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Comparison of metal hydride alloys for solid-state hydrogen storage: Mg-, Ti-, and La-based systems and high-entropy alloys

Hainuo Bao

University of Manchester, Manchester, UK

hainuo.bao@student.manchester.ac.uk

Abstract. Hydrogen is seen as an ideal fuel due to its high reaction enthalpy, environmental friendliness, and renewability. Currently, gaseous hydrogen storage is the most mature technology. Unfortunately, it suffers from low volumetric density. Meanwhile, liquid hydrogen storage needs to overcome the problems of high energy consumption and cost. As a result, solid-state hydrogen storage is well known in academic circles. In this work, different hydrogen storage approaches, including gaseous, liquid, and solid-state methods, are reviewed and compared. Representative hydrogen storage alloys, including Mg-based, Ti-based, and La-based systems, are systematically analyzed. The results indicate that hydrogen storage performance is fundamentally governed by a trade-off between hydrogen binding strength and reversibility. No single material simultaneously satisfies all key requirements. However, solid-state storage materials show significant potential for future development. Further research should focus on compositional optimization and microstructural engineering to achieve a balance between key requirements.

Keywords: solid-state hydrogen storage, high-entropy alloys, metal hydrides, hydrogen absorption/desorption, hydrogen storage alloys

1. Introduction

With the increasing emissions of CO_2, there is an increasingly urgent need to develop new energy sources in order to reduce or partially replace our reliance on fossil fuels. Fossil fuels are non-renewable, and their combustion produces greenhouse gases. At the same time, harmful pollutants, which include Sulfur Oxides (SO_X) or Nitrogen Oxides (NO_X), are usually produced in this process. Worldwide, hydrogen is widely recognized as a key component of future low-carbon energy systems. China has established targets to reach "carbon peak" by 2030 and "carbon neutrality" by 2060 [1]. Furthermore, in 2022, the Chinese government published the "Medium- and Long-Term Development Plan for the Hydrogen Energy Industry (2021–2035)" [2]. These policies have provided a strong impetus for the development of hydrogen energy technology.

Hydrogen is considered an ideal fuel due to its high energy density and environmental benefits. However, the wider application of hydrogen energy still faces challenges. Hydrogen storage methods can be categorized into gaseous, liquid, and solid-state storage. Solid-state hydrogen storage technology is attracting increasing attention due to its greater safety and higher volumetric hydrogen density.

In this paper, different hydrogen storage methods are compared. Representative solid-state hydrogen storage systems, including Mg-, Ti-, and La-based alloys as well as high-entropy alloys, are systematically analyzed.

2. Properties and production of hydrogen

2.1. Properties of hydrogen

Hydrogen, chemical formula H_2, has a molecular weight of 2.01588. Hydrogen is a highly flammable gas, and it is difficult to dissolve in water. The reaction of hydrogen with large electronegativity shows reduction and oxidation with active metals. In industry, hydrogen is generally produced from methane [3].

Hydrogen has a wide flammability range in air (4–75 vol%) and a high autoignition temperature of approximately 858 K [4]. The total hydrogen releases 143 kJ per gram when it is completely burned. As shown in Table 1, it is significantly higher than conventional fuels such as gasoline and ethanol [5].

Table 1. Comparison of several fuels

Fuel	Energy (kJ/g)	Main products	Whether renewable
H_2	143	water	depends
C_2H_5OH	26.77	Water, CO_2	yes
Petrol	44	Water, CO_2	no
CH_4	50	Water, CO_2	no (fossil-based)

Data for hydrogen is from Ref. [5], gasoline and ethanol from Ref. [6], and methane from Ref. [3].

The combustion of hydrogen follows the reaction: $2H_2 + O_2 \longrightarrow 2H_2O$. At the same time, since the product is water, the pollution of the environment is minimal. Moreover, hydrogen can be reproduced by water. However, in industry, hydrogen is usually the by-product of other reactions instead of directly electrolyzing water since the cost is high.

2.2. Production of hydrogen

Hydrogen is often generated as a by-product from many systems. For example, for chlor-alkali enterprises [7], there would be about 0.02 to 0.03 tons produced when producing 1 ton of NaOH, depending on the specific production method [8]. However, a considerable amount of by-product hydrogen remains underutilized, indicating significant potential for hydrogen recovery and application [3].

Plus, hydrogen can be classified into different types based on production methods. They are grey hydrogen (from fossil fuels), blue hydrogen (with carbon capture), and green hydrogen (from water electrolysis) [9], as shown in Table 2. Currently, grey hydrogen dominates global production due to its low cost, while for green hydrogen, it is expected to play a key role in reducing carbon emissions despite its higher cost.

Table 2. Comparison of three types of hydrogen

Type	Production method	CO_2 emission	Cost (approx.)	Current share
Grey hydrogen	Steam Methane Reforming (SMR)	High	Low (~1–2 $/kg)	~95%
Blue hydrogen	SMR + Carbon Capture and Storage (CCS)	Medium	Moderate (~2–3 $/kg)	< 5%
Green hydrogen	Water electrolysis (renewables)	Near-zero	High (~3–6 $/kg)	< 1%

Data adapted from Ref. [9].

3. Different ways to store hydrogen

Since hydrogen is easily burned and in a gaseous state in standard conditions, storing hydrogen plays a very important part in using hydrogen. Until now, there are three main ways to store hydrogen.

3.1. Gaseous hydrogen storage

The advantage of this kind of hydrogen storage mode is its simple operation. Then, the hydrogen filling and discharging speeds are fast, and the hydrogen can be inflated and released by adjusting the valve.

The disadvantages of this hydrogen mode are also obvious. The hydrogen gas is compressed to the gas storage cylinder. It takes a lot of compression work. Secondly, the gravimetric density of high-pressure hydrogen tanks is typically in the range of 1–5 wt%, depending on the tank design and operating pressure [6]. In addition, compressed hydrogen storage systems present safety challenges. The high operating pressure (typically 350–700 bar) increases the risk. Furthermore, hydrogen's wide flammability range and low ignition energy (~0.02 mJ) make it sensible to ignition and explosion [8, 10].

3.2. Liquid hydrogen storage

The second way is to use low temperature to store liquid hydrogen (approx. 20 K). It is suitable for large-scale storage and long-distance transportation because of its high gravimetric density. Yet the liquefaction process is extremely energetically intensive and requires complex insulation systems. It leads to high cost and boil-off losses [3].

Consequently, as compressed hydrogen is more commonly used for storage due to cost and safety considerations, liquid hydrogen is primarily used as rocket fuel rather than in conventional vehicles [5].

3.3. Solid-state hydrogen storage

For solid-state hydrogen storage, hydrogen is stored either through chemical bonding (e.g., metal hydrides) or physical adsorption, rather than as free molecular hydrogen as in gaseous or liquid storage systems. For metal hydrides, hydrogen is released upon heating, which provides the energy required to break the metal–hydrogen bonds. The hydrogen desorption process typically involves diffusion, phase transformation, and surface reactions. It is strongly influenced by thermodynamic and kinetic factors.

Solid hydrogen storage has few requirements about high-pressure or heat-insulation containers and little explosion risk. These advantages make it a very ideal hydrogen storage technology. Since about 70 years ago, different kinds of alloys have been found, and some kinds of alloys have demonstrated excellent properties until now.

3.4. A summary of the 3 ways

As shown in Table 3, gaseous hydrogen storage is the most mature technology, while solid-state hydrogen storage has potential for future applications.

Table 3. Comparison of three storage methods for hydrogen in different phases

Storage method	Gravimetric density (wt%)	Operating conditions	advantages	disadvantages
Compressed hydrogen storage	1-5	High pressure	Mature, fast charging	Low gravimetric density, safety concerns
Liquid hydrogen storage	10-15	Low temperature	High hydrogen density	High energy consumption, boil-off losses
Solid-state hydrogen storage	1-10	Moderate temperature or pressure	Relatively safe, high volumetric density	Slow kinetics, immature

Data adapted from Refs. [3, 5, 6].

4. Different methods of solid-state hydrogen storage

Generally, solid-state hydrogen storage can be classified into four methods: physisorption, chemisorption, spillover mechanisms, and Kubas interaction [11].

For physisorption, H_2 binds to the compound by intermolecular force (van der Waals). The binding energy of this method is about 4-10 $kJ \cdot mol^{-1}$ [12], which is relatively small compared to the other three methods. This value indicates that this process is reversible. However, this process generally requires low temperatures (77 K) [13].

For chemisorption, H_2 binds to compounds (especially for metals) by forming covalent bonds. This mechanism has high gravimetric density. Nevertheless, binding energy is usually greater than 50 $kJ \cdot mol^{-1}$. This value is high, and it indicates that a relatively high temperature is required when releasing hydrogen [5, 11].

The spillover mechanism may be regarded as a supplementary mechanism to physisorption. It can improve the gravimetric density of carbonaceous materials at moderate temperatures. This process involves two steps. Start with the dissociative chemisorption of gaseous H_2 on a secondary catalytic phase (Pd or Pt). Hydrogen atoms are then migrated onto the high-surface-area support [14, 15].

The desorption mechanism does not have a specific binding energy value. This is because the mechanism involves multiple steps, including hydrogen dissociation, migration, and adsorption. The dissociation of H_2 on metal catalysts typically exhibits binding energies in the range of 40–100 $kJ \cdot mol^{-1}$, while the subsequent adsorption of atomic hydrogen on carbon supports is in the range of 10–30 $kJ \cdot mol^{-1}$ [14, 16]. But the reproducibility and reversible kinetics of the spillover effect remain a subject of intense debate in the scientific community [12].

The Kubas interaction refers to the non-dissociative coordination of molecular hydrogen to transition metal centers. The Kubas mechanism involves a synergistic bonding scheme: H_2 acts as a ligand, which uses its sigma bond to form a coordination bond with the metal. While there is pi back-donation from the metal's d electrons to the anti-bonding sigma orbital of H_2. Overall, this method weakens the H-H bond without breaking. The binding energy has a range of 20-30 $kJ \cdot mol^{-1}$. It is more reversible than most chemisorptions [17, 18].

Table 4. Comparison of four methods

Method	Mechanism	Binding energy	Advantages	Disadvantages
Physisorption	Van der Waals	4-10 $kJ \cdot mol^{-1}$	Reversible	Low temperature
Chemisorption	Covalent bonds	> 50 $kJ \cdot mol^{-1}$	High density	slow
Spillover mechanism	Catalyzed dissociation, surface diffusion	(multiple steps)	Improve volume	Still debate
Kubas interaction	Coordination bond	20-30 $kJ \cdot mol^{-1}$	Reversible	High demands on metal centres

Data summarized from Refs. [5, 12-18].

Among these mechanisms, physisorption dominates in porous carbon materials, and chemisorption dominates in metal hydrides, while spillover and Kubas interactions have been proposed to improve hydrogen storage performance. The key characteristics of these hydrogen storage mechanisms, including their mechanism, binding energies, advantages, and disadvantages, are summarized in Table 4.

4.1. Hydrogen storage in activated carbons

Carbonaceous materials, particularly Activated Carbon (AC), have been extensively studied since the mid-to-late 20th century. Experimental studies have shown that hydrogen storage in activated carbon is primarily governed by physisorption. In other words, H_2 has a weak intermolecular force to the carbon atoms on the surface [5].

Hydrogen storage in activated carbon is primarily governed by physisorption. It is therefore strongly dependent on temperature and pressure. At low temperatures (e.g., 77 K), the adsorption capacity of hydrogen increases due to enhanced adsorption within the micropores. The adsorption can reach as high as 5–6 wt% at higher pressures [19]. However, at moderate temperatures, the gravimetric density decreases sharply to approximately 1–2 wt% even at high pressures (20–70 MPa) [20].

Recent advances in the field of porous carbon materials indicate that their performance has been enhanced. For instance, activated carbons with an ultra-high surface area (~3,000 $m^2 \cdot g^{-1}$) have achieved high gravimetric density (7.08 wt%) at 77 K [21]. Furthermore, under conditions close to ambient temperature and at moderate pressure (~45 bar), biomass-derived activated carbon has demonstrated a gravimetric density of approximately 2–3 wt% [22].

These results indicate that, although activated carbon exhibits an acceptable gravimetric density at low temperatures, its performance at room temperature remains inadequate.

4.2. Hydrogen storage in alloys

Hydrogen storage alloys used as a source of hydrogen for fuel cells should possess the following properties:

1. High storage density: Superior gravimetric and volumetric hydrogen capacities.

2. Favorable thermodynamics: capable of releasing hydrogen at moderate temperatures (60–120 °C) and low pressures (0.1–1 MPa), thereby utilizing waste heat from fuel cells or vehicle exhaust gases [23].

3. Excellent kinetics: Rapid hydrogen absorption and desorption rates to meet real-time power demands

4. Optimal reaction enthalpy: A relatively low heat of formation (about -37.62 $kJ \cdot mol^{-1}$). As the heat released during the adsorption process is relatively low, this simplifies thermal management; meanwhile, the low heat absorption during desorption makes it easier to utilize external waste heat [24].

5. Long-term cycling stability and poisoning resistance: The alloy must maintain its reactivity over thousands of cycles and demonstrate high tolerance to impurities such as oxygen and moisture within the closed system.

Three main alloy systems have been widely studied: Mg-based, Ti-based, and La-based alloys.

4.2.1. Mg-based alloys

Most of these have garnered significant attention because of their abundant reserves, low costs, and high gravimetric density. Mg-based materials exhibit a high theoretical gravimetric density of 7.6 wt% [25]. Notwithstanding these advantages, the technology is currently some way from practical application due to slow adsorption/desorption kinetics and high thermodynamic stability [26].

Particularly, Mg_2Ni has attracted considerable attention due to its relatively high gravimetric density. Recent studies have shown that Mg–Ni alloys can achieve a gravimetric density of approximately 3.5–3.8 wt%. At 588 K and 20 MPa, the Mg-Ni (75:25) alloy achieved a gravimetric density of 3.76 wt%, which is higher than Mg-Ni (66.7:33.3) with a gravimetric density of 3.53 wt%. Furthermore, this alloy demonstrated excellent cycle stability over 10 cycles. These findings supported Mg-Ni (75:25) as a potential candidate for an efficient, reversible hydrogen storage alloy [27]. This highlights the importance of adjusting the percentage of components in improving magnesium-based systems.

4.2.2. Ti-based alloys

They predominantly are in the form of AB-type (e.g., TiFe) [28] and AB_2-type (e.g., $TiMn_2$) [29]. These alloys are renowned for their excellent cyclic stability [30]. Furthermore, they offer moderate raw material costs and favorable thermodynamic properties, and their relatively low decomposition temperatures make them suitable for room-temperature applications. However, two major challenges exist: difficulty in activation and susceptibility to gaseous impurities. The former is primarily due to surface oxidation layers, while the latter relates to the oxygen in the air or impurities from hydrogen (e.g., H_2O, CO), which significantly inhibit the alloys' gravimetric density [31].

One study investigated the activation behavior of TiFe hydrogen storage alloys. It focused on the enhancement of their performance through the addition of elements such as Al, Cr, Co, and Cu. The results indicate that Al-containing alloys are capable of immediate hydrogen absorption, while Cr-doped alloys activate rapidly due to the existence of $TiCr_2$ compounds. In contrast, Co- and Cu-doped alloys require a longer activation time [32].

Consequently, $TiMn_2$ possesses abundant rare-earth resources. However, it also presents several issues, including mediocre hydrogen adsorption/desorption kinetics. It also lacks in-depth mechanistic analysis of its hydrogenation/dehydrogenation behavior. Therefore, additional components are added. $Ti_{0.9+x}Zr_{0.1-x}Mn_{1.4}Cr_{0.4}V_{0.2}$ (x = -0.05, 0, 0.05) hydrogen storage alloy powder is prepared. By partially substituting titanium (Ti) with zirconium (Zr), hydrogenation is improved. The synthesized $Ti_{0.85}Zr_{0.15}Mn_{1.4}Cr_{0.4}V_{0.2}$ hydrogen storage sample exhibits acceptable hydrogenation kinetics (with virtually no pre-treatment time) and an outstanding gravimetric density (1.73 wt%) [33].

4.2.3. La-based alloys

Lanthanum-based alloys, specifically the AB_5-type intermetallic compound, $LaNi_5$, are among the most extensively studied materials [34].

$LaNi_5$ is characterized by its excellent reversible capacity and superior kinetics under ambient conditions, typically operating at near-room temperature and moderate pressures (< 2 MPa). It can react with H_2 to give a compound in the formula of $LaNi_5H_6$. Unlike Ti-based alloys, $LaNi_5$ exhibits exceptional activation ease and a relatively high tolerance to surface impurities. However, the large-scale industrial application of $LaNi_5$ is primarily constrained by the high cost of rare-earth elements and a relatively low gravimetric density (approximately 1.4-1.6 wt%). This value is lower than that of Mg-based and some Ti-based systems [16, 30].

Recent research showed that the hydrogen gravimetric density of $LaNi_5$ reached 2.07 wt% under 6 GPa. This indicated the formation of $LaNi_5H_9$. These results represent that, under practical conditions, there are approximately one third of the available interstitial sites, which are not occupied by hydrogen atoms [35].

4.2.4. Summary of three metal-based alloys

In summary, the hydrogen storage performance of Mg_2Ni, TiFe, $TiMn_2$, and $LaNi_5$ alloys reflects a clear trade-off between gravimetric density, thermodynamics, and kinetics, as shown in Table 5.

Table 5. Comparison of four types of alloys

Properties	Mg_2Ni	TiFe	$TiMn_2$	$LaNi_5$
Storage density (wt%)	3.6	1.8	1.5-2.0	1.4
Reaction enthalpy	High	Moderate	Moderate	Moderate
Kinetics	Slow	Moderate	Fast	Fast
Cycling Stability	Moderate	High	High	High
Poisoning resistance	Low	Low	Moderate	Moderate

Data summarized from Refs. [27, 32, 35].

Values may vary depending on different conditions and reactants.

At present, only La-based and some Ti-based alloys can be primarily applied to the thermal management requirements of low-temperature Proton Exchange Membrane Fuel Cells (PEMFCs). Additionally, $LaNi_5$ alloys are generally more expensive than the other Mg-based and Ti-based alloys because of the use of lanthanum. In this case, using more mixed rare earth elements has been researched recently [36]. Instead, Mg-based alloys still face challenges due to their high reaction enthalpy [5, 16].

4.3. High-entropy alloys

High-Entropy Alloys (HEAs) are first introduced by Yeh et al. [37]. Typically, for traditional hydrogen storage alloys, a metal is used as the base with small amounts of other elements added. Differently, HEA consists of several major elements that form a single-phase solid solution with high configurational entropy. It comprises five or more elements in stoichiometric or near-stoichiometric proportions (typically from 5% to 35%) [38]. High entropy arises from the random distribution of multiple principal elements in the crystal lattice. Entropy (S) is defined by $S = k_B \ln \Omega$. Since there are more ways to arrange the metal atoms, it leads to a large configurational entropy. Hydrogen atoms will occupy the interstitial sites in the lattice. HEAs have four core effects [39]:

1. High-Entropy Effect: In thermodynamics, Gibbs free energy is defined by $\Delta G = \Delta H – T\Delta S$. When hydrogen binds to metal, it is a chemical reaction. Thus, it has enthalpy and entropy change. When ΔS increases, ΔG becomes more negative, which makes this reaction more feasible.

2. Severe Lattice Distortion: As the size and radius of the metal atoms are different, they will cause significant distortion. This affects the material's physical properties (hardness, electrical resistivity, and the diffusion path of hydrogen atoms).

3. Sluggish Diffusion: When atoms exchange positions, the complex chemical environment creates significant resistance. As a result, diffusion rates of HEAs are far lower than those of conventional alloys. These properties make HEAs have excellent thermal stability and creep resistance.

4. Cocktail Effect: When different elements are combined, there will be a synergistic effect. By adjusting the percentage of components, some physical properties (e.g., the magnetic properties, corrosion resistance, or hydrogen storage pressure) of customized materials can also be changed.

In many high-entropy alloys (such as the Ti-Zr-V-Nb-Hf series), the hydrogen-to-metal atom ratio can reach 2.0 [40]. This ratio exceeds the conventional limit of $LaNi_5$, but its cycle stability and dehydrogenation kinetics still require improvement. It suppresses the formation of multiple phases, as in the case of Mg_2Ni, which leads to uneven hydrogen absorption kinetics as well.

Although it is still in the early stages of development, HEAs provide a potential pathway to overcome the trade-off between gravimetric density and thermodynamic stability observed in conventional alloys [38].

5. Conclusion

Several hydrogen storage approaches, including gaseous, liquid, and solid-state storage, have been widely investigated. Among them, gaseous hydrogen storage is the most mature but suffers from safety issues and relatively low volumetric hydrogen density, while liquid hydrogen storage is mostly applied in aerospace and large-scale hydrogen transport due to its high gravimetric density [16].

By contrast, solid-state hydrogen storage technology offers the potential for safer and more efficient hydrogen storage. Hence, this technology has attracted considerable attention in recent years. In this work, representative hydrogen storage alloys, including Mg-based, Ti-based, and La-based systems, have been systematically discussed and compared. Significant trade-offs exist between these materials in terms of gravimetric density, thermodynamics, kinetics, cost, cycle life, and resistance to deactivation [27, 41].

Hydrogen storage performance is fundamentally governed by a trade-off between hydrogen binding strength and reversibility. No single hydrogen storage alloy simultaneously satisfies hydrogen gravimetric density, thermodynamics, kinetics, cost, cycle life, and resistance to deactivation. At the same time, given the large number of components, it is impossible to exhaustively test all possibilities experimentally. In this case, it should rely more on Density Functional Theory (DFT, first-principles calculations) [42] and machine learning [43] to identify the optimal composition. Through high-throughput computational screening of the atomic compositions of HEAs, identify the best candidate materials with binding energies in an ideal range. In addition, future research is expected to focus on optimizing alloy compositions, nanostructuring, and developing hybrid systems [41] to achieve a balance between gravimetric density and thermodynamic properties, rather than exploring new alloy systems.

References

[1] State Council of the People's Republic of China. (2021, October 25). *Working guidance for carbon dioxide peaking and carbon neutrality in full and faithful implementation of the new development philosophy*. https://english.www.gov.cn/policies/latestreleases/202110/25/content_WS61760047c6d0df57f98e3c21.html

[2] National Development and Reform Commission & National Energy Administration. (2022, March 29). *Medium- and long-term plan for hydrogen energy industry development (2021–2035)*. https://en.ndrc.gov.cn/news/pressreleases/202203/t20220329_1321487.html

[3] International Energy Agency. (2019, June). *The future of hydrogen: Seizing today's opportunities*. https://www.iea.org/reports/the-future-of-hydrogen

[4] National Institute of Standards and Technology (NIST). (n.d.). *Hydrogen. In NIST chemistry WebBook (NIST Standard Reference Database Number 69).* Retrieved May 15, 2026, from https: //webbook.nist.gov/cgi/cbook.cgi?ID=1333-74-0

[5] Züttel, A. (2003). Materials for hydrogen storage. *Materials Today, 6*(9), 24–33.

[6] U.S. Department of Energy. (2020). *Fuel properties comparison. Alternative Fuels Data Center*. https: //afdc.energy.gov/fuels/properties

[7] Schmittinger, M. (2006). Chlorine. In *Ullmann's encyclopedia of industrial chemistry*. Wiley-VCH. https: //onlinelibrary.wiley.com/doi/10.1002/14356007.a06_399.pub2

[8] Schmittinger, M. (2011). Chlorine. In *Ullmann's encyclopedia of industrial chemistry*. Wiley-VCH. https: //onlinelibrary.wiley.com/doi/10.1002/14356007.a06_399.pub3

[9] International Energy Agency. (2022). *Global hydrogen review 2022*. IEA. https: //www.iea.org/reports/global-hydrogen-review-2022

[10] International Organization for Standardization. (2026). *Hydrogen technologies — Basic considerations for the safety of hydrogen systems* (ISO/TS 15916: 2026). Hydrogen technologies — Basic considerations for the safety of hydrogen systems (ISO/TS 15916: 2026)

[11] Alharthi, L., Hazazi, K., Alanazi, A., & Bokhari, A. (2026). Hydrogen storage in carbon materials: A review of mechanisms, performance, and optimization strategies. *Renewable and Sustainable Energy Reviews, 231*, Article 116751.

[12] Broom, D. P., & Hirscher, M. (2016). Irreproducibility in hydrogen storage material research. *Energy & Environmental Science, 9*(11), 3368–3380.

[13] Dillon, A. C., Jones, K. M., Bekkedahl, T. A., Kiang, C. H., Bethune, D. S., & Heben, M. J. (1997). Storage of hydrogen in single-walled carbon nanotubes. *Nature, 386*(6623), 377–379.

[14] Yang, R. T. (2008). Hydrogen storage by spillover. *Catalysis Reviews, 50*(4), 395–418.

[15] Li, Y., & Yang, R. T. (2010). Hydrogen storage in metal–organic frameworks by bridged hydrogen spillover. *Journal of Physical Chemistry C, 114*(14), 595–600.

[16] Schlapbach, L., & Züttel, A. (2001). Hydrogen-storage materials for mobile applications. *Nature, 414*(6861), 353–358.

[17] Kubas, G. J. (2007). Fundamentals of H_2 binding and reactivity on transition metals underlying hydrogenase function and H_2 production and storage. *Chemical Reviews, 107*(10), 4152–4205.

[18] Li, J., & Yang, R. T. (2006). Hydrogen storage in metal–organic frameworks by Kubas interaction. *Journal of the American Chemical Society, 128*(25), 8136–8137.

[19] Nijkamp, M. G., Raaymakers, J. E. M. J., van Dillen, A. J., & de Jong, K. P. (2001). Hydrogen storage using physisorption—materials demands. *Carbon, 39*(11), 1863–1872.

[20] Hirscher, M., Becher, M., Haluska, M., von Zeppelin, F., Chen, X., Dettlaff-Weglikowska, U., Roth, S., & Stepanek, M. (2003). Hydrogen storage in carbon nanostructures. *Journal of Alloys and Compounds, 356–357*, 433–437.

[21] Furukawa, H., Ko, N., Go, Y. B., Aratani, N., Choi, S. B., Choi, E., Yazaydin, A. Ö., Snurr, R. Q., O'Keeffe, M., Kim, J., & Yaghi, O. M. (2010). Ultrahigh porosity in metal–organic frameworks. *Journal of the American Chemical Society, 132*(33), 11886–11887.

[22] Wang, S., Wang, Z., Li, Y., & Zhang, X. (2024). Hydrogen storage in biomass-derived activated carbon materials. *Fuel, 353*, Article 129363.

[23] Sakintuna, B., Lamari-Darkrim, F., & Hirscher, M. (2007). Metal hydride materials for solid hydrogen storage: A review. *International Journal of Hydrogen Energy, 32*(9), 1121–1140. https: //doi.org/10.1016/j.ijhydene.2006.11.022

[24] Dantzer, P. (1997). *Properties of intermetallic compounds: Hydrogen-metal systems*. CRC Press.

[25] Jain, I. P., Lal, C., & Jain, A. (2010). Hydrogen storage in Mg: A most promising material. *International Journal of Hydrogen Energy, 35*(10), 5133–5144.

[26] Xie, X., Chen, M., Hu, M., Wang, B., Yu, R., & Liu, T. (2019). Recent advances in magnesium-based hydrogen storage materials with multiple catalysts. *International Journal of Hydrogen Energy, 44*(21), 10694–10712. https: //doi.org/10.1016/j.ijhydene.2019.02.237

[27] Lai, D. V., Nguyen, S. H., Nguyen, A. H., Nguyen, T. V., Dinh, L. C., Doan, P. D., Pham, T. T., Phung, V. H. T., Tonezzer, M., La, D. D., Nguyen, T. T., & Tran, T. B. (2025). Tailoring hydrogen storage performance of Mg-Mg_2Ni alloys: Synergistic effects of composition and phase formation with first-principles insights. RSC Advances, 15, 31240–31254. https: //doi.org/10.1039/d5ra04356e

[28] Reilly, J. J., & Wiswall, R. H. (1974). Formation and properties of iron titanium hydride. *Inorganic Chemistry, 13*(1), 218–222.

[29] Liu, B.-H., Kim, D.-M., Lee, K.-Y., & Lee, J.-Y. (1996). Hydrogen storage properties of $TiMn_2$-based alloys. *Journal of Alloys and Compounds, 240*(1–2), 214–218. https: //doi.org/10.1016/0925-8388(96)02245-1

[30] Sandrock, G. (1999). A panoramic overview of hydrogen storage alloys from a multinational perspective. *Journal of Alloys and Compounds, 293–295*, 877–888.

[31] Sandrock, G. D., & Goodell, P. D. (1980). Surface poisoning of LaNi5, FeTi and (Fe, Mn)Ti by O2, CO and H2O. *Journal of the Less-Common Metals, 73*(1), 161–168. https: //doi.org/10.1016/0022-5088(80)90355-0

[32] Garelli, F., Dematteis, E. M., Stavila, V., Di Florio, G., Carbone, C., Agostini, A., Palumbo, M., Baricco, M., & Rizzi, P. (2025). Enhancing TiFe alloy activation for hydrogen storage through Al, Cr, Co, and Cu substitutions as a step towards future recycling. International Journal of Hydrogen Energy. https: //doi.org/10.1016/j.ijhydene.2025.150720

[33] Zhang, H., Ma, Z., Wang, Z., Liu, Y., Lin, F., Miao, G., Ju, A., Qu, X., & Li, P. (2025). Tuning of Zr content in $TiMn_2$ based multinary alloys by powder metallurgy to fabricate superior hydrogen storage properties. *Journal of Colloid and Interface Science, 682*, 1040–1050.

[34] van Mal, H. H. (1973). A LaNi5-hydride thermal absorption compressor for a hydrogen refrigerator. *Chemie Ingenieur Technik, 45*(2), 80–83.

[35] Sato, T., Saitoh, H., Utsumi, R., Ito, J., Nakahira, Y., Obana, K., Takagi, S., & Orimo, S. i. (2023). Hydrogen absorption reactions of hydrogen storage alloy LaNi5 under high pressure. *Molecules, 28*(3), Article 1256. https: //doi.org/10.3390/molecules28031256

[36] Kojima, Y., Miyata, Y., & Nakanishi, H. (2024). $MmNi_5$-based hydrogen storage alloy as an electrocatalyst. *International Journal of Hydrogen Energy, 87*, 450–456. https: //doi.org/10.1016/j.ijhydene.2024.09.057

[37] Yeh, J.-W., Chen, S.-K., Lin, S.-J., Gan, J.-Y., Chin, T.-S., Shun, T.-T., Tsau, C.-H., & Chang, S.-Y. (2004). Nanostructured high-entropy alloys with multiple principal elements: Novel alloy design concepts and outcomes. *Advanced Engineering Materials, 6*(5), 299–303.

[38] Miracle, D. B., & Senkov, O. N. (2017). A critical review of high entropy alloys and related concepts. *Acta Materialia, 122*, 448–511.

[39] Zhang, Y., Zuo, T. T., Tang, Z., Gao, M. C., Dahmen, K. A., Liaw, P. K., & Lu, Z. P. (2014). Microstructures and properties of high-entropy alloys. *Progress in Materials Science, 61*, 1–93.

[40] Sahlberg, M., Karlsson, D., Zlotea, C., & Jansson, U. (2016). Superior hydrogen storage in high entropy alloys. *Scientific Reports, 6*, Article 36770. https: //doi.org/10.1038/srep36770

[41] Hirscher, M., Yartys, V. A., Baricco, M., Bellosta von Colbe, J., Blanchard, D., Bowman, R. C., Jr., Broom, D. P., Buckley, C. E., Chang, F., Chen, P., Cho, Y. W., Crivello, J.-C., Cuevas, F., David, W. I. F., de Jongh, P. E., Denys, R. V., Dornheim, M., Felderhoff, M., Filinchuk, Y., ... Zlotea, C. (2020). Materials for hydrogen-based energy storage: Past, recent progress and future outlook. *Journal of Alloys and Compounds, 827*, Article 154186.

[42] Züttel, A. (2004). Hydrogen storage methods. *Naturwissenschaften, 91*(4), 157–172.

[43] Ward, L., Agrawal, A., Choudhary, A., & Wolverton, C. (2016). A general-purpose machine learning framework for predicting properties of inorganic materials. *npj Computational Materials, 2*, Article 16028. https: //doi.org/10.1038/npjcompumats.2016.28