight yet strong materials (*e.g.*, carbon composites) improve the payload efficiency. Overall, storing hydrogen in high-pressure tanks is currently a widely adopted and relatively reliable method. However, ongoing research focuses on material improvements, energy-efficient compression, and optimization of thermal insulation and safety systems to further enhance these systems' effectiveness.[51]

Storing hydrogen in liquid form requires cooling it to -

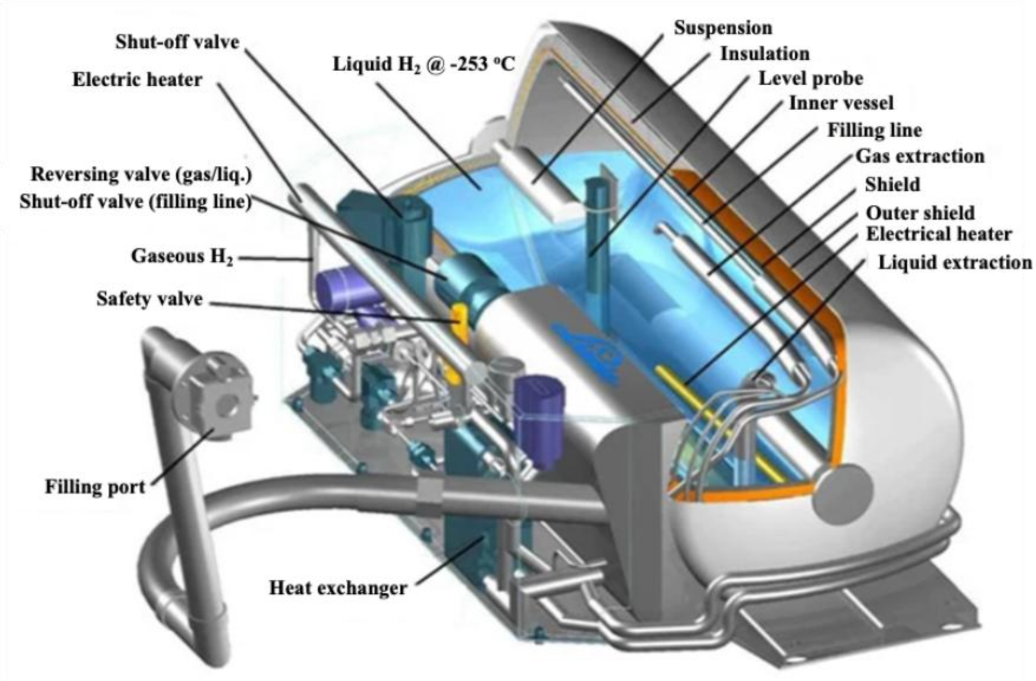

Fig. 3: Structure of a High-Pressure liquid Hydrogen storage tank. Reproduced from.[54]

Table 1: Comparison between Compressed Hydrogen and Liquefied Hydrogen storage methods.

Feature	Compressed Hydrogen	Liquefied Hydrogen
Physical State	Gaseous	Cryogenic Liquid
Typical Pressure	350 - 700 bar (5000–10,000 psi)	Near ambient pressure (~1 - 3 bar)
Temperature Required	Ambient (25°C)	- 253°C (20 K)
Volumetric Energy Density	~20 - 40 kg/m³	~70 - 71 kg/m³
Gravimetric Energy Density	Lower (heavy tanks)	Higher (lighter per volume)
Storage Tank Type	High-pressure carbon composite tanks	Double-walled vacuum-insulated tanks
Main Use Cases	Fuel cell vehicles (*e.g.*, Toyota Mirai), buses	Aerospace, long-distance trucking, storage depots
Energy Required to Store	Moderate (compression energy)	High (liquefaction energy)
Boil-off Loss	None (sealed)	Yes (evaporation over time)
Safety Concerns	High-pressure leaks, risk of rupture	Extreme cold, boil-off, fire/explosion risk
Advantages	Simpler Infrastructure, No Cryogenic Needs, No Boil-Off, Wider Application.	Higher Volumetric Density, Lighter Per Energy Unit, Suitable for Large-Scale Transport, Efficient for Large-Scale Storage.
Disadvantages	Lower Volumetric Density, Heavy Tanks, Energy Loss, High Pressure Risks.	High Energy Cost, Boil-Off Losses, Complex Equipment, Safety Hazards.

253°C. This method is advantageous for storing large volumes of hydrogen due to its high volumetric density. Liquid hydrogen is kept in cryogenic tanks (see Fig. 3), which are equipped with specialized vacuum insulation. This approach is predominantly used in aerospace applications. The drawbacks of this storage method include the complexity of cryogenic systems and their high energy consumption. Additionally, hydrogen loss due to boil-off may occur.[52, 53]

Physical storage methods are technologically advanced today; however, they still require optimization to ensure long-term, safe, and cost-effective storage. Numerous research groups are striving to develop alternative or hybrid storage systems. Physical storage involves preserving hydrogen in its pure form through physical means, such as under pressure or at low temperatures. This method is currently the most widely adopted and technically developed approach. The comparison between compressed hydrogen and liquefied hydrogen storage methods is presented in Table 1.

3. Chemical storage

Chemical storage is a method of preserving hydrogen in a chemically bonded form, where hydrogen interacts with specific chemical substances to form stable compounds. This approach enables the safe, long-term storage of hydrogen, typically in solid form, rather than in gaseous or liquid phases. Chemical storage systems offer several advantages, including high energy density, environmental safety, and ease of use. This method is widely considered for applications in automotive, aviation, stationary energy systems, and space technologies.

3.1. Metal hydrides

Metal hydrides are materials used to store hydrogen, resulting from the interaction of hydrogen with metal atoms to form solid-phase compounds (hydrides). This process can occur at low temperatures and under atmospheric or higher pressures. Commonly studied hydrides include magnesium hydride (MgH_2), titanium-iron hydride ($TiFeH_2$), and lanthanum-nickel hydride ($LaNi_5H_6$). These materials can absorb hydrogen at specific temperatures and pressures and release it through a reverse reaction.[55,56] Metal hydrides offer several advantages, including high energy density exemplified by MgH_2, which can theoretically store up to 7.6 wt% hydrogen along with enhanced safety due to storage in a solid state that minimizes the risk of spontaneous combustion or leakage, and reversibility, as many hydrides can be charged and desorbed multiple times over several cycles. However, these materials also present notable disadvantages, such as the high temperature requirement for desorption, often necessitating temperatures between 250 - 400°C, slow reaction kinetics that cause some hydrides to absorb and release hydrogen inefficiently, and material instability, which may lead to phase changes or degradation during long-term use. The operating and comparative parameters of complex metal hydride hydrogen storage systems are summarized in Table 2 and Fig. 4.

Hydrogen-fueled electric power plants (Table 3) are facilities that generate electricity using hydrogen as the primary fuel, typically employing fuel cells (which convert hydrogen electrochemically into electricity) or combustion in

Table 2: Operating Conditions of Metal Hydride-Based Hydrogen Storage Systems.

Metal Hydride	Dehydrogenation enthalpy ΔH (kJ/mol)	Hydrogen Release Temperature (°C)
MgH_2	75 - 80	250 - 400
$TiFeH_2$	27 - 41	400 - 450
$LaNi_5H_6$	30.8	25 - 100
$NaAlH_4$	37	150 - 200
LiH	181.2	500 - 750
CaH_2	210 - 220	>700
ZrH_2	169	>700
Mg_2FeH_6	77 - 98	450
$LiBH_4$	67	300 - 400
$NaBH_4$	47	400 - 500 (with hydrolysis)

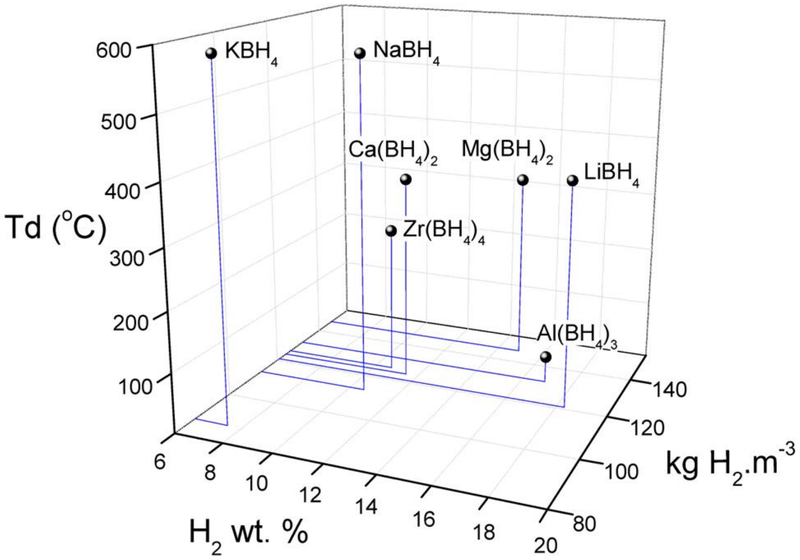

Fig. 4: 3D Performance Comparison of Complex Metal Hydrides for Hydrogen Storage. Reproduced from.[57]

Table 3: Hydrogen-Fueled Electric Power Plants (By Capacity).

Plant Name / Location	Capacity (MW)	Fuel Type / Technology	Operational Since
Antwerp Hydrogen Production Plant Port of Antwerp, Belgium	1.0	Byproduct H_2 from industrial electrolysis / Fuel cell	2011
Hydrosol II Pilot Plant Almería, Spain	0.1	Green H_2 via high-temperature electrolysis powered by solar / Fuel cell integration	2008
Idaho National Laboratory HTSE Demo Idaho, USA	0.5	Green H_2 via high-temperature steam electrolysis using nuclear electricity / Fuel cell	2023
HYFLEXPOWER Demonstration Plant Saillat-sur-Vienne, France (Smurfit Kappa site)	12	Green H_2 via renewable electrolysis / Gas turbine (100% H_2 capable)	2023
Fusina Hydrogen Power Station Fusina, near Venice, Italy	12 (plus 4 MW steam reuse)	Grey H_2 from petrochemical cracker / Combined-cycle gas turbine	2009 (decommissioned 2018)
Shinincheon Bitdream Hydrogen Fuel Cell Power Plant Incheon, South Korea	78.96	Green/grey H_2 / Phosphoric acid fuel cells (PAFC)	2021
Bridgeport Fuel Cell, LLC Bridgeport, Connecticut, USA	17 (single unit; part of larger 384	Pipeline natural gas-derived H_2 (with biogas options) / Fuel cells	~2010s (part of U.S. fleet operational since early 2000s)

Plant Name / Location	Capacity (MW)	Fuel Type / Technology	Operational Since
	MW U.S. fuel cell fleet)		
Voestalpine Green Hydrogen Plant (Integrated Power) Linz, Austria	6	Green H_2 via electrolysis powered by renewables / Fuel cell	2019
Lingen Emsland H_2-Ready Plant Lingen, Germany	30-34	Green H_2 via electrolysis / Gas turbine (Kawasaki L30A, 100% H_2)	2024
Hekinan Coal-Fired Power Plant (H_2/Ammonia Co-Firing Test) Hekinan, Japan	1,000 (full plant; 20% H_2 co-firing)	H_2/ammonia blend / Coal turbine with H_2 injection	2024 (testing phase)

turbines (often adapted combined-cycle gas turbines designed for hydrogen use). As of 2024-2025, operational hydrogen-fueled power generation capacity remains limited globally. Fuel cell plants, which are highly efficient (up to 60%), are typically smaller in scale and are utilized for baseload or backup power; while most currently rely on hydrogen derived from reformed natural gas, the adoption of green hydrogen is steadily increasing. In contrast, turbine plants operate on a larger scale through combustion and often begin with hydrogen-natural gas blends (*e.g.*, 30%) before transitioning to full hydrogen use, with an efficiency range of approximately 40-50% for hydrogen.

3.2. Liquid organic hydrogen carriers

Liquid Organic Hydrogen Carriers refer to organic compounds that chemically bond hydrogen atoms within a liquid phase. This storage mechanism allows for the transport and storage of hydrogen at ambient conditions, distinguishing it from traditional gas or solid-state hydrogen storage methods. The process involves the hydrogenation of an unsaturated organic compound, converting it into a hydrogen-rich form, and the subsequent dehydrogenation to release hydrogen gas when needed. The appeal of LOHCs lies primarily in their high volumetric energy density, which surpasses that of gaseous hydrogen storage, making them conducive for integration into pre-existing fuel infrastructure without requiring extensive modifications. The reversible nature of the hydrogenation and dehydrogenation processes enables LOHCs to be cycled multiple times, thus presenting a robust solution for energy storage.[58-61]

Hydrogen is stored in LOHCs through covalent bonding. When hydrogen gas interacts with a hydrogen-lean organic compound, it undergoes catalytic hydrogenation, resulting in the formation of a hydrogen-rich compound. Organic compounds such as toluene and naphthalene have been widely studied for their ability to act as LOHCs, providing substantial hydrogen storage capacity.[79] The hydrogenation process improves energy density while maintaining the liquid state, allowing for efficient transport and utilization.[80,81] In dehydrogenation, the hydrogen-rich organic compound is subjected to heat or catalytic action, which breaks the bonded hydrogen and releases it as molecular hydrogen. This process typically requires optimized conditions (temperature, pressure, and catalyst choice) to ensure efficient hydrogen release without excessive energy input and degradation of the carrier material.[82,83] Table 4 presents the physical parameters and hydrogen storage capacities of selected liquid organic hydrogen carriers (LOHCs).

Table 4: Physical parameters and hydrogen storage capacity of some LOHCs.

LOHCs	Melting Point (°C)	Boiling Point (°C)	H_2 Storage Capacity wt%	Reference
Benzene (Ben)	5.5	80	7.2	[62]
Toluene (TOL)	- 95	111	6.2	[62]
Naphthalene	80	218	7.3	[62]
Carbazole	245	355	6.7	[62]
N-ethylcarbazole (NEC)	69	378	5.8	[62]
N-propylcarbazole (NPC)	48	336	5.43	[63]
Dibenzyltoluene (DBT)	- 39~ - 34	390	6.2	[64]
1-methylindole (1-MID)	- 20	239	5.76	[65]
2-methylindole (2-	57	273	5.76	[66]

LOHCs	Melting Point (°C)	Boiling Point (°C)	H_2 Storage Capacity wt%	Reference
MID)				
1,2-dimethylindole (1,2-DMID)	55	260	5.23	[67]
N-ethylindole (NEID)	- 17.8	253.5	5.23	[68]
Dibenzyltoluene (DBT) / Perhydro-dibenzyltoluene (H18-DBT)	-	-	6.2 wt%	[69]
Methylcyclohexane (MCH)	-126.3 °C	101 °C	Approximately 6.5 wt%	[70]
N-Ethylcarbazole (NEC)	68-70	166°C	7.0 wt%	[71]
Toluene	- 95.0	110.60	7.0 wt%	[72]
diphenylmethane	22 - 25	264	6.9 wt %	[73]
decalin /naphthalene			7.3	[74]
Bis-BN Cyclohexane	*6.47*	80.74	4.7 wt%.	[75]
indole			1.7%.	[76]
dodecahydro-*N*-ethylcarbazole/*N*-ethylcarbazole	-	-	5.8	[77]

LOHCs present several significant advantages over traditional hydrogen storage methods:

1. Safety and handling: LOHCs operate at ambient temperature and pressure, reducing the risks associated with high-pressure hydrogen storage systems. Their liquid state makes them easier to handle and transport using current fuel logistics, ensuring compatibility with existing fuel supply chains and minimizing safety concerns related to gas handling.[84]

2. High energy density: Compared to compressed hydrogen and liquid hydrogen storage, LOHC systems exhibit a superior volumetric energy density—allowing more energy to be stored in a given volume, which is crucial for applications like vehicular storage where space is limited.[85]

3. Versatility: A wide range of organic compounds can be utilized as LOHCs, providing flexibility in selection based on availability, cost, and desired operating conditions. This allows for a broad application scope across different sectors, including transportation, industrial processes, and energy storage.[86]

4. Long-term storage: LOHCs enable long-term hydrogen storage without significant losses or performance degradation. This trait is particularly beneficial for applications in seasonal energy storage and as backup power sources.[86]

The efficiency of LOHC systems hinges on the performance of the catalysts used in the hydrogenation and dehydrogenation reactions. Research has identified various metal-based catalysts (*e.g.*, ruthenium, platinum) that facilitate both reactions under mild conditions, enhancing reaction kinetics and lowering energy requirements. Notably, catalytic activity is not solely dictated by the metal type; it is also significantly influenced by the support materials, preparation methods, and the specific reaction environment. Studies have demonstrated that modifying catalytic surfaces to optimize active site accessibility can lead to considerable improvements in hydrogen storage performance.

Despite their potential, LOHCs also face several challenges that need addressing to enhance their viability for large-scale applications:

1. Thermal management: The heat associated with dehydrogenation reactions can pose operational challenges, particularly in maintaining optimal temperatures for reaction kinetics. Consequently, advanced heat management strategies are required in commercial implementations to mitigate energy losses during the dehydrogenation phase.[84]

2. Catalyst stability and activity: While many catalysts show promise, their long-term stability during multiple reaction cycles remains a concern. Deactivation due to coking, leaching, or sintering can significantly hamper performance, necessitating continuous research into more robust catalytic materials.[85]

3. Water management: Managing water produced during the dehydrogenation process is critical for sustaining catalyst activity and ensuring efficient operation. Advanced systems need to be developed for synchronized water removal and handling without compromising overall hydrogen yield or purity.

4. Economic viability: Although LOHC systems are favorable for hydrogen storage, the economic aspects associated with synthesis, catalyst development, and operational costs dictate their market adoption. Ongoing innovations in catalyst design and LOHC selection are vital for enhancing cost-effectiveness and facilitating large-scale deployment.[84]

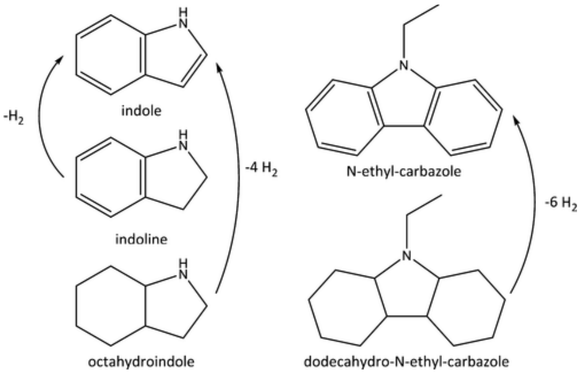

Fig. 5: Left: octahydroindole/indoline/indole LOHC system. Right: dodecahydro-*N*-ethylcarbazole/*N*-ethylcarbazole LOHC system. Reproduced from.[78]

The future of liquid organic hydrogen carriers (LOHCs) appears highly promising, as demonstrated by representative systems shown in Fig. 5. On the left, the octahydroindole/indoline/indole system and, on the right, the dodecahydro-N-ethylcarbazole/N-ethylcarbazole pair, exemplify the diversity and tunability of nitrogen-containing heterocyclic LOHCs. Continuous progress in catalyst design, reaction condition optimization, and molecular engineering is expected to further enhance their hydrogen storage capacity, reversibility, and thermal stability. As the role of hydrogen as a clean energy vector continues to expand, such LOHC systems are likely to play a pivotal role in enabling safe, high-density, and easily transportable hydrogen storage. Advancements in hydrogenation/dehydrogenation catalysis will deepen understanding of the underlying reaction mechanisms, facilitating the rational design of next-generation LOHC molecules with improved energy efficiency and recyclability. Collaborative efforts among academia, industry, and policymakers are essential to integrate these LOHC technologies into sustainable hydrogen supply chains. Moreover, with growing global emphasis on renewable energy and carbon-neutral solutions, LOHC systems like those depicted in Fig. 5 could become critical components of broader carbon-capture, utilization, and storage (CCUS) strategies — bridging the gap between hydrogen production and emissions reduction in a future clean energy economy.

Methods of Physical and Chemical Activation of Carbon

Physical activation is a widely applied method to increase the specific surface area and porosity of activated carbon. This process consists of two stages: carbonization (charcoal formation) and activation. At first, carbon-rich raw materials such as coconut shells, wood, or coal are thermally decomposed via pyrolysis in an inert atmosphere (typically nitrogen or argon) at temperatures between 600 - 900°C. At this stage, volatile substances are removed, resulting in carbon frameworks with an initial porous structure (pores).[87] Subsequently, these frameworks are treated with oxidizing agents like steam or carbon dioxide at temperatures ranging from 700 - 1100°C. In this phase, the disordered regions of the carbon undergo slow degradation through chemical gasification reactions (*e.g.*, $C + H_2O \rightarrow CO + H_2$ or $C + CO_2 \rightarrow 2CO$), leading to the formation of new pores and the enlargement of existing ones. However, excessively high temperatures or prolonged exposure may cause the collapse of the porous structure, thereby reducing efficiency.[88] Physical Activation Parameters like Temperature, Gas Type, Steam Concentration and Activation Time of Carbon Materials is presented in Table 5.

Table 5: Physical Activation Parameters of Carbon Materials.

Parameter	Typical Range	Effect on Structure
Temperature	700 - 1100°C	↑ Temperature → ↑ Pore formation; excessively high → reduced efficiency
Gas Type	Steam, CO_2, or mixtures	Steam → mixed micro/mesopores; CO_2 → primarily micropores
Steam Concentration	~10 - 30%	Highest surface area ~20%; excessive → structure damage
Activation Time	0 - 60 min	Longer time → larger pores; excessively long → structure collapse

The advantages of this method include its simplicity, low cost, and the ability to produce micro- and mesopores in carbon. As a result, the specific surface area of activated carbon typically reaches 600 - 1200 m^2/g, with a pore volume of up to 0.4 cm^3/g.[89] Steam activation not only creates wider pore sizes but also allows the introduction of oxygen-containing functional groups that improve adsorption properties. In contrast, activation with carbon dioxide enhances microporosity, making it more effective for gas-phase applications. Studies indicate that the highest porosity is observed after 30 minutes of processing at 800°C, with a 20% steam concentration yielding optimal results; higher values may lead to structural breakdown.[90] For instance, carbon fibers processed with steam at 500 - 700°C for one hour demonstrated well-developed porosity and a strong capacity for CO_2 adsorption.[91] Thus, physical activation serves as a key method widely employed for controlling the structural characteristics of activated carbon, playing a significant role in ecological and industrial applications.

Chemical Activation of Carbon

Chemical activation of carbon is an effective method for transforming carbon-rich materials into activated carbon with high porosity and a large specific surface area. This process involves impregnating raw materials such as nutshells, wood shavings, or straw with strong chemical reagents like potassium hydroxide (KOH), phosphoric acid (H_3PO_4), or zinc chloride ($ZnCl_2$). Initially, the raw material is dried, then mixed with the activating agent in a specific ratio (*e.g.*, 1:1, 2:1, or higher), followed by drying the mixture at 110 - 120°C. Subsequently, the mixture is heated to 400–850°C in a nitrogen atmosphere for activation. At high temperatures, chemical reactions occur; for instance, with potassium hydroxide: $6KOH + 2C \rightarrow 2K + 3H_2 + 2K_2CO_3$, resulting in the expansion of the carbon structure and the formation of numerous micropores. After heating, the product is washed with acid (*e.g.*, HCl) and water to neutralize it. Finally, the dried activated carbon is obtained. This method yields a BET specific surface area of 1000–3200 m^2/g and a pore volume ranging from 0.4 - 1.2 cm^3/g. Phosphoric acid imparts meso- and microporosity and operates at relatively lower temperatures, while KOH leads to deep microporosity. Table 6 presents the chemical activators commonly utilized in the synthesis of carbon materials. Such activated carbons are widely used in water and air purification, gas adsorption, energy storage devices, and catalysis. The process is simple, efficient, and flexible to control; however, thorough washing and neutralization of activating agent residues are crucial for environmental safety. Table 7 summarizes the hydrogen storage performance of biomass-derived activated carbons. Activation at 700 - 800 °C with KOH yields high-surface-area carbons suitable for physisorption-based hydrogen storage. Hydrogen uptake increases significantly at low temperature (77 K) and high pressure (20 - 40 bar), confirming the synergistic effect of these conditions on adsorption.

Table 6: Comparison of Chemical Activators Used in Carbon Material Synthesis.

Chemical Substance	Full Name	Role	Type of Pores Formed
KOH	Potassium Hydroxide	Reacts with carbon to form micropores	Primarily micropores
H_3PO_4	Phosphoric Acid	Dries and stabilizes the carbon structure	Micro- and mesopores
$ZnCl_2$	Zinc Chloride	Dehydrates and acts as a template	Meso- and macropores
NaOH	Sodium Hydroxide	Functions similarly to KOH, but slightly weaker	Micropores

Table 7: Hydrogen Storage Capacity of Biomass-Derived Activated Carbons under Various Activation Conditions.

Raw Material/Material	Activation Conditions	BET Surface Area (m^2/g)	Hydrogen Storage (wt%)	Temperature/Pressure	Literature Source
Polypyrrole	700°C, KOH	3480	7.0	77K, 20 bar	[92]
Bamboo	700°C, KOH	3208	6.6	77K, 4 MPa	[93]
PAN Fiber	700°C, KOH	2686	1.1	303K, 30 MPa	[94]
Rice Husks	800°C, KOH	2713	1.0	303K, 27 MPa	[95]
Wood-Based Charcoal	700°C, KOH	1830	0.9	298K, 35 bar	[96]
Coconut Shell	750°C, KOH	2320	6.8	77K, 2 MPa	[97]
CO_2 and KOH Dual Activation	800°C	3190	7.08	77K, 20 bar	[95]
Mushroom Biomass	700°C, KOH	2432	2.6	77K, 1 MPa	[98]
Pine Powder (Extract)	600°C - 800°C	4097.49	7.73	77K, 40 bar	[99]
Waste Wood Chips	800°C	1486.2	3.03	77K, 1 bar	[100]

4. Carbon nanotubes (CNTs)

Carbon nanotubes (CNTs) have garnered significant attention in the field of hydrogen storage due to their unique properties. They possess high mechanical strength, lightweight characteristics, and excellent electrical conductivity. This section provides a comprehensive analysis of the structure of carbon nanotubes and their hydrogen storage potential, including the differences between single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs), the mechanisms of hydrogen storage, the effects of doping and functionalization, as well as the challenges related to scalability and reproducibility.

Carbon nanotubes are primarily categorized into two types: single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs). The key difference lies in their structure: SWCNTs consist of a single layer of carbon atoms arranged in a cylindrical shape, while MWCNTs are composed of multiple concentric cylindrical layers of carbon. This structural distinction influences their physical and chemical properties, impacting the mechanisms and capabilities of hydrogen storage. SWCNTs stand out for their high surface area-to-volume ratio, which enhances their hydrogen adsorption capacity. Theoretical studies suggest that SWCNTs can store 5 - 10 wt% hydrogen.[101] On the other hand, MWCNTs are distinguished by their mechanical stability, making them suitable for applications requiring a robust structure.[102] However, their more complex structure can sometimes lead to reduced performance. Both types play a significant role in hydrogen storage technology, and their selection should be based on their specific characteristics, tailored to the intended application, as the choice between SWCNTs and MWCNTs can directly affect the efficiency of a hydrogen storage system.

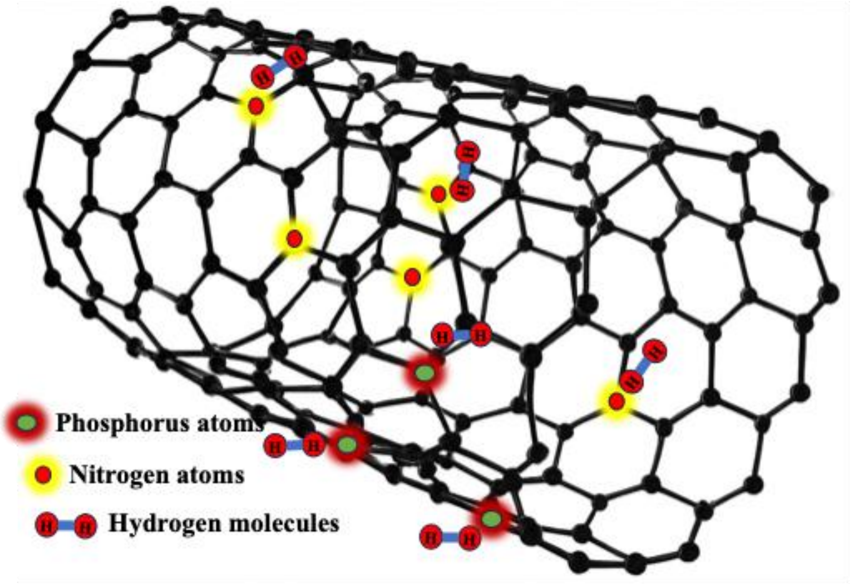

Fig. 6: Mechanism of hydrogen storage in nitrogen- and phosphorus-doped carbon nanotubes.

Hydrogen Storage Mechanisms and Capacity

Hydrogen storage in carbon nanotubes occurs through physisorption and chemisorption. Physisorption involves the weak adsorption of hydrogen molecules onto the carbon surface via van der Waals forces, while chemisorption entails the formation of strong chemical bonds between hydrogen molecules and the carbon surface.

Research indicates that the one-dimensional structure of single-walled carbon nanotubes provides greater accessibility for hydrogen molecules. For instance, pure SWCNTs can adsorb approximately 1 wt% hydrogen, and this capacity can be further increased with structural defects or functional groups.[103] In contrast, multi-walled carbon nanotubes, due to their lower surface area, exhibit a reduced storage capacity; however, their structural durability makes them suitable for use in challenging conditions.

Doping (the introduction of other atoms) and functionalization also significantly influence hydrogen storage capacity. Doping involves incorporating heteroatoms such as nitrogen, boron, or lithium into the carbon lattice, altering the electronic properties and hydrogen interaction energy of the nanotubes (Fig. 6). For example, nitrogen-doped carbon nanotubes have shown improved hydrogen adsorption and increased binding energy.[104,105]

Effects of Doping and Functionalization

Doping with heteroatoms modifies the electronic structure, thermal stability, and chemical reactivity of carbon nanotubes. Nitrogen doping, in particular, has been extensively studied and is known to enhance the interaction between hydrogen and the carbon surface. Synthesis of nitrogen-doped carbon nanotubes using methods like chemical vapor deposition (CVD) has led to a significant improvement in hydrogen storage capacity.[104,105]

Boron doping also enhances hydrogen adsorption, as the interaction between hydrogen molecules and boron-doped sites is strengthened.[106,107] This structural modification enables storage capacities that exceed those of undoped carbon nanotubes.

Functionalization methods improve the hydrophilicity of carbon nanotubes and create additional adsorption sites, thereby enhancing their storage potential. For example, the covalent attachment of hydroxyl or carboxyl groups can strengthen the binding of hydrogen molecules.[108,109] Such modifications increase the usable surface area and improve the efficiency of hydrogen storage.

The unique properties of carbon nanotubes make them promising for hydrogen storage; however, their large-scale production and quality reproducibility present several challenges. One major issue is the synthesis methods themselves. For instance, carbon nanotubes produced via chemical vapor deposition (CVD) or arc discharge methods may vary in quality, with incomplete growth, inconsistent diameters, and the presence of unwanted byproducts, all of which can negatively impact hydrogen storage capacity.[110,111]

Additionally, ensuring uniform distribution of nitrogen or other elements during doping remains a complex task. Variations in the distribution of these elements can alter material properties and complicate the reproducibility of experimental results. Large-scale production of carbon nanotubes also poses difficulties. As demand for carbon nanotubes in hydrogen storage increases, developing high-yield production processes without compromising quality has become a pressing concern. Various solutions are being proposed to achieve continuous production and obtain defect-free, uncontaminated products, though these goals still require multidisciplinary research.[112,113] Furthermore, integrating carbon nanotubes into practical hydrogen storage systems presents additional challenges. The unique characteristics of carbon nanotubes can complicate their compatibility with existing storage solutions. Addressing these issues requires studying the interactions between materials and enhancing their compatibility.

The comparison between single-walled and multi-walled carbon nanotubes necessitates careful selection based on specific applications. A deeper understanding of the effects of doping and functionalization on hydrogen storage mechanisms can pave the way for developing strategies to improve storage efficiency. Nevertheless, challenges related to the production and reproducibility of carbon nanotube materials remain unresolved. Refining reliable synthesis methods and gaining a deeper understanding of material properties will open pathways to developing efficient and sustainable hydrogen storage systems in the future.

5. Graphene and its derivatives for hydrogen storage

Hydrogen is considered one of the most promising energy carriers of the future due to its high energy density, the production of clean byproducts upon combustion, and the potential for production from renewable sources. One of the primary challenges in implementing a hydrogen economy is the development of efficient, safe, and cost-effective hydrogen storage technologies. Among the various materials studied for hydrogen storage, graphene and its derivatives graphene oxide (GO) and reduced graphene oxide (rGO) have garnered significant interest due to their exceptional physicochemical properties. These properties include a large surface area, tunable porosity, chemical functionalization capability, and excellent mechanical strength.[114,115]

Graphene is a single-atom-thick layer of carbon atoms arranged in a two-dimensional honeycomb lattice. Graphene and its derivatives have attracted attention for their potential to enhance hydrogen storage capabilities. Graphene oxide (GO) and reduced graphene oxide (rGO) possess unique properties that facilitate the hydrogen storage process, thereby making a significant contribution to energy applications. This chapter examines the role of graphene and its derivatives in hydrogen storage, analyzing their properties, composite structures, methods to improve efficiency, and strategies for performance optimization.[116-118]

Graphene-based materials for hydrogen storage pure graphene

Graphene is a material consisting of a single layer of carbon atoms arranged in a two-dimensional (2D) hexagonal lattice. Since its discovery in 2004, it has been widely studied due to its exceptional electrical, thermal, and mechanical properties.[119] Theoretical predictions suggest that graphene, owing to its high surface area (~2630 m^2/g), can adsorb up to 7.7 wt% hydrogen under ideal conditions.[120]

Hydrogen can bind to graphene through physical adsorption (via van der Waals interactions) or chemical adsorption (via the formation of C–H bonds). Physical adsorption predominates at low temperatures, while chemical adsorption plays a significant role at higher temperatures or under surface modification conditions.[114] However, pure graphene exhibits limited storage capacity under normal conditions due to its low binding energy with hydrogen molecules (~0.04 eV).

Graphene Oxide (GO)

Graphene oxide is produced by oxidizing graphite. During this process, oxygen-containing functional groups such as hydroxyl, epoxy, and carboxyl are introduced into the graphene structure. These groups disrupt the sp^2 bonding network of graphene, creating defects and increasing interlayer spacing. These functional groups enhance the hydrophilicity of graphene oxide, making it a stable dispersion in water, which is crucial for subsequent chemical transformations and hydrogen storage applications.[121]

Studies have shown that graphene oxide holds significant potential for hydrogen storage. For instance, Rajaura and colleagues demonstrated that the functional groups in graphene oxide improve its interaction with hydrogen molecules, thereby increasing adsorption.[122] The high surface area and specific chemical properties of GO create favorable conditions for use in composite materials for hydrogen storage. The presence of functional groups enhances accessibility and reactivity to hydrogen. Furthermore, the increased interlayer spacing (over 6 Å for GO compared to 3.4 Å for pure graphene) ensures easier access for hydrogen molecules. GO can store 2–3 wt% hydrogen at moderate pressure and temperature.[123]

Reduced graphene oxide (rGO)

Reduced graphene oxide (rGO) is a material obtained by thermally, chemically, or electrochemically reducing graphene oxide (GO) to remove oxygen groups. rGO retains some functional groups and defects, which aid in hydrogen adsorption. Additionally, the material's electrical conductivity and structural integrity are restored. Effective reduction methods can optimize the material's structure, enhancing its hydrogen uptake capacity.

For example, Jain and colleagues showed that rGO can store 1.5 wt% hydrogen under normal temperature and moderate pressure conditions.[124] Compared to pure graphene, rGO generally stores hydrogen more effectively due to a synergistic effect between residual defects and the restored π-conjugation system. Under optimal conditions, rGO can store 3 - 5 wt% hydrogen.[125] Ariharan and colleagues demonstrated that nitrogen doping during the reduction of graphene oxide improves interaction with hydrogen molecules, thereby increasing storage capacity.[126]

6. Conclusion and future prospects

Hydrogen storage remains a critical component in the development of a sustainable hydrogen economy, with multiple strategies physical, chemical, and hybrid demonstrating unique benefits and technical challenges. High-pressure and cryogenic systems offer near-term feasibility for transportation and industrial deployment but are limited by safety, cost, and energy efficiency concerns. Advanced materials such as metal hydrides, porous carbon materials, and liquid organic hydrogen carriers (LOHCs) show strong potential for compact, high-density, and reversible hydrogen storage. These systems benefit from tunable properties, the potential for integration with renewable energy sources, and compatibility with various energy applications. However, issues such as material degradation, kinetic limitations, thermal management, and economic viability remain active areas of investigation. Moreover, the role of catalysts, support structures, and composite design is essential in optimizing the sorption/desorption cycles and ensuring stable operation over prolonged periods. In conclusion, while no single method meets all DOE targets (*e.g.*, 6.5 wt%, 50 g/L volumetric), hybrid systems combining LOHCs with nanomaterials offer synergistic paths forward. By synthesizing recent research, this review underscores that interdisciplinary progress in material design and process optimization is vital for realizing a hydrogen economy, ultimately curbing CO_2-driven climate and health crises.

Looking forward, the future of hydrogen storage will depend on a combination of materials innovation, system integration, and cross-disciplinary collaboration**.** Research must focus on developing novel nanostructured and hybrid materials with high gravimetric and volumetric capacities under mild conditions. Simultaneously, rational catalyst design including the use of bimetallic and interface-engineered systems can improve hydrogenation / dehydrogenation kinetics. Successful deployment of storage technologies will also require comprehensive lifecycle assessments (LCA), thermal management strategies, and standardization efforts to ensure safety and infrastructure compatibility. Additionally, integrating artificial intelligence (AI) and machine learning for predictive material design and real-time system optimization can significantly accelerate progress. With ongoing investment and coordinated global research efforts, hydrogen storage technologies are poised to become pivotal enablers of decarbonized energy systems, facilitating the transition to net-zero targets and reshaping the global energy landscape.

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Conflict of 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.

Supporting Information

Not applicable.

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