

An Overview of Chemical Hydrogen Storage Materials

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Abstract

The potential of hydrogen energy as a source of clean energy is now widely acknowledged, and the scientific community is directing its attention towards the advancement of storage technologies for this energy source. Such materials can be divided into two principal categories: (1) the utilization of chemical reactions, and (2) the application of physical adsorption. These materials can be classified into three categories: hydrogen storage alloys, metal hydrides, and liquid organic hydrogen carriers (LOHCs). Presently, the advancement and investigation of these materials is predominantly concentrated on the synthesis of intricate materials through the incorporation or partial substitution of specific elements to enhance their intrinsic characteristics, including storage capacity, volumetric energy density, hydrogen uptake and desorption kinetics, and enthalpy of dehydrogenation. Our work presents a review of the three types of improved hydrogen storage materials mentioned above, with the objective of assessing their respective benefits and shortcomings. A comparison of the enhanced attributes of the various materials is presented, along with an analysis of some of their shortcomings.

Keywords

Chemical Hydrogen Storage Materials; Hydrogen Storage Property; Hydrogen Storage Alloy; Metal Hydrides; Liquid Organic Hydrogen Carrier.

1. Introduction

The diminishing reserves of traditional energy sources, including fossil fuels such as coal, oil, and natural gas, coupled with the mounting environmental concerns, have prompted a shift in the global energy landscape. The advent of renewable energy sources represents a substantial transformation in the global energy landscape, with hydrogen emerging as a pivotal element in this transition [1]. As a highly sustainable and clean energy vector, hydrogen is positioned to serve as a pivotal contributor in the development of new energy sources, offering a promising pathway for achieving a green transition. Due to its typical gaseous state, hydrogen is flammable, explosive, and diffusible. This presents a substantial challenge with regard to the storage and transportation of hydrogen at ambient temperatures and pressures. The primary concern, therefore, is the development of an energy-efficient, secure, and effective method of hydrogen storage.

This paper is divided into three sections. The initial section presents an overview of the four principal types of hydrogen storage alloys, namely AB₅, AB₂, AB and A₂B. The subsequent section provides a detailed examination of two distinct categories of metal hydrides, namely magnesium-based hydrides and lithium-based hydrides. The third section discusses the three major classes of organic hydrogen carriers-Cycloalkane, N-heterocycles, and O-heterocycles,

and discusses hydrogen storage. Metal hydrides have emerged as a promising area of research, given their high hydrogen storage capacity and favorable cycle stability.

2. Chemical Hydrogen Storage Materials

2.1. Hydrogen Storage Alloy

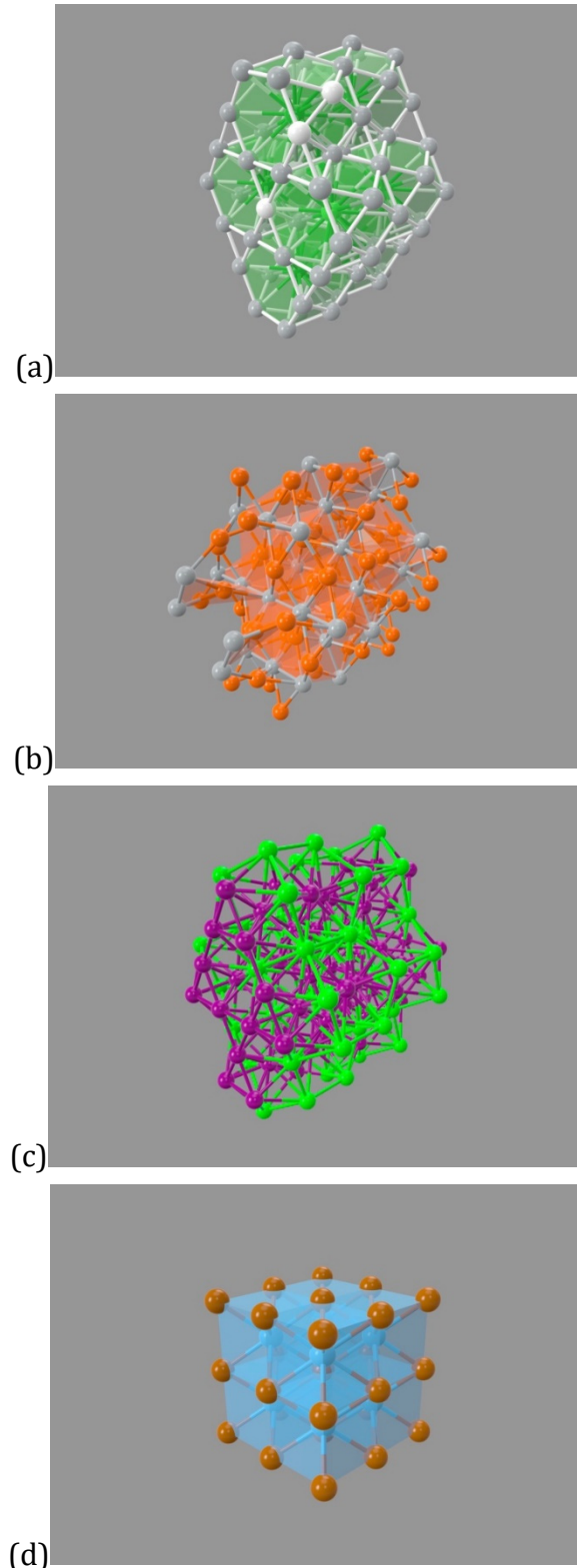


Fig 1. The structures of Hydrogen alloy materials of (a) AB_5 type, (b) A_2B type, (c) AB_2 type, (d) AB type.

In the mid-twentieth century, reversible absorption-desorption patterns of hydrogen under environmental conditions were discovered in specific alloys, thus opening a new field of material which was named hydrogen storage alloys. They have the advantages of large capacity, low energy consumption and convenient transportation. The principle is metal (M) from alloy and hydrogen form metal hydride (MH_x). This process is reversible, positive reaction is hydrogen absorption which release heat, and the reverse reaction is hydrogen release which absorb heat. Hydrogen storage alloy can be classified into 4 types by different composition ratio (crystal shape): AB_5 , AB_2 , AB and A_2B . At present, the research on them mainly focuses on improving their properties by adding other elements or alloys, or mechanical deformation. The structures of these types of alloys as shown in **Fig 1**.

2.1.1. AB_5 - Type Alloy

For AB_5 type alloy, A is normally a rare earth metal element. It has the strengths of high-volume energy density, excellent hydrogen absorption and discharge performance, and fast reaction speed. However, it has the problem of high cost, serious cycle degradation and easy to powder. Nowadays, $LaNi_5$ has been a typical of AB_5 alloy, which shows fast kinetics, low activation energy and in room temperature, the hydrogen storage reaction is reversible [2].

Singh & Bhogilla discovered that compare with the powder $LaNi_5$ hydride, the thermal conductivity of expanded natural graphite (ENG) compacts-based type is increased from 0.5 W/mK to 4 W/mK. The data of comparison is and shows that when the gas supply pressure is 24 bar and the fluid temperature is 293 K, the duration to reach the most stable hydrogen storage capacity is as follows: 1.209 wt%, decreased from 464 s to 232 s [3]. Almeida Neto et al. designed the acrylonitrile-EPDM-styrene (AES) composite materials that containing $LaNi_5$ for hydrogen storage is displayed in **Fig 2**. From the current stage of many scientific research results, no matter changing the synthesis method or the material specific surface of AES- $LaNi_5$, the hydrogen storage reaction kinetics and hydrogen storage capacity will be reduced, however, AES is highly adaptable and can inhibit the air exposure impact of $LaNi_5$ adsorption kinetics. It significantly reduces the time to achieve the peak stable storage capacity [2].

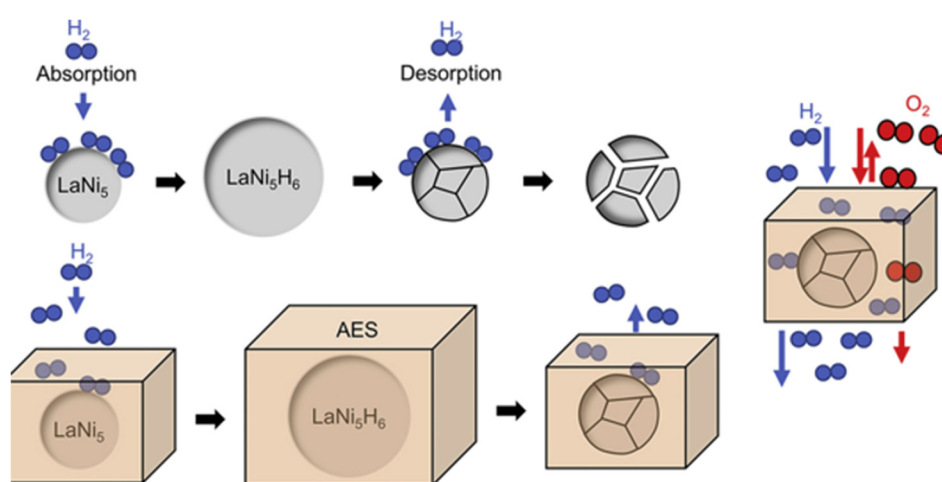


Fig 2. The hydrogen storage process of AES $LaNi_5$ [2]

Moreover, rare earth hydrogen storage alloys of A_2B_7 -type, AB_3 -type have been widely studied in recent years. In summary, for A_2B_7 alloy, a typical one – La-Y-Ni-based was researched, if the Y/La ratio is incremental, it will increase the storage capacity in the meantime. However, the activation performance and cycle life need to be improved.

2.1.2. AB₂ – Type Alloy

For AB₂ alloy, is often referred to as AB₂ – Laves phase alloy, the Laves phase is an intermetallic phase with AB₂ composition. Its main advantages are low reaction activation energy, slightly high hydrogen density and commerciality. Zr – based, Ti– based are the most common types.

HEAs (high-entropy alloy) material with C₁₄ Laves phase of this type can have the reversible hydrogen storage reaction. Multiple sets of data show that, firstly, according to data, (Ti_{1.3} Zr_{0.7})_{1.1} Cr_{1.1} Mn_{1.8} Co_{0.4} V_{0.4} Fe_{0.3} hydrogen storage performance is the best, at 15 °C, reversible hydrogen storage amount for close to 2 wt %. Secondly, Zhou *et al.* research that after Ti hyperstoichiometry was introduced, Ti – Zr – Mn – Cr - V based AB₂ – HEAs with lower V content decrease the pressure of hydrogen equilibrium and enhance the storage capacity, to be specific, the most befitting density of storing hydrogen device is Ti_{0.95}Zr_{0.07}Mn_{1.15}Cr_{0.7}V_{0.15}, which has 1.83% saturated hydrogen capacity, the useable hydrogen capacity yield can reach 58% of the saturated value in 10 °C and 3.2 MPa. This ratio of alloy shows good activity and still has good hydrogenation kinetics after many cycles [4]. Thirdly, when part of Ti in these materials is replaced with the rare earth metal yttrium, Ti_{0.552}Y_{0.048}Zr_{0.4}Cr_{0.6}Mn_{1.4} properties are best at 5 MPa and 298 K can achieve the largest capacity of 1.98 wt % in the condition of inactivated. And the stability and enthalpy of the hydride are reduced, causing the hydrogen release to become simpler. Also, after 100 cycles of absorption and dehydrogenation, the capacity retention rate is less than 4 % away from 100%, and the durability is excellent [5].

2.1.3. AB – Type Alloy

AB alloy has two categories: TiFe and TiNi. For the most common TiFe-type, the alloy is low cost, and the storage capacity is high, up to 1.9 wt%. However, high activation energy results in a low hydrogen absorption kinetics (the difficult first hydrogenation process) due to the surface oxide layer passivation.

Adding some elements will change the performance of AB hydrogen storage alloy, for example, for as-cast Ti-Fe based alloy, after adding ZrCr₂ and Zr, causing a harder hydrogen absorption under moderate conditions, thus, it respectively reduced the absorption capacity to about 1.4 wt % and 1.6 wt %. However, the absorption reaction kinetics are significantly improved. Ha *et al.* researched the hydrogen storage characteristics of Ti₅₀Fe₄₈V₂ alloys which containing a fraction of Ce and the absorption process of Ce is displayed in Fig 3. [6]. The results show that at 25 °C, the particles formed by mixing FCC structure γ -Ce with cerium oxide provide a starting point for the alloy initial absorption capacity and hydrogen absorption kinetics were enhanced. Moreover, an arc- melted AB – type HEAs TiZrNbCrFeNi alloy which have two C₁₄ Laves phases was studied. This AB – HEAs has high potential for hydrogen storage in medium temperature cycle. Because at 473 K, although the capacity is only 1.1 wt%, it can reversibly absorb and desorption [7].

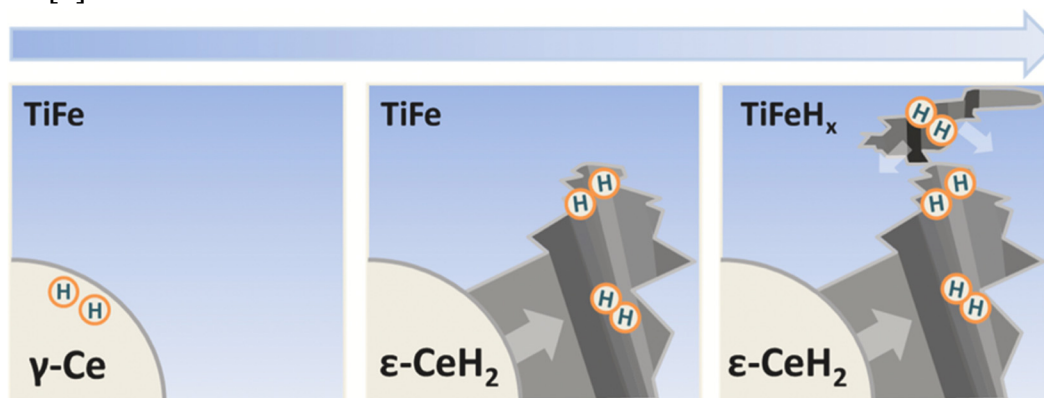


Fig 3. Schematic illustration of the role of the Ce particle during initial hydrogen absorption [6].

2.1.4. A₂B – Type Alloy

The A₂B – type alloy is based on Mg₂Ni and partially replaces Mg and Ni with different elements, which is hexagonal and rhombic structure. The advantages are high storage capacity, rich resources, and the bargain price. However, it has the drawbacks of easy decay as well as short cycle life.

Mg₆₇Ni₃₂Y alloy replaced by yttrium was found to have better dynamic properties, it showed 3.79 wt% hydrogen absorption capacity at most. Moreover, not more than 10 minutes, it can reach the 96% of the maximum capacity [8]. Moreover, Zhong *et al* replaced part of Ni with three M (Al, Mn and Ti) to obtain Mg₂Ni_{0.7}M_{0.3}. The statistics indicate that the adsorption and desorption properties of hydrogen can be enhanced though using this alloy, the dehydrogenation activation energies are -46.12, -59.16 and -73.15 kJ/mol respectively, and the dehydrogenation enthalpy is significantly reduced. And the corrosion resistance has been enhanced. In addition, the Mg₃MNi₂ phase can further improve performance [9].

2.2. Metal Hydrides

Metal hydride is a material composed of metal and hydrogen which can be stored and released as hydrogen repeatedly. Metal hydride storage reaction is as follow:



It's used in new energy electric automobiles, portable electronics and renewable energy systems, etc [1]. The main types are magnesium-based hydrides, lithium-based hydrides, and so on.

2.2.1. Magnesium-based Hydrides

Magnesium is a low-density, non-toxic, abundant metal that is predominantly found in the form of compounds in the Earth's crust. The theoretical hydrogen storage capacity of magnesium hydroxide has been the subject of extensive investigation, with studies indicating a potential capacity of up to 7.6 wt% H₂ [10]. However, the high desorption temperature (300 °C to 400 °C), susceptibility to oxidation in air, and high kinetic barriers have thus far impeded the development of magnesium hydride.

Peng *et al.* showed that by combining NiS@C and MgH₂ and ball-milled, the composite absorbed 6.02 wt% H₂ and release 1.89 wt% up to 523 K; and at 323 K, the hydrogen uptake capacity reached 3.23 wt% within 3.5 hours. Moreover, hydrogen release activation energy can be as low as 60.45 KJ mol⁻¹; secondly, the hydrogen absorption and release rate after 50 cycles is guaranteed to be not less than 98%. The dehydrogenation rate and the stability of the cycle were effectively improved, and the rapid oxidation of magnesium in air or oxygen was avoided [10]. Ali *et al.* designed 3D-TiVCT_x MXene structure and formed MgH₂@3D-TiVCT_x MXene nanocomposite by ball-milled with MgH₂. The material effectively lowered the hydrogen emission temperature to 443 K and stabilized the MgH₂ nanocrystal structure. Moreover, the material absorbed 6.5 wt% hydrogen at 373 K and release 84.62% wt% H₂ at 300 °C in three mins. Then, the capacity of the material only decreased by 0.2 wt% from 6.5 wt% after 180 cycles at 250 °C [11].

2.2.2. Lithium-based Hydrides

Lithium is a lightweight material that reacts with hydrogen to produce stable ionic hydrides (LiH), which have the highest hydrogen content of all hydrides, which can reach 12.6 wt%. Nevertheless, it is not regarded as a material suitable for universal hydrogen storage applications, given that it necessitates the release of hydrogen at temperatures reaching 700 K and exhibits slow reaction kinetics [12].

Bahou and colleagues examined the hydrogen storage capabilities of lithium hydride (LiH) through the use of lithium null defects, identifying that the weight density of LiH could be

increased up to 14.62 wt% when the concentration of lithium nulls reached 16%. Moreover, a notable reduction in desorption temperature was observed, accompanied by enhanced thermodynamic properties [13]. Arharbi and Ez-Zahraouy conducted a series of experiments involving the mixing of fluorine and nitrogen with LiH. The study examined the hydrogen storage properties of lithium hydride (LiH) and investigated the impact of triaxial strain (display in **Fig 4**) on the structural stability thereof. The incorporation of a 4% fluorine atom was found to augment the hydrogen storage capacity of LiH, while concurrently reducing the decomposition temperature to 301.83 K. Furthermore, the application of triaxial compressive stress to these compounds was observed to augment their thermodynamic stability by approximately two-fifths[14].

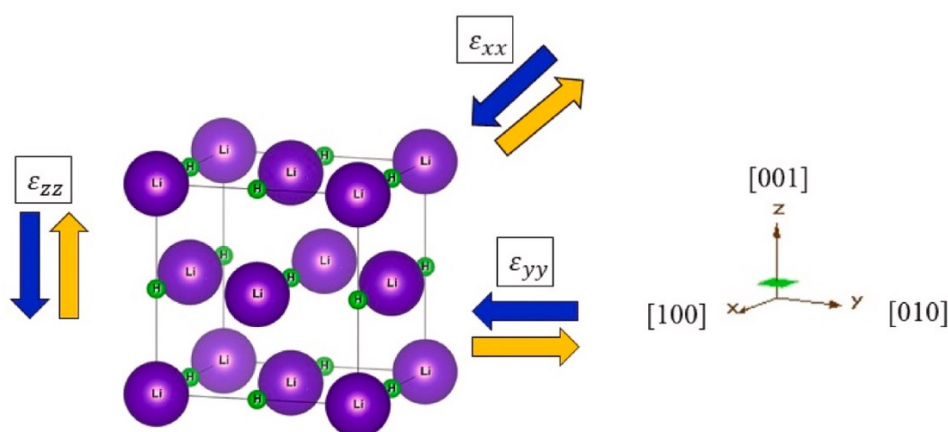


Fig 4. Schematic representation of the crystal structure of LiH under triaxial strains [14].

2.3. Liquid Organic Hydrogen Carrier

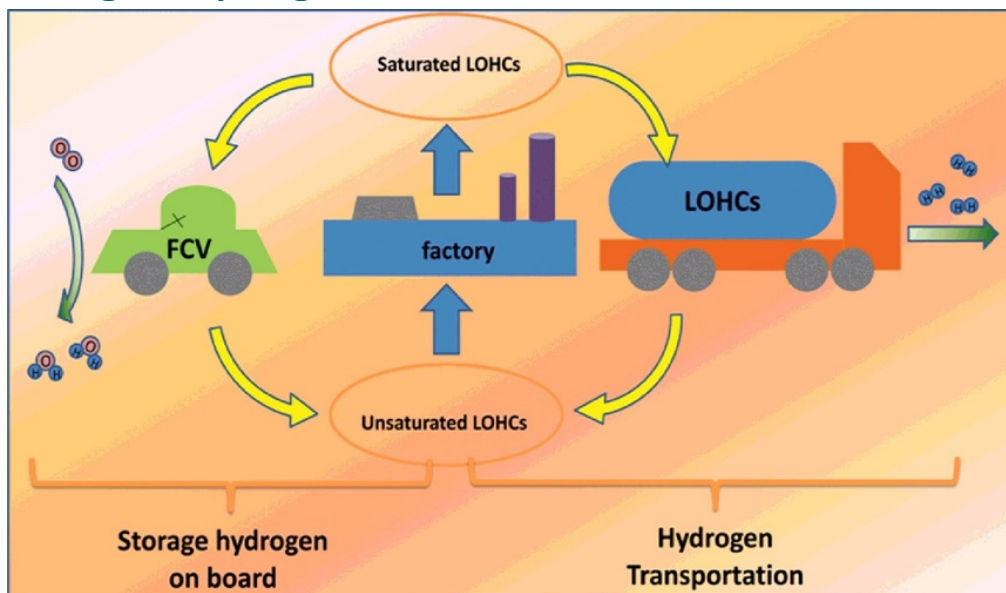


Fig 5. LOHC hydrogen storage industrial process [15]

Liquid Organic Hydrogen Carrier (LOHC) represents a relatively novel technology, developed in the 1970s. The general process is illustrated in **Fig 5**. LOHC employs liquid organic molecules to store and release H_2 in both hydrogenation and dehydrogenation reactions. The storage of H_2 is achieved through the formation of a covalent bond between the selected organic liquid molecules and the H atoms. The hydrogenation reaction occurs under high hydrogen pressure, while the dehydrogenation reaction occurs under low hydrogen pressure. This approach mitigates the risk of explosion and enhances the safety of handling [15]. However, LOHC also

has some disadvantages comparatively. One of the biggest drawbacks is that most of the LOHC molecules are toxic. Moreover, the side reaction after multiple hydrogenation/dehydrogenations can affect the performance of LOHC, and the expensive cost of Platinum group metals catalyst will also be a problem for expanding the production [16]. The potential of LOHC can be evaluated based on its dehydrogenation enthalpy value, as well as its H₂ equilibrium pressure, volumetric and gravimetric energy densities, and energy storage efficiency (wt%). Additionally, the stability of its performance across multiple applications is a crucial factor.

2.3.1. Cycloalkane

MCH/Tol is one of the best-known LOHC systems in the early research of the LOHC technique. Both gravimetric and volumetric densities of Tol/MCH reach 6.2 wt% H₂ and 48 g H₂/L, respectively. MCH/Tol system has 68.3 kJ/mol dehydrogenation enthalpy of H₂. Sinfelt reported the Pt-based catalysts as the best catalyst for the dehydrogenation of cycloalkane represented by Tol for its good efficiency and selectivity [17]. Moreover, Gonda and coworkers show that the Pt catalyst exhibits good activity when H₂S act as a catalyst inhibitor [18].

Dec/Nap is another good aromatic LOHC system, with a larger hydrogen capacity of 7.3 wt% and 66 g H₂/L. However, compared with the MCH/Tol system the higher molecular density makes the rising melting temperature of Dec. Hodoshima and colleagues exploited a Pt-Re bimetallic composite catalyst on granular activated carbon, this catalyst works in a "superheated liquid-film-type" and was proven to increase the dehydrogenation efficiency [19].

2.3.2. N-heterocycles

12H-NEC/NEC is one of the good N-heterocycle LOHC systems with 5.8 wt% of the gravimetric density of H₂, with the possible hydrogenation pathway shown in **Fig 6**. Compared with carbazole NEC has a much lower melting temperature (70 °C) which reduces its restrictions, so it does not need to be diluted. Liu and co-workers developed a new hydrogenation system with the participation of hydrogen-methane mixtures, which increases the maximum degree of hydrogenation to 0.909 [20].

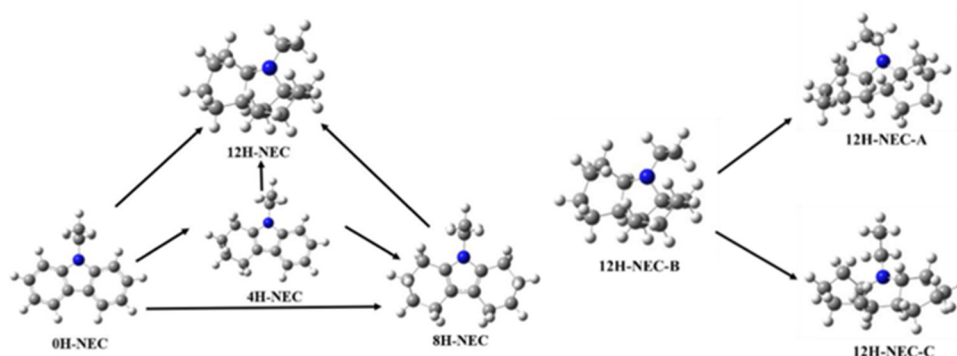


Fig 6. The possible hydrogenation reaction pathway of NEC [20].

The 8H-2-MID/2-MID system has similar structures with carbazole, and its hydrogenation pathway shown in **Fig 7**, but its lower melting point (57 °C), comparably low dihydrogen temperature, and 5.76 wt% of H₂ storage capacity make it an attractive potential LOHC system. Li and colleagues reported a Ru/Al₂O₃ catalyst system, the research reveals the reaction kinetic intermediate through the reaction route and achieved the full dehydrogenation under 4 hours [21].

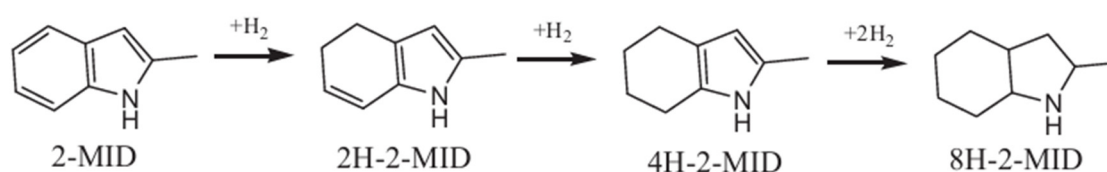


Fig 7. The schematic hydrogenation route from 2-MID to 8H-2-MID [21].

2.3.3. O-heterocycles

One of the primary limitations of O-heterocycles, when compared to N-heterocycles, is that the O atom within the molecule is unable to undergo the process of hydrogenation. The dehydrogenation enthalpy of O-heterocycles is higher compared to the N-heterocycles but still lower than homocyclic LOHC. Several research has shown that Pd/COK-12 catalyst has a good performance on hydrogenation and dehydrogenation, especially on the selectivity of O-heterocycles but slightly lower in hydrogenation efficiency [22].

3. A Characteristics Comparison between the Different Materials Used to Store Hydrogen

The paper presents a summary of several hydrogen storage materials, accompanied by their respective hydrogen storage capacities, advantages and disadvantages. This information is presented in Table 1 for ease of reference. Metal hydrides have the highest hydrogen storage capacity and are among the most promising materials for hydrogen storage. A variety of hydrogen storage alloys are in existence, yet the hydrogen storage capacity of these alloys is typically inferior to that of metal hydrides. Among the latter, the A₂B alloy, represented by a magnesium-based alloy, exhibits the highest hydrogen storage capacity. It has the advantages of good safety, reversibility, hydrogen absorption and decomposition kinetics, and so forth. LOHC also has relatively good hydrogen storage density. Furthermore, it does not need to be liquefied, which reduces thermodynamic and energy losses during hydrogen storage and transport. However, there are still many technical challenges due to the complexity and high cost of hydrogen storage and dehydrogenation devices, as well as the relative susceptibility to side reactions during dehydrogenation.

4. Conclusion

Extensive research has been conducted into the utilization of hydrogen as an energy source due to several factors. These include the high calorific value, versatility, and non-toxic and innocuous nature of hydrogen, adaptability in storage and transportation, environmental benefits, and green credentials. This paper considers three principal categories of chemical material used for hydrogen storage: hydrogen storage alloys, LOHC (liquid organic hydrogen carbons) and metal hydrides. The article examines the most prominent chemical compounds utilized in hydrogen storage, investigates strategies to enhance their hydrogen storage capacity, and assesses their respective merits and limitations.

Table 1. Summary of three storages.

Type of Storages	Structure Type	Materials	H ₂ storage capacity (wt%)	Advantages	Disadvantage
Hydrogen storage alloy	AB ₅	LaNi ₅ with expanded natural graphite (ENG) structure [3]	1.209	1) High the thermal conductivity. 2) Shorter time to reach the most stable hydrogen storage capacity.	\
		AES-LaNi ₅ [2]		1) High adaptable. 2) Shorter time to reach the most stable hydrogen storage capacity.	1) Poor hydrogen storage kinetics and poor hydrogen storage capacity.
	A ₂ B ₇ /AB ₃	La-Y-Ni-based		1) The higher ratio of Y/La, the higher capacity.	1) Weak activation performance and short cycle life.
	AB ₂	(Ti _{1.3} Zr _{0.7}) _{1.1} Cr _{1.1} Mn _{1.8} Co _{0.4} V _{0.4} Fe _{0.3}	2 at 15 °C	1) Good reversibility.	\
		Ti _{0.95} Zr _{0.07} Mn _{1.15} Cr _{0.7} V _{0.15} [4]		1) Good hydrogen absorption kinetics.	\
		Ti _{0.552} Y _{0.048} Zr _{0.4} Cr _{0.6} Mn _{1.4} [5]	1.98 at 25 °C	1) Excellent durability. Easy to release hydrogen.	\
	AB	TiFe	1.9	1) Low cost, and high capacity.	1) Low hydrogen absorption kinetics.
		ZrCr ₂ -Zr-TiFe	1.4 - 1.6	1) Good hydrogen absorption kinetics.	1) Poor hydrogen storage capacity.
		Ti ₅₀ Fe ₄₈ V ₂ [6]		1) Good hydrogen absorption kinetics.	\
		TiZrNbCrFeNi [Z]	1.1	1) High potential for hydrogen storage in medium temperature cycle. 2) Good reversibility.	1) Poor hydrogen storage capacity.
	A ₂ B	Mg ₆₇ Ni ₃₂ Y [8]	3.79	1) Good dynamic properties. 2) High capacity and shorter absorption time.	\
		Mg ₂ Ni _{0.7} Al _{0.3} [9]		1) Lower enthalpy and apparent activation energy of dehydrogenation. 2) Good corrosion resistance.	1) Poor cyclic stability.
Mg ₂ Ni _{0.7} Mn _{0.3} [9]					
Mg ₂ Ni _{0.7} Ti _{0.3} [9]					
Metal hydrides	Magnesium-based hydrides	NiS@C-MgH ₂ [10]	6.02 at 250 °C	1) Rapid hydrogen absorption in a short time. 2) Stable hydrogen absorption and release performance after many cycles.	\
		MgH ₂ @3D-TiVCTx MXene nanocomposite [11]	6.5 at 100 °C	1) Large hydrogen absorption capacity. 2) Hydrogen absorption capacity is basically unchanged after many cycles.	\
	Lithium-based hydrides	LiH-4% F- N [12]	More than 12.6	1) Effectively reduce the decomposition temperature. 2) Increased hydrogen storage capacity.	\
Liquid Organic Hydrogen Carrier	Cycloalkane	MCH/Tol [17]	6.2	1) Good efficiency and selectivity	\
		Dec/Nap [19]	7.3	1) Larger hydrogen capacity. 2) Higher melting temperature makes it efficient in high-temperature environment.	\
	N-heterocycles	12H-NEC/NEC [20]	5.8	1) No need to be diluted. 2) Higher degree of hydrogenation.	\
		8H-2-MID/2-MID [21]	5.76	1) Rapid dehydrogenation .	\
	O-heterocycles [22]		Lower than N-heterocycles		1) O atom cannot store hydrogen in hydrogenation process.

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