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Nanocomposite modelling, synthesis and applications in clean energy (hydrogen) storage -A comprehensive review

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Abstract. Hydrogen, as a clean and efficient energy carrier, has gained significant attention for its potential in addressing global energy challenges. Efficient and safe storage is a critical aspect of harnessing hydrogen as an energy source, and various materials and mechanisms have been developed to optimise this process. The review begins by elucidating the fundamental mechanisms governing hydrogen storage in materials, encompassing physical adsorption, chemical bonding, and hybrid storage mechanisms. Subsequently, it delves into an extensive examination of different types of hydrogen storage materials, including metal hydrides, porous materials, chemical hydrides, and liquid hydrogen carriers. Each type is scrutinised for its unique properties, advantages, and limitations in hydrogen storage applications. Additionally, the review focused on newly developed materials and possible utilisation for efficient hydrogen storage for future applications. Finally, the review highlights the prospective challenges of computational modelling of those materials before their real-time applications.

Keywords: adsorption; hydrogen; machine learning; sorption; storage materials;

1. Introduction

Hydrogen, hailed as a clean and efficient energy carrier, is increasingly recognized as a critical player in mitigating global energy challenges. This review meticulously explores the pivotal role of efficient and safe hydrogen storage in unlocking the full potential of hydrogen as a sustainable energy source. The investigation begins by elucidating the fundamental mechanisms governing hydrogen storage in materials, spanning physical adsorption, chemical bonding, and hybrid storage mechanisms. Hydrogen, the lightest and simplest chemical element, is a colourless and odourless gas, well-known for its extreme flammability. It consists of a nucleus containing a positively charged proton and a negatively charged electron (Kothari *et al.* 2004). Its low density means hydrogen can escape Earth’s gravitational pull, potentially dissipating into space. At room temperature, hydrogen tends to remain inert, displaying limited reactivity with other elements. However, when heated to approximately 450°C, it undergoes a highly explosive reaction when combined with oxygen, resulting in the release of an immense amount of energy (Dillon and Heben 2001, Lewandowski 1996) Conventional and Renewable Sources of Energy, Polski Klub, Ekologiczny, n.d.). These unique characteristics position hydrogen as a valuable fuel source with vast potential for diverse applications (refer to Fig. 1). Barthelemy (2012) has dedicated his research to providing a comprehensive historical and technical overview of hydrogen storage. The subject of hydrogen storage has garnered significant attention due to its potential as a clean energy source. Throughout history, the primary method for storing gases, including hydrogen, has involved the use of pressure vessels. These vessels can be categorized into four distinct types based on the materials used in their construction. The initial exploration of hydrogen adsorption was documented in a seminal paper authored by Kidney and Hiza (Timmerhaus 1972). This study focused on the behaviour of adsorbents under cryogenic conditions, wherein the adsorption process was carried out using coconut shell charcoal. Abe *et al.* (2019) contribute to the field with a concise review that delves into the utilization of hydrogen as an energy source. Additionally, the paper offers insights into the current state of solid-state hydrogen storage in metal hydrides. The review highlights recent advancements aimed at enhancing hydrogen storage within metal hydrides. These improvements encompass catalysis, the formation of alloys with other elements, nano structuring, and other innovative techniques. Mandal and Gregory (2009) describe the present state of contemporary solid-state hydrogen. It also emphasized the understanding of storage mechanisms and their evolution and their impacts on future materials design. Hydrogen, hence, is undergoing considerable research in the field of storage due to its wide variety of applications and the advantages it offers.

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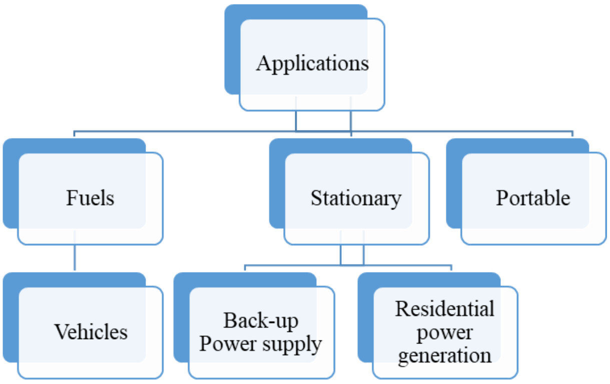

Fig. 1 The diverse applications of Hydrogen

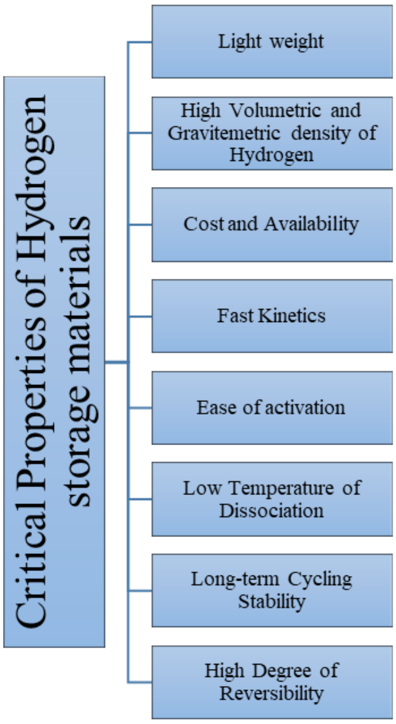

Fig. 2 Critical properties required for a hydrogen storage material

Selecting an effective hydrogen storage material necessitates careful consideration of critical properties to ensure optimal performance and safety. The key properties that are crucial for a hydrogen storage material are presented in Fig. 2.

To establish the current research question about hydrogen storage, relevant novel materials, and their possible applications, the discussion has been extended to different possible orientations. This review mainly puts forward an effort to provide an overall view of materials, mechanisms, and modelling approaches taken globally for design engineers, and corresponding combinations may be adopted when and where they are deemed fit. The present review introduces the hydrogen/hydrogen storage and its futuristic applications and extends further to the sources and synthesis (heading 2). Again, the discussion has been extended to the mechanics and mechanisms, including the modelling steps (headings 3, 4 and 5). The discussion includes the strategy of material selection due to the diversified field of hydrogen applications, i.e., material selection steps, porous material and their influences, nano materials with new polymers (under headings 6, 7 and 8). Further, an established simulation technique for the material modelling, future scope and subsequent closures for the selected research avenues in the directions of hydrogen storage (sections 9, 10 and 11) are discussed in this article.

2. Sources and synthesis of hydrogen (H_2)

Hydrogen, like many other gases, has synthetic and natural modes of synthesis and preparations. The synthesis processes of hydrogen can be cumbersome, especially when water is used as a source.

2.1 Fossil Fuels

Hydrogen is primarily employed in ammonia production and refining processes. Remarkably, over 90% of hydrogen production relies on fossil fuels like coal, gasoline, methanol, and natural gas (Hassmann and Kühne, 1993). Notably, hydrogen is inherent in the chemical composition of these fossil fuels. The challenge lies in the safe and efficient extraction of hydrogen while ensuring the elimination of all other elements present in the original compounds (Hassmann and Kühne, 1993, Kothari *et al.* 2004).

2.2 Water

Hydrogen is abundantly present in water, a readily available and inexpensive resource found in our oceans, lakes, and rivers. Therefore, developing methods to produce hydrogen from water is a crucial and challenging endeavour with the potential to address future energy demands. Splitting water molecules necessitates a source of energy, typically achieved through direct current, solar energy (photolysis), or heat/electricity at high temperatures (Willner and Steinberger-Willner 1988). Various approaches to hydrogen production from water will be explored in the following sections. Although the availability of hydrogen is abundant in various sectors, the separation of hydrogen and its storage involve intricate methodologies.

2.3 Fermentative hydrogen production from organic compounds

Fermentative hydrogen production, although less explored than hydrogen production by photosynthetic microorganisms, offers distinct advantages for industrial applications. This method boasts a notably high rate of hydrogen evolution. Roychowdhury et al. (Roychowdhury *et al.* 1988) found that certain bacteria, when exposed to sugars at temperatures of 37°C and 55°C, produced high concentrations of hydrogen (up to 87%) without generating methane, showing the potential for efficient hydrogen production from various sources. Furthermore, recent

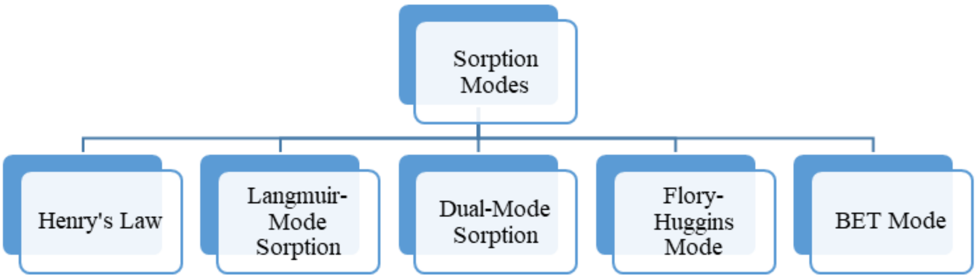

Fig. 3 Various Sorption Modes may take place during hydrogen

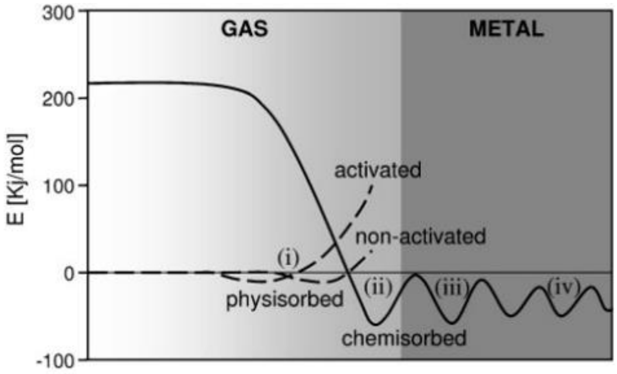

Fig. 4 Potential energy curve for the Lennard-Jones potential for hydrogen binding to a metal

research on fermentation by a strain of E. aerogenes suggests that, under specific conditions, this organism can produce one mole of hydrogen for every mole of glucose consumed. Importantly, these microorganisms can continuously produce hydrogen day and night using organic substrates, thanks to their suitable growth rate for sustaining the production process. In light of these findings, fermentative hydrogen production stands as a more advantageous method compared to photochemical evolution for large-scale hydrogen production by microorganisms. Effective optimization of fermentative hydrogen production can be achieved by ensuring access to abundant electron sources, establishing a robust biochemical electron pump, and maintaining an active hydrogenase enzyme. This synergy of factors maximises the potential of fermentative hydrogen production (Brosseau and Zajic 1982, Kumar and Das 2000, Narendra Kumar and Das 2000, Talapko *et al*. 2023, Tanisho *et al*. 1987). The reviews indicate that effort has been made in the past, and it's an ongoing development process to establish a safe, suitable and sustainable method. Also, the processes should maintain the necessary ecological balance and have a low societal impact.

3. Mechanics

Klopffer and Flaconnèche (Klopffer and Flaconnèche 2001, Wang and Guo 2020) have focused their work on the transportation of gases in polymers and the effect of various parameters on the transportation properties of gases. Various physical laws related to transportation properties have been discussed and various sorption modes related to gas sorption have been discussed. Various sorption modes are represented in Fig. 3.

3.1 Hydrating mechanism

The mechanism can be explained using long-range attractive/short-range repulsive Lennard-Jones potential (shown in Fig. 4). During the approach of molecular hydrogen, it is encountered by successive minima in the adsorption potential curve. This molecular hydrogen is first physiosorbed on the surface of the metal. This process is governed by Langmuir isotherms (Sarkar and Bhattacharyya 2012). The reviews on mechanics and mechanisms are well understood, but they cannot be scaled up from the storage point of view for one or more reasons.

4. Mathematical Models

Every physical situation can be represented using some kind of mathematical model. Similarly, the hydrogen adsorption capabilities and mechanisms can be modelled using various mathematical models. These models can be differentiated primarily based on the principles and mechanism of the adsorption process.

4.1 Henry's Model

The Henry model, derived from the Gibbs adsorption and Peng-Robinson equations, describes gas adsorption on a solid surface under specific conditions. It's applicable at low gas pressures (below 1 MPa) and assumes minimal surface coverage (only 10%). The model simplifies adsorption by treating adsorbed molecules as an ideal gas.

The equation, $V = KP$

The equation relates the unit mass solid adsorption capacity (V) to equilibrium pressure (P) through the Henry constant (K). This linear isothermal model asserts that gas adsorption on the solid surface increases linearly with pressure. It's valuable for analysing gas-solid interactions when pressure is low, and interactions among adsorbed molecules are negligible (Oliveira *et al*. 2024, Wang *et al*. 2016b).

4.2 Freundlich's model

The Freundlich model (F model) is an extension of the

Henry model, offering a more rigorous statistical thermodynamic foundation. Underlying assumptions include non-uniform adsorption energies across the solid surface and monolayer adsorption, meaning each adsorption site can host just one adsorbed molecule. This model is best suited for medium-pressure conditions and low gas concentrations, particularly when dealing with single-molecule-layer adsorption.

The equation, $V = KP^n$ links the unit mass solid adsorption capacity (V) to equilibrium pressure (P) through the Freundlich constant (F) and an exponent (n). The value of 'n' indicates the adsorption strength, as it approaches 1, the model simplifies to the Henry model, while higher 'n' values represent continuous adsorption, and lower values suggest intermittent adsorption. At a specific temperature, the Freundlich equation illustrates how gas adsorption capacity relates to pressure, indicating that as pressure surpasses a certain threshold, the rate of gas adsorption capacity increase slows (Wang *et al*. 2016a).

4.3 Langmuir's Model

Between 1916 and 1918, Langmuir formulated the Langmuir adsorption model (L model), derived from kinetic principles. This model posits several key assumptions: it involves single-molecule layer adsorption (akin to the Freundlich model), assumes a homogeneous solid surface with constant adsorption capacity and heat, postulates no molecular interactions influencing adsorption or desorption, maintains a dynamic adsorption equilibrium, and treats the fluid as an ideal gas with equal adsorption capacities for each component.

The Langmuir equation, $V = \frac{V_l bp}{bP+1}$

The equation relates the unit mass solid adsorption capacity (V) to equilibrium pressure (P), with VL representing the maximum adsorption capacity and 'b' reflecting the temperature-dependent adsorption/desorption ratio. This model finds application in describing the physical and chemical adsorption of single-layer molecules on solid surfaces (Clarke *et al*. 1916, Wang *et al*. 2016a).

4.4 Dubini-Radushkevich Model

The Dubini-Radushkevich (DR) model, rooted in the Polanyi adsorption potential theory, differs from surface coverage-based adsorption models. It's suitable for microporous materials, focusing on filling the tiny pore volumes rather than forming molecular layers on the surface. Here, molecules adhere within micropores due to cohesive forces. The narrow pore diameter enhances the attraction between molecules, leading to volumetric filling rather than wall coverage. However, a limitation of the D-R model is its inability to revert to Henry's law when pressure approaches zero. Thus, it's only applicable when the filling rate exceeds 15% (Dubinin 1947, Wang *et al*. 2016a).

The D-R equation, $V = e^{-a[\ln(\frac{c}{p})]^2}$

The equation describes unit mass solid adsorption capacity (V), equilibrium pressure (P), and constants (a and c) unique to the D-R model.

4.5 Radke-Prausnitz Model

The Radke-Prausnitz (R-P) model is founded on the ideal adsorption solution theory, which treats adsorbed molecules as if they were in an ideal solution. This model is versatile and applicable across a broad concentration range in adsorption processes (Wang *et al*. 2016b).

The R-P equation, $V = \frac{bP}{(bP)^n+1}$,

The equation describes the adsorption capacity per gram of adsorbent (V), with constants 'b' and 'n' characterizing the R-P model (where 'n' falls between 0 and 1).

At high pressure, the equation simplifies to $= \left(\frac{A}{B}\right) P^{1-n}$, while at low pressure, it aligns with the Henry adsorption model: $V = AP$.

This model can also be extended to handle multi-component adsorption scenarios similar to the Langmuir isothermal adsorption equation.

4.6 Toth Model

The Freundlich and D-R equations deviate from Henry's law at low pressures and lack a defined threshold value with increasing pressure. To address these limitations, the semi-empirical Toth model (T model) was introduced. In this model, 'n' is a parameter linked to the heterogeneity of the adsorbent. The Toth model, rooted in adsorption potential theory, is particularly useful for heterogeneous adsorption (Terzyk *et al*. 2003, Wang *et al*. 2016a).

$V = \frac{V_l bP}{(1+bP^n)^{1/n}}$,

The equation describes the unit mass solid adsorption capacity (V) concerning equilibrium pressure (P), with 'b' and 'n' as constants unique to the Toth model. This model provides a more accurate representation of adsorption behaviour, especially in cases of heterogeneous adsorption.

4.7 Langmuir-Freundlich Model

In 1984, Sips introduced the L-F adsorption model, which considers the complex interactions among adsorbed molecules. While it can be simplified as a single-layer model, it doesn't adhere to Henry's law. At lower concentrations, it approximates the Freundlich adsorption model. When '*n*' equals 1, the L-F adsorption model simplifies to a single-component Langmuir adsorption model, suitable for homogeneous surfaces (Quiñones and Guiochon 1998, Sips 1948).

The equation is given as $V = \frac{V_l bP^n}{1+(bP)^n}$, where 'V' represents the unit mass solid adsorption capacity, '*P*' is the equilibrium pressure, and 'VL' and '*b*' are constants specific to the L-F model. The '*n*' parameter, influenced by temperature and pore size distribution, helps correct adsorption characteristics and molecule interactions. When '*n*' equals 1, it essentially becomes the Langmuir model (Wang *et al*. 2016a).

Various mathematical models have been adopted before finalising any specific process and/or techniques that have evolved following the material-relevant research's complexities and desired outcomes. Also, the material model gives an

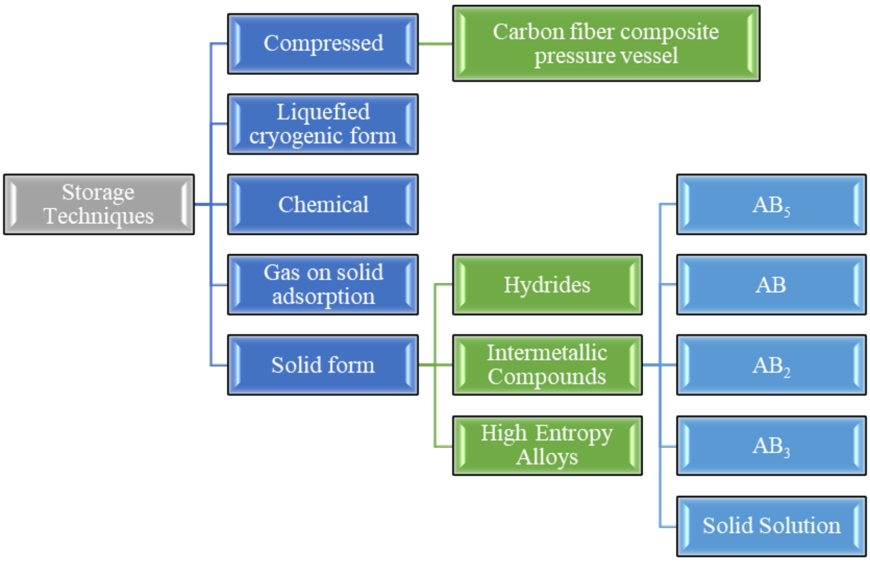

Fig. 5 List of storage techniques

intrinsic understanding of any product/ process before its final design and implementation.

5. Methods and materials

Hydrogen storage techniques play a crucial role in harnessing hydrogen as a clean and efficient energy carrier, with diverse methods addressing the unique challenges associated with storage and release. Physical storage methods include compressed hydrogen storage (CHS), where hydrogen is pressurized and stored in vessels, and liquid hydrogen storage (LHS), involving cryogenic cooling to transform hydrogen into a dense liquid. Chemical storage methods encompass metal hydride storage, where metals react with hydrogen to form hydrides, and Ammonia Borane (AB), a solid-state compound releasing hydrogen through reversible chemical reactions. Adsorption-based storage utilizes porous materials like activated carbon or metal-organic frameworks to adsorb hydrogen onto surfaces, either through physisorption or chemisorption. Liquid organic hydrogen carriers (LOHC) involve chemically binding hydrogen to organic compounds, offering safe and reversible storage. Hybrid systems, such as advanced compressed hydrogen and complex hydride-based Systems, combine different storage materials to enhance overall efficiency. Each technique presents a trade-off between factors like storage capacity, kinetics, safety, and cost, driving ongoing research for improved solutions to propel the adoption of hydrogen as a sustainable energy source. The more detailed storage techniques are found in Fig. 5.

Several hydrogen storage techniques have been developed to address the unique challenges associated with storing and releasing hydrogen for various applications. The structural and hydrogen storage properties of Mg binary alloys were studied by synthesising materials like Mg60-Ni40 and Mg80-Ni20 using the melt spinning method (Sünbül *et al*. 2020). The corrosion mechanism of L245NS steel and L360QS steel gas injection/withdrawal pipeline has been investigated under gas storage in acid gas environments (Zhao *et al*. 2024).

5.1 Compressed form

In this form, the gaseous form of hydrogen is stored in cylinders at pressurised conditions. Compressed hydrogen can also be stored in the form of geological storage setups and underground technologies (Elberry *et al*. 2021). These underground technologies include underground pipes, underground lined rock caverns, salt caverns, etc., (Papadias and Ahluwalia 2021). To increase the storage capacity, an innovative design based on glass capillary arrays with a honeycomb-like structure (Preuster *et al*. 2017). Ni (2006) has focused on how to store hydrogen effectively using high-pressure gas compression, liquefaction, metal hydride storage, and CNT adsorption technologies. It has also been seen that high-pressure gas compression has been mostly used due to its high energy efficiency, and liquefaction has been used mainly for space applications due to high volumetric and gravimetric efficiency. Hence, the compressed form of hydrogen storage has been a go-to form of hydrogen storage in the past and still remains one of the most used ways of hydrogen storage and the major storage apparatus being high-pressure gas cylinders.

5.2 Liquefied Cryogenic form

In this method, hydrogen is stored in pressure vessels that can operate at cryogenic temperatures (as low as 20K) and high pressures (around 350 atm). These systems require thick insulations for proper thermal performance, which may impact the volumetric hydrogen storage capacity (Aceves *et al*. 2010). This form of hydrogen is emerging as an alternative fuel for many applications like aerospace and automotive applications (Mital *et al*. 2006). Some of the materials for the cryogenic tanks that have been looked into include stainless steel, aluminium alloys, titanium alloy, and cryogenic composites like CYCOM 5320-1/IM7 composite material (Qiu *et al*. 2021). This form of hydrogen storage is employed majorly in the ever-growing cryogenic propulsion technology and thus is slowly gaining popularity in many fields especially the aerospace field.

5.3 Chemical storage techniques

This technique includes hydrogen storage by forming chemical bonds in compounds like complex hydrides, amine-borane adducts, ammonia, hydrazine, metal hydrides, and organic compounds (Demirci and Miele, 2011). Boron and nitrogen-based hydrides are also expected to be potential carriers for PEM fuel cells. These hydrides include borohydrides, ammonia borane, and nitrogen-based systems like metal N-H systems, ammonia, Hydrazine, etc. Due to their high hydrogen contents, these systems exhibit high potential as hydrogen carriers for PEM cells (Sun *et al*. 2020, Umegaki *et al*. 2009). Andersson and Gronkvist (2019) have reviewed the large-scale hydrogen techniques and compared them. Hydrogen storage techniques like liquid hydrogen, methanol, ammonia, and dibenzyl toluene have been considered advantageous due to their high storage density, cost of storage, and safety. These advantages of chemical storage techniques can become crucial for applications requiring the storage of hydrogen on a small scale.

5.4 Gas on solid adsorption

The major materials that have been in use for this technique involve fullerenes, CNTs, which can be either SWCNT or MWCNT, activated carbons, metal and alloys for hydrogen storage. This storage technique follows the mechanism of physisorption, where the gas molecules get adsorbed on the surface of the adsorbent. (David 2005, Züttel 2003). Klangt *et al*. (1997) focused on the storage of hydrogen in single-walled carbon nanotubes. The paper mainly focuses on thermal programmed desorption tests on SWNTs to observe and analyze the quantity of hydrogen adsorbed in the SWNTs. Niemann *et al*. (2008) focused on the application of nanostructured materials like doped nano catalyst in complex borohydrides, carbonaceous nano-materials like CNTs, fullerenes, and nanofibers, and nanocomposite conducting polymers. These materials have shown a lot of potential due to advantages like intrinsically high-surface-area and unique adsorbing properties of nanophase materials that can assist the dissociation of gaseous hydrogen. Feng *et al*. (2025, 2023) studied the surface modification strategies inspired by previous works and employed them to simultaneously enhance the damping and mechanical properties of CFRPs and nature inspired sandwich composite through tailored interfacial interactions. The lightweight nature of these materials makes them an excellent choice for both aerospace and automotive applications, where weight is a crucial factor in design. It is imperative to ensure that appropriate insulation arrangements are implemented to prevent the adverse effects of direct exposure of nanomaterial arrangements to sudden temperature changes.

5.5 Solid form of hydrogen storage

In this technique, the hydrogen gas is stored in solid substances like hydrides, intermetallic and high entropy alloys (Schneemann *et al*. 2018). Schneemann *et al*. (2018) review nanostructured metal hydrides for hydrogen storage and its current progress. The preparation of nanostructured metal hydrides and structure analysis methods have been deeply looked into. The main reason why nanostructured metal hydrides have been analyzed so deeply is due to their advantages compared to the bulk, like improved reversibility and altered heats of hydrogen adsorption/desorption. Guther and Otto (Güther and Otto 1999) have deeply reviewed the use of metal hydrides for hydrogen storage applications. It has mentioned some of the advantages of metal hydride tanks over pressure tanks, like no requirement for additional power supply, no loss of hydrogen, the tendency to supply hydrogen at optimum and constant pressure and improved safety. It has looked into the optimized use of a combination of a metal hydride tank with a low-power PEM fuel cell due to their high energy densities. In this form of solid-state storage of hydrogen, the storage of hydrogen takes place through physisorption on metal hydrides. Some of the types of hydrides on which this technique has been applied include Magnesium-based metal hydrides and complex hydrides like sodium alanates, Lithium and potassium alanates, Lithium nitrides, Lithium boron and beryllium hydrides (Sakintuna *et al*. 2007, Sclüth *et al*. 2004).

5.6 Metals and Intermetallic compounds:

Metal hydrides are one of the most common compounds, according to Rusman and Dahari (2016), the most convenient and feasible technique to store hydrogen is to store it in solid-state compounds, and metal hydrides have been primarily used in this regard. Sahlberg *et al*. (2016) have focused on hydrogen storage in high-entropy metal hydride alloys. Due to the need for rare-earth metals, the paper focused on high entropy alloys for storage, which is a recent method being used. These high entropy alloys were synthesized using arc-melting methods of various elements like Ti, V, Zr, Nb and Hf. This set of compounds has a wide range of applications over a wide range of temperatures. It has been found that intermetallic compounds have been more efficient and reliable in storing hydrogen than in gaseous and liquid forms (Dantzer 2002, Rusman and Dahari 2016). It has been found that A_x and B_y type of intermetallic would show more encouraging and enhanced hydrogen storage capabilities when partially substituted (Lys *et al*. 2020). Mechanical alloying and ball milling are some of the few methods useful in the synthesis of intermetallic compounds for solid-state hydrogen storage (Liu *et al*. 2021). Ionic polymer metal composite (IPMC) actuators are used with electrolyte polymer membrane for hydrogen storage. The results indicates, deformation depends upon the applied voltage, palladium-electrode thickness, and actuator length (Omiya and Kurokawa 2023). The sandwich structure composed of concave hexagonal Negative Poisson’s ratio (NPR) is utilized in protecting the

Table 1 Types and configurations of different kinds of intermetallic compounds (Dantzer, 2002)

Intermetallic Compound	Reference Alloy	Structure
AB_5	$LaNi_5$	Haucke phase, Hexagonal
AB_2	$TiMn_2$	Laves phase, hexagonal or cubic
AB	TiFe	Cubic, CsCl-type or orthorhombic, CrB-type
AB_3	$CeNi_3$	Hexagonal, $NbBe_3$-type
Solid Solution	V, Ti-V	Body-centred cubic

Table 2 The hydrogen storage density and the energy density exhibited by different materials

Material	Hydrogen Density		Energy Density	
	wt%	g/dm^3	MJ/kg	MJ/dm^3
Gas H_2, 100 bar, 293 K	100	7	14.0	1
Liquid H_2 (20 K)	100	70	141.0	10
$LaNi_5H_{6.7}$	1.37	89	2.0	12.7
$FeTiH_{1.95}$	1.75	96	2.5	13.5
MgH_2	7	101	9.9	14.0

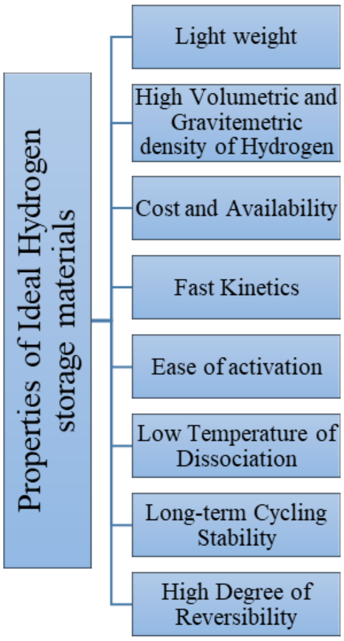

Fig. 6 Necessary properties for an ideal Hydrogen storing materials

hydrogen storage tank (Zhou *et al.* 2024). The various kinds of intermetallic compounds have been represented in a tabular form in Table 1. A clear comparison has been drawn between the hydrogen storage capacities of various materials in Table 2. It can be observed that the energy density per kg of material is highest for liquid H_2, which means the least amount of liquid can give the highest amount of energy and the highest energy density per unit volume was seen for the metal hydrides. Hence, metal hydrides play a pivotal role in maximum hydrogen storage applications where space is a major constraint.

Abdin *et al.* (2020) have reviewed hydrogen as an energy vector. The literature has analyzed a few of the hydrogen storage techniques and options like Gaseous hydrogen, Liquid hydrogen, Solid hydrogen, Fuel Cells, and some alternate hydrogen carriers like synthetic methane, methanol, ammonia etc. Zhou *et al.* (2004) have focused on the storage of hydrogen in activated carbon at liquid nitrogen temperature, which gets considerably enhanced in terms of compression and adsorption on activated carbon. A comparison between adsorption characteristics at 77K and 298K were looked into, and it was found that a higher capacity of adsorption took place at 77K as per the isotherm plots obtained. A clear comparison is drawn between storage properties in different storage methods in Table 2.

The reviews on materials, method and their final selections indicate that the processes depend on many factors, and are correlated with types of material, service conditions and their exposures.

6. Material selection technique

For any engineering and scientific purpose, it is extremely important to focus primarily on material selection and its technique so that the best possible output can be obtained for that purpose. Coppola *et al.* (2019) focus on the material selection techniques for hydrogen storage for aerospace applications. Some of the desirable traits that have been looked into for this purpose are high storage capacities, low weight and materials cost, high cyclability and full reversibility. Two primary approaches for hydrogen storage have been mentioned, which include a physical-based approach and a material-based approach, where in the first case, hydrogen is stored in its molecular form, and in the second case, it is stored in materials either through physisorption or chemisorption.

It also includes the algorithms and methodology used behind this process. Materials of the class clathrate hydrogen hydrates have been closely looked into in the literature. The critical properties that can be observed into for an ideal hydrogen storage material have been mentioned in Fig. 6. The primary properties that need to be considered into while designing a system to be propelled by hydrogen power for its locomotion or movement would be lightweight, high volumetric and gravimetric density of hydrogen, and optimized cost can lead to low material usage and hence low added weight to the propulsion system. Selective methodologies have already been established for choosing any material, considering the process parameters and its allied application field.

7. Use of Nanoporous materials for hydrogen storage

Hydrogen storage is a critical component of utilizing hydrogen as an energy carrier, particularly for applications like fuel cells and transportation, where efficient storage methods are essential. There are various methods for storing hydrogen, each with its own advantages and challenges. One of the most straightforward ways to store hydrogen is by using simple tanks, similar to how we store natural gas or propane. However, there are limitations to this approach (Zhou *et al.* 2004). To store a significant amount of hydrogen in a tank, it requires either extremely low temperatures or high pressures. These extreme conditions make the storage process energy-intensive and potentially hazardous. An alternative approach to hydrogen storage involves chemically binding hydrogen to a material, such as metal or nonmetal hydrides. While this method has its merits, there are significant challenges related to the reversibility of the hydrogen release process, kinetics, and heat management. The energy difference between stored and released hydrogen can complicate the efficient release of hydrogen when needed. Researchers have been exploring various materials to improve hydrogen storage, including Metal-Organic Frameworks (MOFs), carbon materials, and zeolites (Budd *et al.* 2007, Chui *et al.* 1999, Irmof- and Tmbdc 1990, Kaye and Long 2005, Langmi *et al.* 2005, Mueller *et al.* 2006, Nijkamp *et al.* 2001, Panella *et al.* 2006, DOE 2007, Wong-Foy *et al.* 2006, Zecchina *et al.* 2005). MOFs, in particular, have shown promise due to their high surface area, which directly correlates with their hydrogen adsorption capacity. In experiments, MOFs, such as HKUST-1, have demonstrated superior hydrogen uptake compared to an empty container at low temperatures and high pressures. It has been noted that the surface area of porous materials plays a crucial role in determining their maximum hydrogen adsorption capacity. In the case of carbon materials and MOFs, their high surface area allows for substantial hydrogen storage, with some MOFs achieving up to 7% wt. at 77 K and 70 bars. In contrast, zeolites, while effective, have limitations due to their relatively lower surface area and heavier weight. To meet the Department of Energy’s targets for practical hydrogen storage, researchers are striving to increase adsorption capacity at or near room temperature. At room temperature, hydrogen’s heat of adsorption is comparable to thermal vibrations, making it challenging to achieve high adsorption capacities. One approach is to increase the adsorption energy, and materials with higher interaction energies, like some MOFs, have shown promise. However, increasing interaction energy alone is not sufficient to achieve high room-temperature hydrogen storage capacity. The density of high-energy sites in the materials needs to be increased significantly. Polymers are also being explored for their potential to enhance hydrogen storage, including the incorporation of tungsten-based organometallic complexes within polymer supports. Another innovative approach is the use of “spillover,” where a metallic catalyst dissociates hydrogen molecules into atoms, enabling them to be absorbed into the material. Initial results have been promising, but further research is needed to determine its feasibility for practical hydrogen storage. Flexibility in MOFs is another avenue of research. Some MOFs have dynamic structures with flexible linkers that can open and close, leading to hysteresis in hydrogen adsorption/desorption isotherms. This property could potentially be harnessed to improve storage properties by allowing selective retention of hydrogen at lower pressures (Bordiga *et al.* 2007, Cooper and Poliakoff, 2007, Li *et al.* 2007, Li and Yang, 2006a, b, Miocic *et al.* 2023, Peterson *et al.* 2006, Spencer *et al.* 2006, Tian *et al.* 2019, Valiev, 2011). Further researchers have utilized normal and bio inspired coating to metal foam to improve the adsorption properties (Feng *et al.* 2023, 2025). In conclusion, hydrogen storage is a complex and evolving field of research with various strategies being explored to enhance hydrogen storage capacity, particularly at room temperature. While materials like MOFs and carbon materials show promise, further advancements are needed to meet the requirements for practical and efficient hydrogen storage, especially in mobile applications where low-temperature cooling equipment can add complexity and cost. The development of materials with high-energy sites and innovative approaches like spillover and flexible MOFs may hold the key to unlocking the full potential of hydrogen as a clean energy carrier (Bhatia and Myers, 2006, Dinča *et al.* 2006, Dincă and Long, 2005, Gigras *et al.* 2007, Lee *et al.* 2006, McKeown *et al.* 2006, 2007, Rowsell *et al.* 2005). Past and recent studies indicate that nanomaterials have the potential to be utilised as a successful storage alternative. However, the hydrogen storage is always associated with some kinds of hazards if any change in operating conditions.

8. Use of Metal hydrides and PIM-1 CNT

Metal hydrides and a composite of PIM-1 and CNT are two extremely important materials used for hydrogen storage applications and hence these materials have been closely compared. Mohan *et al.* (2010) focus on different types of materials being used for hydrogen storage and the manufacturing techniques behind these materials. The adsorption properties of various materials have been studied as well. The paper also focuses on comparing the hydrogen storage capacity of different carbon materials and the impact of structures on hydrogen storage in different carbon materials. Free *et al.* (2021) focused on advanced manufacturing practices for hydrogen storage applications. To manage the storage of hydrogen, different advanced manufacturing practices and 3D printing are being studied. This will help in the rapid prototyping of different pressure vessels, varied in geometry and material composition.

Agarwal *et al.* (2019) have evaluated and analyzed the preparation of thin film composite membranes from PIM-1 using layer by layer method. It provides a more chemical point of view to the synthesis of thin film composites that can largely be useful for the storage of gas. Budd *et al.* (2004) focus on the derivation of PIM-1 through chemical processes. The surface area determination using nitrogen adsorption has indicated that PIMs are microporous with surface areas, and thus, this can be used for storage of other gases like hydrogen. Rathinavel *et al.* (2021a) have reviewed the synthesis, properties, functionalization, characterization, and application of CNTs. This paper has attracted the focus as CNTs have been primarily used for hydrogen storage applications. CNTs have some very useful properties that make them good candidates for hydrogen storage, as they are lightweight and strong. They are used in composite to strengthen hydrogen storage materials. Single-

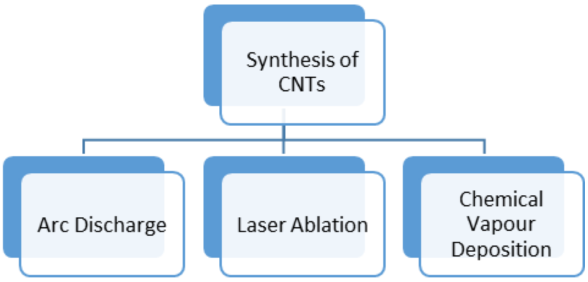

Fig. 7 Some of the methods used for the synthesis of CNTs

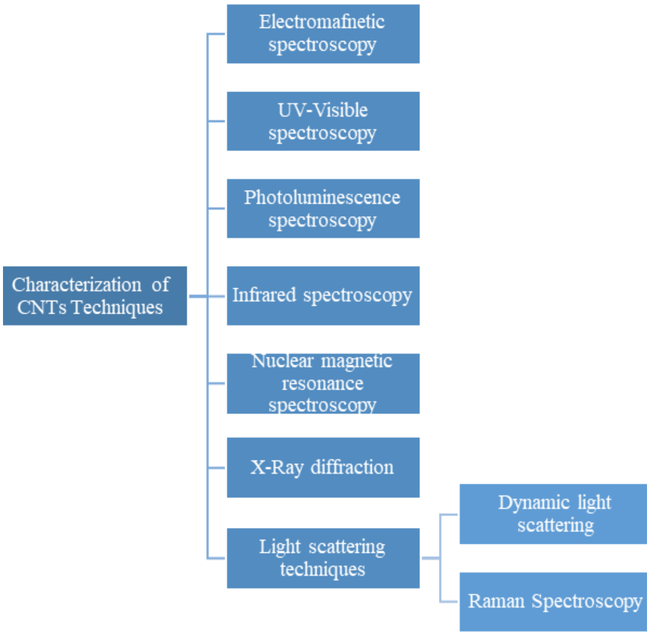

Fig. 7 Some of the methods used for the synthesis of CNTs

walled CNTs have been predominantly attractive for hydrogen storage. Hence, Single-walled CNTs are gaining popularity as hydrogen storage materials for various applications. This can lead to its inclusion in various aerospace applications when hydrogen-based fuels are extensively used. One of the main comparison criteria that has been considered is the manufacturing technique, as this criterion dictates most of the material properties and the economic factors. Researches have also studied the flexural behaviour of steel for the application of storage (Xianzhong 2019). Further research have also been performed on the feasibility study of Ni use in steel for LNG storage (Myungjin Chung 2019).

8.1 Synthesis of CNT

Carbon nanotubes (CNTs) have emerged as extraordinary materials with unique structural and electronic properties, making them highly promising candidates for various applications, including hydrogen storage. The synthesis of CNTs involves diverse methods that cater to specific requirements, enabling the production of nanotubes with varying structures and properties. Among these methods are chemical vapors deposition (CVD), arc discharge, and laser ablation, as shown in Fig. 7. These techniques offer control over the size, alignment, and purity of CNTs, providing a versatile platform for tailored material design.

Understanding and improving the properties of CNTs for hydrogen storage necessitates thorough characterization. Various analytical techniques play a pivotal role in unveiling the structural and morphological intricacies of CNTs. Fig. 8 presented scanning and transmission electron microscopy (SEM and TEM), Raman spectroscopy, X-ray diffraction (XRD), thermogravimetric analysis (TGA), and gas adsorption measurements. Additionally, nuclear magnetic resonance (NMR) spectroscopy provides intuitions into functionalization and hydrogen interaction. This array of characterization techniques forms the foundation for advancing our understanding of CNTs, steering their potential application in efficient hydrogen storage systems.

8.1.1 Arc Discharge

The arc discharge setup, as shown in Fig. 9, the method used to generate plasma through the electrical breakdown of gases, has been employed since 1991 for carbon nanotube (CNT) synthesis. This setup typically consists of two electrodes, one filled with a carbon precursor and catalyst (anode) and the other with a pure graphite rod (cathode). A gas or liquid environment surrounds them. Applying power initiates an arc between the electrodes, requiring a stable gap of 1-2 mm for consistent discharge. The resulting high-temperature plasma (~4000-6000 K) sublimes the anode's carbon precursor and the vaporized carbon aggregates, forming CNTs and soot on the cathode. Understanding this growth mechanism, whether vapour phase, liquid phase, or solid phase, remains a topic of debate, but it plays a critical role in optimizing CNT production (De Heer *et al*. 2005, Ezekowitz 1991, Gamaly and Ebbesen 1995, Ugarte 1994).

8.1.2 Laser Ablation

Laser ablation uses pulsed lasers, as shown in Fig. 10. Pulsed lasers, with their ultra-short bursts of high-energy light, create rapid, non-equilibrium conditions. In processes like pulsed laser vaporization (PLV), a laser rapidly heats materials, vaporizing them into a superheated plasma plume. As this plasma cools and expands, it enables the synthesis of unique nanostructures within nanoseconds, a feat impossible under equilibrium conditions. This technique finds applications in nanomaterial synthesis and advanced materials research (Chrzanowska *et al*. 2015, Hsiou *et al*. 2004).

8.1.3 Chemical Vapor Deposition

Stainless steel micro fibrous composite supports were created via a wet lay-up papermaking process and subsequent sintering. Cellulose and stainless-steel fibers were combined, formed into circular precursors, sintered to remove cellulose, and then calcined to form a three-dimensional network structure. CNTs were synthesized on these supports using chemical vapor deposition (CVD) in a quartz tube with varying parameters like temperature, time, gas flow rates, and acid pretreatment. This process enabled the production of CNTs on the supports with controlled properties (Couteau *et al*. 2003, Yang *et al*. 2019).

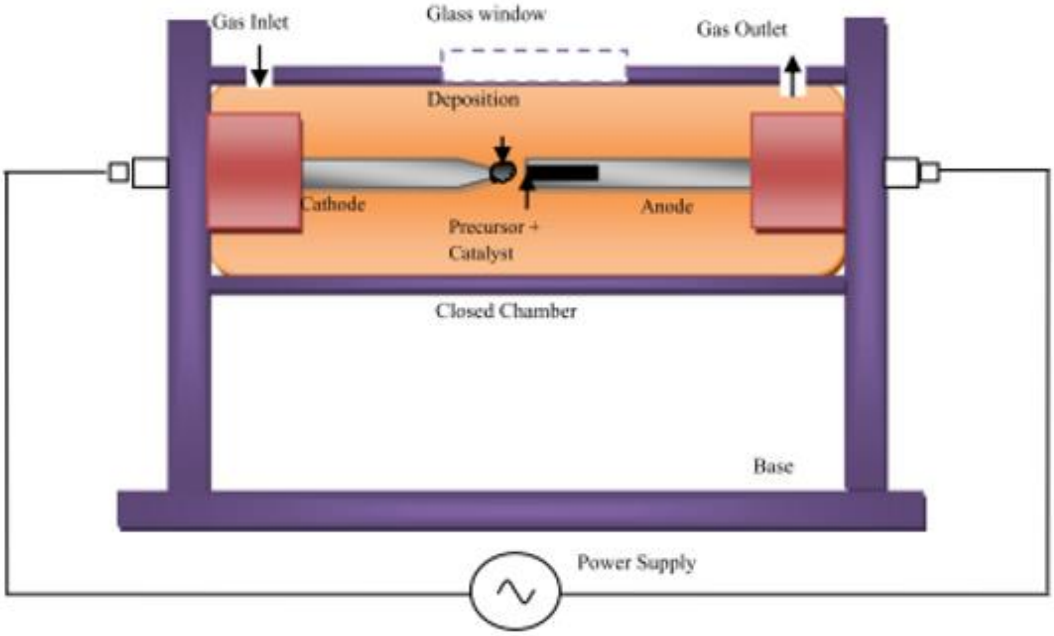

Fig. 9 Schematic diagram of arc discharge setup

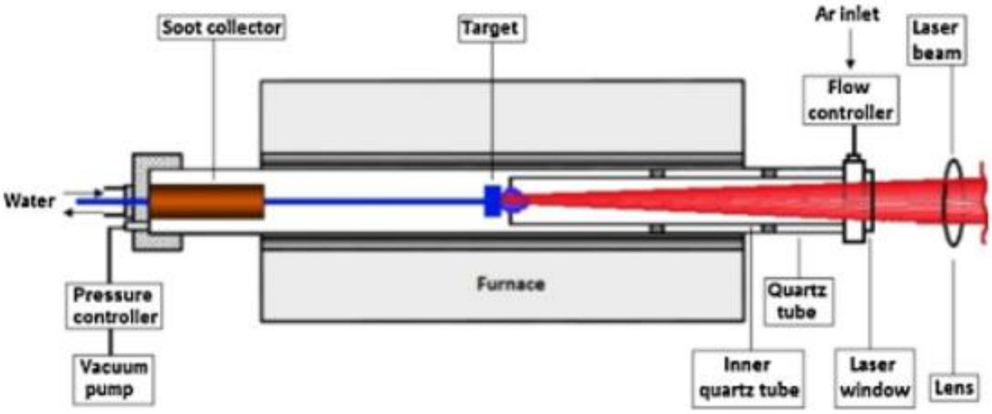

Fig. 10 Schematic diagram of laser ablation setup

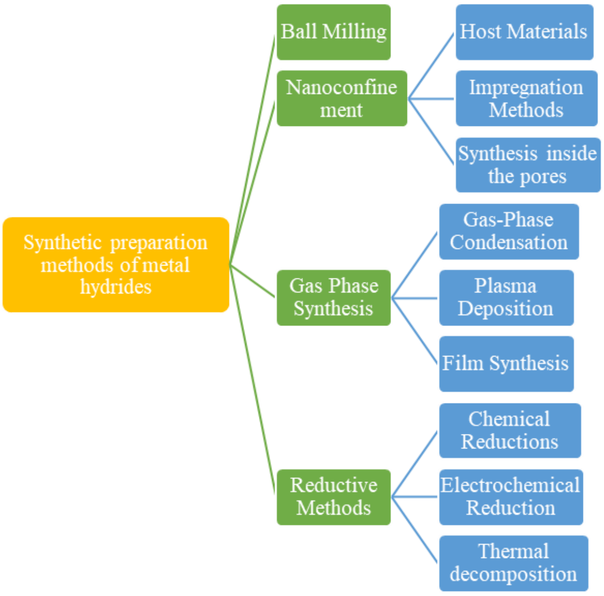

Fig. 11 Synthetic preparation methods of metal hydrides

8.2 Synthesis of metal hydrates and intermetallic compounds

Metal hydrides and intermetallic compounds can be synthesized using various synthetic methods. These methods can be of four major types as has been specified in Fig. 11.

8.2.1 Ball Milling

There are four distinct approaches to synthesizing metal hydrides through ball milling. The most prevalent method involves milling a metal powder, like titanium, in a hydrogen atmosphere to produce the corresponding hydride. Alternatively, a binary hydride can be milled with another metal to create a ternary hydride. Another option is a metathesis reaction, where one metal hydride is transformed into another through anion exchange. Lastly, a relatively rare approach, similar to our method, involves milling methanol with elemental titanium aluminium powder, resulting in titanium hydride formation, although this

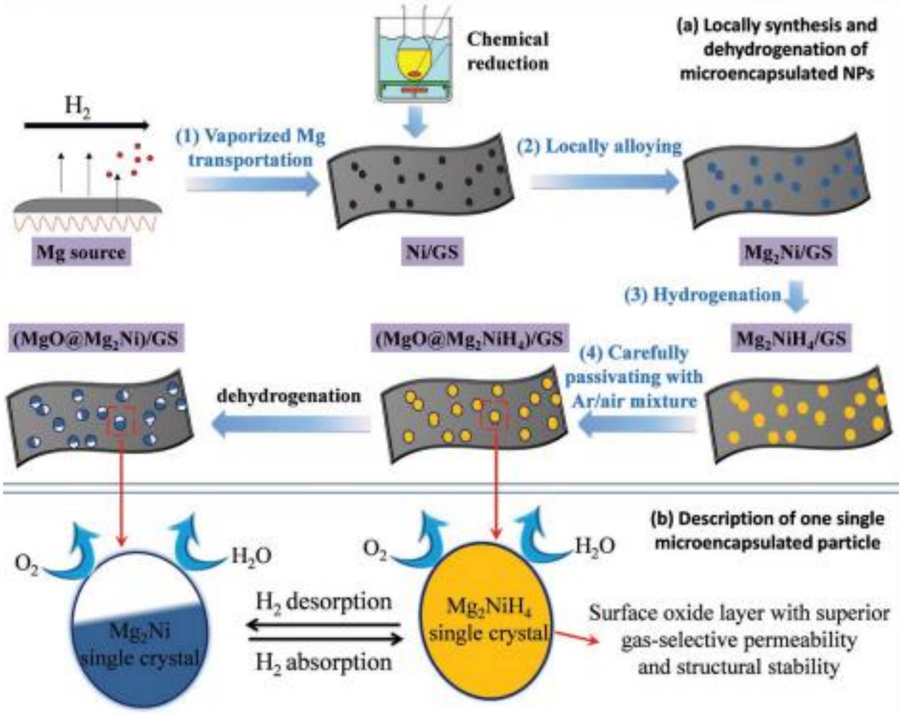

Fig. 12 The schematic of the nanoconfinement process (Zhang *et al*. 2017)

appears to be a somewhat serendipitous discovery, as the authors did not specify the role of methanol's reduction agent (Ney *et al.* 2011). Here, we introduce a novel approach to hydride synthesis through reactive ball milling, utilizing a room-temperature solid acid in conjunction with metal as the reducing agent (Goidin *et al*. 2004, Liang *et al*. 2010, Morales-Hernández *et al*. 2005, Ni, 2006, Rochat *et al*. 2017, Skupov *et al*. 2023, Zhang and Kisi, 1997).

8.2.2 Gas-phase synthesis

This method of synthesis involves the reaction of metal-containing gases with hydrogen to form metal hydrides. This method of synthesis is mostly carried out in controlled conditions of pressure and temperature, and different methods can be employed depending on the required composition. Calizzi *et al*. (2016) have worked on this method of metal hydride and intermetallic compound formation. Calizzi *et al*. (2016) worked on Mg-Ti inter-metallic compound formation. The process involved the compaction of nanoparticles that were grown by inert gas condensation, and the two metals had independent vapour sources. The starting material in this preparation was taken to be Mg ingots and Ti powder, and these materials were heated under a flow of He gas. A compaction process followed the above process, and after compaction, pure oxygen gas was admitted slowly to form a passivating oxide layer.

8.2.3 Nanoconfinements

This method involves the confinement of materials at nanoscale, and this technique of metal hydride synthesis has gained immense attention due to its capability to improve the hydrogen storage capacity of metals. Zhang *et al*. (2017) have focused on this method of synthetic synthesis of metal hydrides. This approach is based on hydriding chemical vapour deposition (HCVD) in which monodispersed Mg_2NiH_4 single-crystal nanoparticles were incorporated into an ultrathin MgO oxide layer. Additionally, graphene sheet-supported microencapsulated Mg_2NiH_4 nanoparticles could also be prepared using this same technique. The synthesis process comprised of gasification of the Mg source, alloying with Ni dopants on the graphene surface, hydrogen adsorption and formation of the MgO layer through passivation. The schematic diagram of the whole process is shown in Fig. 12.

This section is mainly attributed to different types of material utilised for the hydrogen storage via the available conventional and emerging novel materials, considering the necessary conducive storage conditions.

9. Simulation methods and analysis

One of the most important procedures for testing the viability and effectiveness of any material for the purpose of engineering applications is the carrying out of numerical-based simulation and analysis. Wang *et al*. (2016) focus on failure analysis of carbon fiber/epoxy composite vessels useful in hydrogen storage. The vessel in this analysis has been subjected to both high pressure and thermal loading. The damage progression models used in these analyses included micromechanics-based failure criteria, which included fiber failure criteria and matrix failure criteria. Xu *et al*. (2015) focus on hydrogen storage techniques for critical applications like aerospace applications. It focuses on the design of lightweight and super-insulated storage tanks for cryogenic liquid hydrogen, which has the potential to act as a fuel for high-altitude, long-endurance unmanned

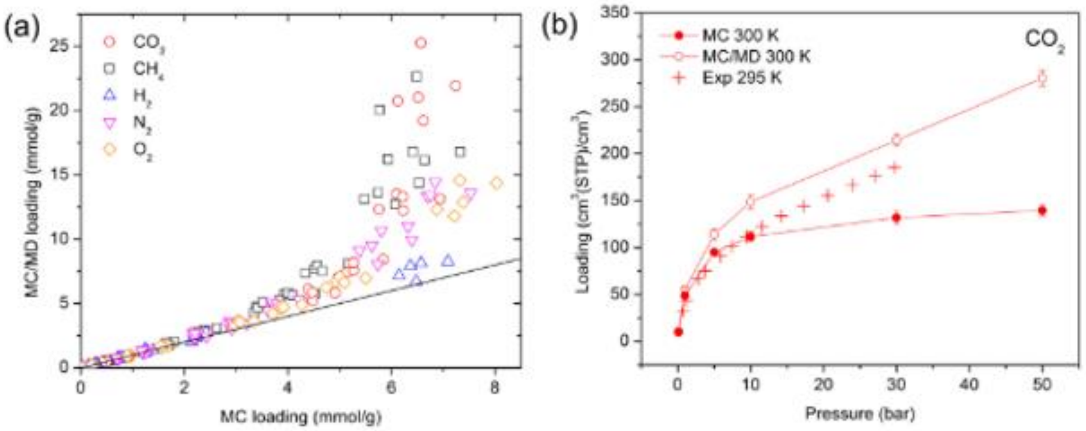

Fig. 13 (a) The MC/MD loading vs MC loading curve for various gases (b) The loading vs pressure for MC, MC/MD and experimental conditions

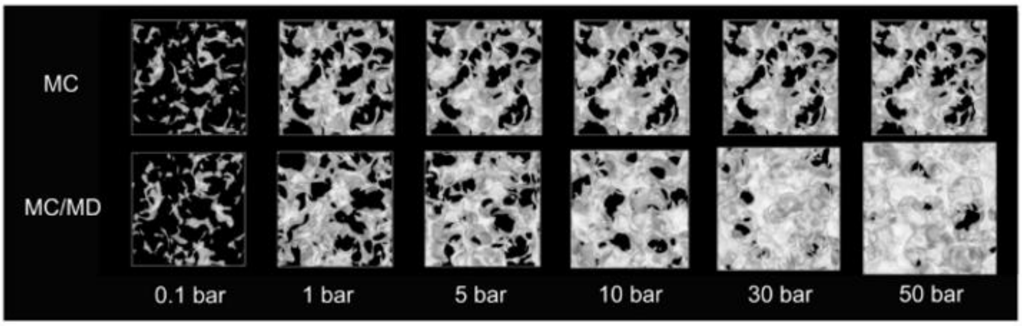

Fig. 14 Adsorption configuration of CO_2 at different pressures for MC and MC/MD

aircraft. The problem of excessive heat leakage was looked into and was resolved by providing a new insulation support structure to the tank. These structures have been analyzed using Hertz contact theory and numerical simulation methods. Hirscher *et al*. (2020) focus on various methods that have been employed for hydrogen storage like the use of porous materials, liquid hydrogen carriers, complex hydrides, intermetallic hydrides, electrochemical storage of energy, thermal energy storage and hydrogen energy systems, etc. The literature has focused on the thermodynamic treatment of storage capabilities of various materials used for hydrogen storage. Techniques like multi-scale theoretical techniques and machine learning techniques for modelling hydrogen storage in metal-organic frameworks have been reviewed. Akkermanns *et al*. (2013) have focused on the Monte Carlo methods of computation used in Materials Studio to carry out Molecular Dynamics simulations. This technique can be used as a configurational sampling method, an important sampling method, and an optimization procedure. These methods have been used by the various modules of Materials Studio to run molecular dynamics simulations. Sunnardianto *et al*. (2021) focus on a combined density function theory and molecular dynamics approach for studying the hydrogen storage process in a hydrogenated graphene structure. The transition in the bonding hybridization leads to a change in tensile strength, and studies have shown that these materials undergo brittle failure. Stan and Cole (Li *et al*. 2015) have studied hydrogen adsorption in nanotubes using a quantum mechanics model. The first quantum correction of the problem has been calculated using the Feynman "effective potential method". A quasi-one-dimensional Lennard-Jones (LJ) classical approximation was used to describe a finite coverage. Hu *et al*. (2009) have focused on techniques to predict failure by using tools like finite element simulations. Shell deformable shell theory was used to theoretically analyze the failure mechanism. The plasticization behavior in PIM-1 can be studied using the Monte Carlo method and molecular dynamics simulations (Kupgan *et al*. 2018). Plasticization is defined as the rearrangement in polymer structure and swelling due to chain relaxation induced by the uptake of adsorbates (Ismail and Lorna, 2002, Wessling *et al*. 1991). Structure generation for this model was done using open-source software, and a sorption-relaxation method was used, which works on a combined Monte Carlo and molecular dynamics approach. Following these, characterization of the ultimate structure was performed using molecular dynamics simulations. In this literature, a clear difference was observed when an MC approach and a combined MC/MD approach were taken. The difference in the loading characteristics with respect to MC loading and pressure (in bar) can be seen in Fig. 13. The comparison of the configuration of CO_2 molecules after CO_2 adsorption found using the MC method and the combined MC/MD approach can be seen in Fig. 14. The radial distribution of CO_2 molecules using both MC and a combination of

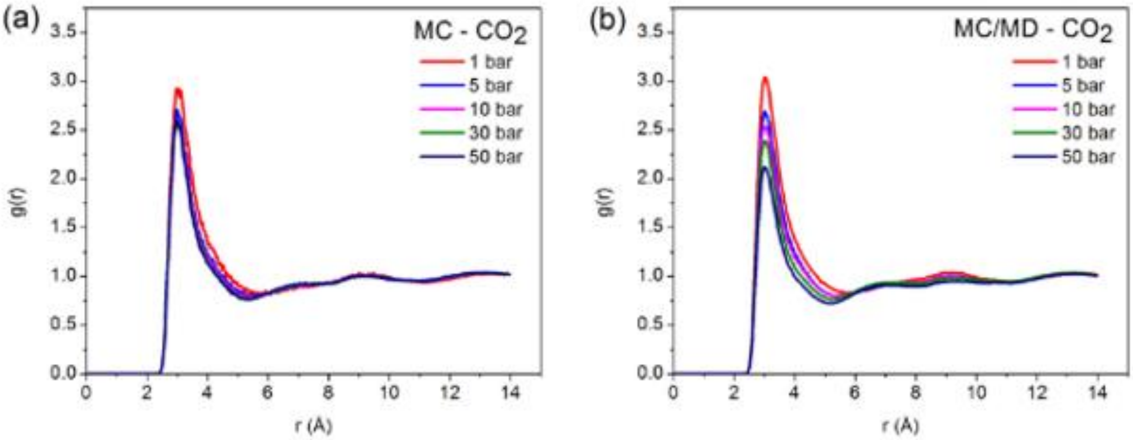

Fig. 15 Radial distribution of CO_2 in (a) MC (b) MC/MD

MC/MD simulations at different pressures have been represented in Fig. 15.

9.1 Damage progression model

Damage detection and prediction is an extremely important step that needs to be taken to understand the consumable limits of a material during its engineering usage. Hassan *et al*. (2021) have reviewed and discussed various storage techniques and methods, and the literature has mainly focused on mechanical properties and aspects of hydrogen storage techniques. The literature has provided suitable insights and recommendations for suitable applications, and the failure mechanisms of some of the methods have been discussed. Onboard storage methods have been investigated for automotive applications. Three feasible methods for hydrogen storage have been considered for automotive applications which include compressed gas, metal hydride adsorption, and cryogenic liquid. Alternative methods have been developed which include pressure vessels with cryogenic capabilities and a combination of metal hydride and liquid hydrogen storage (Berry and Aceves, 1998). Hydrogen storage has important applications in the aerospace field. The methods that have been studied for these applications include gaseous hydrogen storage, where pressure tanks, metal hydrides, CNTs and glass microspheres are used, cryogenic hydrogen storage, where gelled hydrogen and cryo-coolers are used, and chemically bound hydrogen storage.

Adopting any method, material and/or process is inseparable from testing and involves various complexities. However, the numerical and/or simulation techniques are cost-effective and safer than all other available methodologies. Hence, to show the importance of simulation techniques, researchers are now and then provided with the scope of imitating real-time cases, considering unseen associated conditions.

10. Future scope and innovative direction

The majority of the literature has covered the existential aspects of hydrogen storage technology. The future of hydrogen storage technology seems extremely promising due to the ever-growing use of renewable and environmentally friendly energy sources. To accommodate this extensive use of technology, there is a necessity to initiate and develop research to minimize the expense of manufacturing hydrogen storage technology and making it viable for industries and the energy sector. On the scientific front, there is an extreme need to fabricate hydrogen storage materials that can sustain the storage of hydrogen for longer periods of time and can be able to sustain any small amount of external supply of energy. It can also be observed from the current scenario that the aerospace industry will be one of the major potential consumers of hydrogen storage technology. Thus, the development of materials and the addition of extra attachments to safely co-exist with other components of the propulsive system becomes an extremely important and salient point of research. From the analysis point of view of hydrogen storage systems, there is always a scope for the incorporation of machine learning with molecular dynamics simulations to accelerate the extremely computationally expensive simulations.

11. Conclusions

This comprehensive review of hydrogen storage materials, mechanisms, and computational modelling underscores the pivotal role of efficient and safe hydrogen storage in realizing the full potential of hydrogen as a clean and efficient energy carrier.

- The examination of various hydrogen storage materials, such as metal hydrides, porous materials, chemical hydrides, and liquid carriers, reveals a diverse landscape of options with unique properties, advantages, and limitations. This comparative analysis serves as a valuable guide for selecting materials tailored to specific application requirements, fostering informed decision-making in the pursuit of sustainable hydrogen storage solutions.
- The integration of computational modelling techniques with experimental studies emerges as a key theme, offering

a promising avenue for accelerating the finding and design of novel materials. The synergy between these approaches enhances our ability to predict and optimize storage capacities, kinetics, and thermodynamics, thus contributing to the advancement of hydrogen storage technologies.

- Despite significant progress, challenges persist, and ongoing research is essential to address issues such as material stability, reversibility, and cost-effectiveness. The review highlights recent developments in the field and identifies future prospects, emphasizing the need for continued collaboration between experimentalists and computational modelers to overcome these challenges.
- This review consolidates current knowledge on hydrogen storage, providing a valuable resource for researchers, scientists and engineers. By fostering a holistic understanding of storage mechanisms, material characteristics, and the evolving landscape of computational modelling, this work aims to catalyze innovations in hydrogen storage technologies, paving the way for a sustainable energy future.

Overall, this review consolidates the current state of knowledge in hydrogen storage materials and computational modelling, providing a valuable resource for researchers, engineers, and policymakers involved in the sustainable development of hydrogen-based energy systems. Developing novel nanomaterials, including the matrix, may handle complexities inclusively.

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CC

Nomenclature

V	Adsorption Capacity
n	Adsorption Strength
AB	Ammonia Borane
CNT	Carbon Nanotube
CVD	Chemical Vapor Deposition
CHS	Compressed Hydrogen Storage
P	Equilibrium Pressure
F model	Freundlich Model
K	Henry Constant
HCVD	Hydriding Chemical Vapour Deposition
L-F model	Langmuir-Freundlich Model
LHS	Liquid Hydrogen Storage
LOHC	Liquid Organic Hydrogen Carriers
MOFs	Metal-Organic Frameworks
MWCNT	Multi Walled CNT
NMR	Nuclear Magnetic Resonance
SWCNT	Single Walled CNT
TGA	Thermogravimetric Analysis
XRD	X-Ray Diffraction