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Hydrogen storage ability of hexagonal boron nitride

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The development of hydrogen energy is capable of solving a number of important issues that modern society is facing, including global warming and various environmental impacts. Currently, there is an intensive search for natural sources of hydrogen as well as low-carbon techniques for mass production of hydrogen from natural gas, associated petroleum gas, and water. In parallel, efforts to develop technologies for the subsequent management of hydrogen are underway, and the creation of its safe and efficient storage is one of the highest priority goals. For the transportation and storage of hydrogen today, a number of solutions are offered, each of which has both positive and negative aspects. The boron nitride family of materials with high thermal and chemical stability, variability of morphologies, and flexibility of structure has been considered as a candidate for efficient hydrogen storage. This review offers to familiarize readers with the progress in the research and application of hexagonal boron nitride (h-BN), as well as BN-based materials in comparison with other materials, as promising hydrogen storage. Experimental and theoretical data obtained for different morphologies and internal structures were reviewed in relevance to the material`s sorption capacity with respect to hydrogen. Various approaches to improve the efficiency of hydrogen storage were analyzed, and the highest storage capabilities published were mentioned. Thus, BN-based materials are very promising as hydrogen storage, even for an automotive application, but the development of new mass production technologies should be carried out.

KEYWORDS

hydrogen storage, sustainability, boron nitride, structure design, functionalization, theoretical modeling, experimental investigation

1 Introduction

Nowadays, industrial sectors are working hard to find ways to reduce greenhouse gas (GHG) emissions and stop climate change. In 2022, the production, transportation, and processing of oil and gas released 5.1 billion tons (Gt) of CO_2-eq. These emissions, categorized as “scopes 1 and 2,” contributed to almost 15% of the overall energy-related greenhouse gas (GHG) emissions. Furthermore, the utilization of oil and gas resulted in an additional 40% of emissions (IEA, 2023). The IEA’s Net Zero Emissions by 2050 (NZE) Scenario assumes an immediate, concerted effort by all the oil and gas industry to limit emissions from its activities. GHG emissions can be cut down in industries where hydrogen is used as an energy source. When burned, it emits no carbon dioxide or other carbon-based gases, and when produced via electrolysis using renewable energy, it has a comparatively low carbon footprint. The majority of hydrogen is currently produced using fossil fuels, but a rapid transition to renewable hydrogen is ongoing, and it is projected that both the overall amount of hydrogen produced and the share of renewable hydrogen will expand considerably over the next several decades (IEA, 2019).

As it was demonstrated in Figure 1A, there are five basic approaches used to achieve a reduction in emissions intensities: tackling methane emissions, eliminating all non-emergency flaring, electrifying upstream facilities with low-emissions electricity, equipping oil and gas processes with carbon capture utilization and storage (CCUS), and expanding the use of low-emission hydrogen in refineries (IEA, 2023).

Thus, the development of hydrogen energy is one of the most promising solutions to the issue of massive GHG emissions. The difficulties of hydrogen energy distribution can be solved by developing methods for its production, transport, and storage at a reasonably low cost. One of the most important and unsolved problems in the scaling of the application of hydrogen energy is the development of attractive options to store hydrogen. In general, there are two types of hydrogen storage methods: physical methods that involve the compression of hydrogen and possibly converting it into a liquid form, and chemical methods that rely on strong interactions between hydrogen molecules or atoms and the accumulating materials. In particular, for the second-type methods, solid adsorbing materials are common, along with liquid organic hydrogen carriers (LOHC). It was demonstrated that the adsorption energy of H_2 molecules must be between 0.1 and 0.8 eV in order to create a solid material with the high-density capability of storing hydrogen under standard pressure and temperature conditions (Jena, 2011).

Storing efficiency is especially important for facilities used in transport. For automotive applications, hydrogen storage capacity of about 6.5 wt% of the mass of the storage system is set as the ultimate goal by the U.S. Department of Energy (DOE) (U.S. Department of Energy, 2022). Even though $LaNi_5H_6$ is employed as a hydrogen storage material, it is capable of accumulating only 1 wt% of H_2 molecules due to the extremely high atomic weights of La and Ni (Schlapbach and Züttel, 2001). On the other hand, carbon-based materials, which are made of light elements such as boron, carbon, and nitrogen, might be able to store a significantly higher amount of hydrogen than metal hydrides. Several studies focused on the usage of carbon nanotubes, fullerenes, and nanomaterials for hydrogen storage have been shown in the past decade. For example, it has been reported that multi-walled carbon nanotubes can absorb hydrogen in amounts up to 4.6 wt% (Schlapbach and Züttel, 2001).

Carbon-based materials, such as porous graphene (Wang et al., 2019; Huo et al., 2021), carbon-nitrogen composites (Bafekry et al., 2019; Varunaa and Ravindran, 2019), covalent organic frameworks (COF) (Cao et al., 2009; Zhao et al., 2020; Shangguan et al., 2021), and metal-organic frameworks (MOF) (Rosi et al., 2003; Sengupta et al., 2023), according to their sorption capacity for hydrogen, show promising characteristics and were previously studied as potential hydrogen storage materials. However, some physicochemical properties and peculiarities of hydrogenation, dehydrogenation, and cyclization processes significantly limit the prospects of their use. Moreover, many of these materials are not stable in ambient conditions in the presence of moisture (Hamilton et al., 2009).

Recently, h-BN structures have also been considered as promising materials for hydrogen storage applications (Tozzini and Pellegrini, 2013). Hexagonal boron nitride is an isostructural graphene counterpart, and the polarity of B-N bonds and partially ionic bond nature make it efficient for hydrogen storage (Li et al., 2022). Complementary modification of h-BN-based structures can additionally extend the capability of the materials in hydrogen storage applications. An extensive review of the theoretical and experimental studies presenting the possibilities of h-BN in relation to hydrogen sorption is presented in this paper. Our manuscript first focuses on the main results, representing the topical developments and achievements in this field. Then a comprehensive comparison and analysis of the mentioned results are presented, and conclusions are made.

2 Outstanding features of hexagonal boron nitride-based materials

H-BN-based nanomaterials, like their carbon counterparts, exhibit an extended surface area and high porosity. Due to the high chemical inertia and thermodynamic stability of h-BN (up to 1273 K in air), as well as the high specific surface area of nanoparticles and B-N polar covalent bonds, this material is of great interest in the issue of its various applications, including usage as hydrogen storage. Traditionally, h-BN materials are considered efficient hydrogen storage operating via chemisorption mechanisms, but recent theoretical studies increasingly show the promise of BN-based structures for high hydrogen physisorption (Cheng et al., 2007; Salazar-Aparicio et al., 2014; Azimirad et al., 2016). As a highly stable hydrogen storage material, h-BN can provide improved performance, cycling, and regeneration. But one of the main limitations in the industrial application of hexagonal boron nitride is the lack of developed techniques for cheap mass production of nanostructures of this material, as well as simple and effective approaches for their modification to increase sorption capacity. Outstanding properties of this material, along with the capacity of its structure with respect to hydrogen, are described in (Lim et al., 2007; Ebrahimi-nejad and Shokuhfar, 2013; Wang et al., 2013; Moussa et al., 2014a; Moussa et al., 2014b; Lei et al., 2014; Liu et al., 2014; Weng et al., 2014; Wang et al., 2017).

For instance, boron nitride nanotubes (BNNT) obtained by annealing ball-milled boron-nickel catalyst in a nitrogen/hydrogen gas mixture at 1298 K demonstrated the ability to sorb hydrogen at room temperature, with a predictable storage capacity up to 2.2 wt% under 6 MPa (Lim et al., 2007). The improved hydrogen storage of this material can be attributed to its nanoscale morphology and the presence of heteropolar B-N bonding. Through ionic B-N bonding, an extra dipole moment is generated, which aids in stronger hydrogen adsorption.

Nanostructured BN has unique physical and chemical properties when compared to bulk and microsized materials. For example, BN nanoparticles (BNNP) can be synthesized via a vapor-phase pyrolysis precursor, then tailored to the nanostructures by annealing at high temperatures (2273 K) (Moussa et al., 2014b).

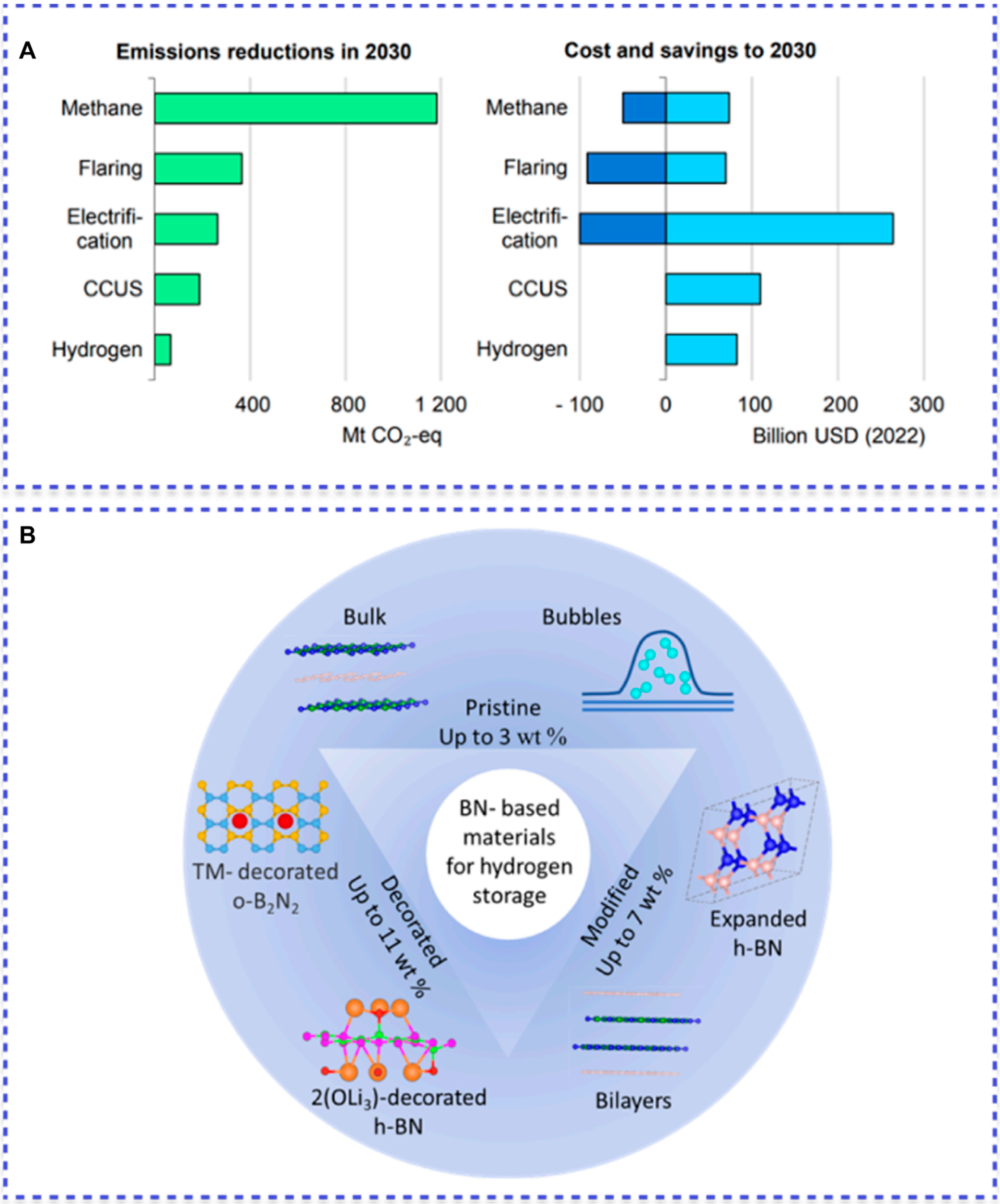

FIGURE 1
(A) Estimated reduction in emissions and total cost and savings accrued resulting from the adoption of measures to curtail emissions from oil and gas operations in the NZE scenario by 2030 [1]; **(B)** Key trends in the development of hydrogen storage in BN-based materials.

Then ball-milling of these nanostructures can be applied to improve the specific surface area. As a result, hollow-cored BNNP with a porous shell structure showing a specific surface area of 200.5 m^2g^{-1} and a total pore volume of 0.287 cm^3g^{-1}, which is conducive to advanced hydrogen accumulation, can be obtained.

Another study (Lei et al., 2014) focuses on oxygen-doped BN nanosheets, which were synthesized through a sol-gel process. The obtained material demonstrated a storage capacity of 5.7 wt% under 5 MPa at room temperature, with each 3 × 3 supercell of BN monolayer capable of absorbing up to 6 H_2 molecules. A theoretical study revealed that the enhanced hydrogen storage capability can be attributed to the oxygen-doping of BN nanosheets, with decreased adsorption distance between H_2 molecules and O atoms compared with pure BN. Additional calculations (Liu et al., 2014) examined the structural durability of metal/BN and investigated metal adsorption sites on the layers. Specifically, the study explored the Na-doped BN layer and found that the electric field generated between the positively charged Na and negatively charged N played a crucial role in enhancing the binding energy between hydrogen and the complex, creating the polarization of hydrogen. As a result, the hydrogen storage ability of this layer was approximately 5.84 wt%.

The key trends in the development of hydrogen storage in BN-based materials are schematically presented in Figure 1B.

To estimate the sorption capacity of h-BN, Wang and colleagues (Wang et al., 2002) milled a commercial powder of BN in a hydrogen atmosphere at 10 bars of pressure and obtained 3-nm crystallites. These crystallites were able to uptake hydrogen in an amount less than 0.5 wt% for a milling time of 5 h. For a much longer milling time of about 80 h, the sorption capacity of h-BN increased up to 2.6 wt%. Indeed, this is quite an impressive result for such a simple method of obtaining material.

In addition to the highlighted material, porous h-BN is also considered for the physical storage of H_2 molecules and cryo-adsorption. Such material was synthesized at 873 K according to a chlorine-assisted method and showed a specific surface area of 960 m^2/g and a specific total pore volume of 0.68 cm^3/g. Thanks to these textural properties, such material is capable of reversibly storing 1.01 wt% of hydrogen at 77 K and 1 bar (Kim et al., 2013). A higher specific surface area was reported for porous BN microbelts. The reversible hydrogen uptake of 2.3 wt% was achieved at 77 K and 10 bars by a sample with a specific surface area of 1,144 m^2/g and a specific pore volume of 0.88 cm^3/g (Weng et al., 2013). Shahsavari and Zhao (Shahsavari and Zhao, 2018) demonstrate a maximum gravimetric uptake of h-BN of 8.65 wt% at 300 K via *ab initio* multiscale simulations. This one has the highest hydrogen uptake on sorbents at room temperature without doping, confirming the positive effect of the specific surface area.

3 Main regularities in accumulating of hydrogen

The hydrogen storage capacities of materials are related to their specific surface areas and, respectively, morphologies. Higher specific surface areas favor faulty architectures with numerous open-edge layers on the external surface. And one of the high specific area promising morphologies of hexagonal boron nitride nanostructures for hydrogen absorption at room temperature is the nanotube. It was shown that with the BN nanotubes, chemisorption of hydrogen predominates (Ma et al., 2002a; Tang et al., 2002; Lim et al., 2007; Leela et al., 2010; Okan et al., 2012) over physisorption almost in all cases. As a result, higher energies are required to remove hydrogen (in the reverse dehydrogenation process). According to Ma et al. (2002a), the hydrogen adsorption on the multiwalled BN nanotubes with a specific surface area of 150 m^2/g and on bamboo-like BN nanotubes with a specific surface area of 210 m^2/g at 293 K and 100 bars was 1.8 wt% of hydrogen and 2.6 wt% of hydrogen, respectively. It has also been experimentally demonstrated that the hydrogen storage capacity of h-BN nanostructures increases with increasing hydrogen pressure. Thus, flower-type BN nanostructures (specific surface area of 180 m^2/g) show a maximum hydrogen storage capacity of 2.5 wt% at around 100 bar hydrogen pressure, while straight-walled BNNTs (specific surface area of 210 m^2/g) show an increased storage capacity of 2.7 wt% at the same conditions. In turn, the bamboo-type nanotubes with the maximum specific surface area of 230 m^2/g have the highest hydrogen uptake capacity of 3.0 wt%.

Tang et al. (2002) looked at the capability to accumulate hydrogen by different BN structures at 10 MPa and room temperature. They found that collapsed BN nanotubes were better at increasing hydrogen adsorption capacity than conventional multiwalled nanotubes. Because of this, there were more dangling bonds, and the specific area of BN nanotubes dramatically increased from 254.2 m^2/g to 789.1 m^2/g. The amount of hydrogen adsorbed by the material consequently goes from 0.9 to 4.2 wt%.

The chemical functionalization of nanomaterials may also play a great role in their hydrogen sorption capacity. For example, oxygen-doped h-BN nanosheets with 2–6 layers that were made using the sol-gel method can accumulate up to 5.7 wt% of hydrogen at room temperature under 5 MPa (Lei et al., 2014). This material exhibits high cycling stability, up to 15 cycles in hydrogen uptake-release. Another paper (Zhang et al., 2015) shows the advantage of using one additional morphology of material based on hexagonal boron nitride - porous boron nitride structures (p-BN). Quantum-chemical calculations based on the first principle show that hydrogen storage of C-doped p-BN led to a maximum of 5.1 wt% hydrogen taken, and Li-doped p-BN adsorbs up to 7.5 wt% hydrogen. In addition, similar calculations can be performed for promising materials like lithium-functionalized BC_2N monolayers that have been doped with boron and carbon (Qiu et al., 2014). Moreover, using the dispersion-corrected semi-empirical method, the hydrogen storage capability of B_mN_m nanocages was investigated, and the highest uptake of 12.01% was demonstrated for $B_{96}N_{96}$ (Kinal and Sayhan, 2016).

It is worth paying attention to the new structures based on boron nitride, the proposed theoretical ones. The theoretically proposed novel structure $B_{20}N_{24}$ (Zhao et al., 2023) developed through the CALYPSO code can be seen as a candidate for hydrogen storage. Results show that 19 H_2 molecules absorbed by the structure correspond to 6.8 wt% of storing capacity. The theoretical insights into the possible use of pristine bilayer h-BN as a potential hydrogen storage medium by means of first-principles calculations (Rai et al., 2021) show the maximum storing ability up to 3.4 wt% with the calculated desorption temperature in the range from 1399 K to 279 K, depending on the specific number of H_2 molecules absorbed. The theoretically predicated by DFT calculations orthorhombic diboron dinitride (o-B_2N_2) monolayer decorated by Ti atoms demonstrates 11.21 wt% capacity with a desorption temperature of 396 K (Chodvadiya et al., 2024). The novel theoretically designed TM-decorated $B_{24}N_{24}$ (TM = Sc, Ti) fullerenes have a hydrogen gravimetric density equal to 7.74 wt% and 7.50 wt% for $Sc_6B_{24}N_{24}$ and $Ti_6B_{24}N_{24}$, respectively, with a hydrogen release temperature in the range of 243–408 K (Ma et al., 2020).

Of course, such results obtained both by theoretical calculations and experimental studies encourage some optimism about the resolution of the issue of creating an effective hydrogen storage facility based on nanostructured h-BN.

With the use of the pseudopotential density functional theory (DFT) method, the effect of substitutional doping and structural defects on the hydrogen adsorption capability of boron nitride nanotubes was studied. As a result, a substantial enhancement of the binding energy compared to the perfect boron nitride structure was revealed. It was also shown that BN nanotubes have about 40% larger binding energy compared to carbon nanotubes, the diffusion of hydrogen is slower in small-diameter BN nanotubes than in larger-diameter ones, and the desorption temperature is expected to be about 123 K (Jhi and Kwon, 2004). The effect of Pt modification of the BN nanotubes, resulting in a high average adsorption energy of −0.365 eV for hydrogen molecules, was studied via DFT calculations in (Wu et al., 2006). It was shown that the adsorption of a hydrogen molecule weakens the interaction between the Pt atom and the BN nanotube. While two Pt atoms are doped on the BN tube, the creation of a Pt dimer weakens the Pt-BN connection and reduces the adsorption energy of a hydrogen molecule on the Pt dimer. In addition, the structure, stability, and hydrogen storage efficiency of hydrogenated h-BN sheets doped with lithium have been theoretically explored in (Banerjee et al., 2016). Li atoms on the h-BN sheets have been found to act as binding sites to absorb up to 6 wt% of hydrogen at a lower temperature (<198 K). At the same time, the *ab initio* simulation indicates a favorable hydrogen desorption temperature of ~398 K. In addition to pure lithium, its compounds also show themselves to be good modifiers for increasing the hydrogen-storing capacity of h-BN. The calculated hydrogen gravimetric density of 2(OLi_3)-decorated h-BN for H_2 molecules storage can reach 9.67 wt% (Zhang et al., 2023). The average adsorption energy per H_2 molecule is −0.175 eV, which falls in the ideal window for reversible uptake-release at ambient temperatures.

However, as theoretical studies of carbon-based materials have shown, metal additives can also lead to the aggregation of metal clusters, which can ultimately reduce the adsorption capacity of the materials with respect to hydrogen (Kim et al., 2008; Panigrahi et al., 2021). The first-principle quantum calculations presented in (Venkataramanan et al., 2009) demonstrate favorable absorption sites for Ni and Rh atoms on the BN sheets and the related hydrogen adsorption rate. In Ni-doped BN sheets, a strong chemical bond develops between the nitrogen and Ni atoms; however, in Rh-doped BN sheets, both boron and nitrogen bonds with the Rh atoms were discovered. Both Ni and Rh atoms can chemically absorb up to three hydrogen molecules, and the distance between the metal atom and the BN sheet increases along with the increase in the number of hydrogen molecules.

The capacity of hydrogen adsorption of 4.2 wt% was achieved on composites of Ti powder mechanically milled with h-BN at a weight ratio of 1:1. This value is equal to the theoretically calculated hydrogen absorption of Ti, which can testify that in the tested mixture, Ti mainly absorbs hydrogen (Kondo et al., 2005). In another study (Chen et al., 2012), the adsorption of transition metals such as Sc, Ti, V, Cr, Mn, Fe, Co, and Ni on carbon-doped h-BN sheets and the cage $B_{12}N_{12}$ was investigated using DFT calculations. Sc, V, Cr, and Mn were energetically favorable to be dispersed on the CN-BN sheet and cage and could uptake up to 6 wt% of hydrogen. As was demonstrated, the carbon dopants in h-BN served as potential wells for trapping metal atoms and preventing their clustering.

The novel approach for hydrogen storage in bubbles of pure h-BN (appeared bulging structures on the h-BN surface) via plasma treatment was proposed (He et al., 2019). Such bubble-type structures produced by the methane plasma have a diameter ranging from 2 to 4 μm and a height of up to 8.5 nm. The stability of the hydrogen bubbles based on geometric evolutions shows the diameters of all the bubbles tended to be stable after about 30 weeks under ambient conditions. This is a promising method for preserving hydrogen, but its extraction remains unsolved.

A comparison of different BN-based materials in their ability to accumulate hydrogen is presented in Table 1.

4 Hydrogen release and recycling

There are few data on the hydrogenation and dehydrogenation of hexagonal boron nitride available in the literature, and these are mostly molecular modeling studies. Especially, it makes sense to perform additional experimental modeling devoted to the investigation of hydrogen release processes from h-BN-based materials. Most publications, though, do not disclose the information about whether the BN materials can be used again after the dehydrogenation/desorption process or how their properties change after keeping and releasing hydrogen at the corresponding desorption temperatures. Also, there are some reports stating that the thermal release of hydrogen from BN materials is slow and inefficient and that catalysts are required to speed up the process. Since the value of a material's ability to hold hydrogen is the most important parameter, there is an abundance of information in the literature related to changes in the structure of hexagonal boron nitride to increase the effectiveness of hydrogen accumulation more than release.

The destruction of strong bonds between atoms of BN-based materials and chemisorbed hydrogen (including hydrogen from hydrogenated functional groups) sometimes requires additional energy to release hydrogen after storage. Since then, high-temperature treatment should be applied to storage materials to emit stored hydrogen. For example, nanostructured h-BN powder, which is able to accumulate about 2.6 wt% of hydrogen, can release all hydrogen only at a temperature of 570 K (Wang et al., 2002). At the same time, chemisorbed hydrogen can be released from boron nitride nanotubes at temperatures above 623 K. But triflic acid can catalyze this process, making the dehydrogenation process effective at a slightly elevated temperature (313–323 K) (Roy et al., 2014). Additionally, the proposed mechanism leads to triflic acid regeneration during the process, ensuring total accumulated hydrogen release after some time. In comparison, collapsed Pt-catalyzed BN nanotubes release 5% of adsorbed hydrogen in the temperature range from 353 to 413 K and another 95% in the temperature range from 573 to 723 K (Tang et al., 2002). BN nanofibers with diameters ranging from 30 to 100 nm and lengths of several μm and a hydrogen storage capacity of about 2.9 wt% (at 293 K and 100 bars) are capable of releasing only 20 wt% of accumulated hydrogen at room temperature (physisorbed fraction) (Ma et al., 2002b). A temperature of 573 K is required to release chemisorbed hydrogen. Similar findings were presented in (Ma et al., 2002b), where BN bamboo-like nanotubes retained about 70% of the accumulated hydrogen after returning to ambient pressure, indicating predominantly chemical adsorption. The adsorbed hydrogen was fully released only when the sample was heated to 573 K. In subsequent cycles,

TABLE 1 Comparison of BN-based materials for hydrogen storage.

Storage ability, wt%	Morphology	Material's features	Storing conditions		References
			P, MPa	T, K	
Experimental data					
2.9	Nanofibers	30–100 nm width and several μm length	10	293	Ma et al. (2002b)
1.8	Multiwalled nanotubes	-	10	293	Ma et al. (2002a)
2.5	Flower-type nanostructures	Specific surface area about 180 m^{2}g^{-1}	10	298	Leela et al. (2010)
2.6	Bamboo-like nanotubes	10–80 nm width and >10 μm length	10	293	Ma et al. (2002a)
3.0	Bamboo-like nanotubes	Specific surface area about 180 m^{2}g^{-1}	10	298	Leela et al. (2010)
0.2	Bulk powder	—	10	293	Ma et al. (2002a)
0.1	Bulk powder	—	6	293	Ma et al. (2002a)
2.6	Nanostructured milled powder	Fine-milled (for 80 h)	1	293	Wang et al. (2002)
4.2	Collapsed nanotubes	Catalyzed by the Pt	10	293	Tang et al. (2002)
5.7	O-doped	Nanosheets with 2–6 atomic layers	5	293	Lei et al. (2014)
2.57	Porous microsponge	Ultrahigh surface area up to 1900 m^{2}g^{-1}	1	77	Weng et al. (2014)
5.6	Micro/meso-porous	High surface area of 1,687 m^{2}g^{-1}, pore volume of 0.99 cm^{3}g^{-1}, rich structural defects	3	298	Li et al. (2013)
2.3	Porous microbelts	High surface area up to 1,488 m^{2}g^{-1}	1	77	Weng et al. (2013)
Theoretical modeling data					
1.5	Pristine	—	5	293	Tokarev et al. (2016)
1.9	O-doped	Interlayer distance 7–7.5 Å	5	293	Tokarev et al. (2016)
5.5	O-doped	—	N/a		Lei et al. (2014)
2.81	Pt-doped sheets	—	N/a		Ren et al. (2015)
4.82	Pd-doped sheets	—	N/a		Ren et al. (2015)
6.33	C-doped nanosheets modified with Ti	—	0.5	298	Wang et al. (2022)
5.1	Porous	Ultrahigh surface area of 3,260 m^{2}g^{-1}	N/a		Zhang et al. (2015)
7.5	Li-decorated porous	One-side decoration	N/a		Zhang et al. (2015)
8.65	Li-doped nanosheets	Distance between sheets 8.3 Å	0.1	300	Shahsavari and Zhao (2018)

(Continued on the following page)

TABLE 1 (*Continued*) Comparison of BN-based materials for hydrogen storage.

Storage ability, wt%	Morphology	Material's features	Storing conditions		References
			P, MPa	T, K	
9.67	h-BN monolayer	2(OLi_3)-decorated	N/a		Zhang et al. (2023)
3.4	h-BN bilayer	Sorption in the interlayer spacing	N/a		Rai et al. (2021)
6.7	h-BN bilayer	Sorption on the h-BN surface	N/a		Chettri et al. (2021)
3.86	eh-BN	Expanded h-BN	20	243	Fu et al. (2017)
11.21	O-B_2N_2 monolayer	Decorated by Ti atoms	N/a		Chodvadiya et al. (2024)

the hydrogen uptake capacity remained stable, indicating reversible adsorption-desorption processes. This shows that bad architecture makes it easier for chemicals to interact with hydrogen, forming chemical bonds.

At the same time, additional experiments showed that about 89% of stored hydrogen can be released from oxygen-doped h-BN nanosheets at room temperature due to the decreasing pressure to the ambient value (Lei et al., 2014). Moreover, hydrogen uptake ability slightly changed from 5.7 to 4.79 wt% by fifteen cycles of hydrogen adsorption-desorption. However, molecular modeling performed in the same study showed only 5.5 wt% for maximum hydrogen absorption by an ideal O-doped BN structure. Quantum-chemical calculations based on the first principle predict that pristine boron nitride has a maximum reversible hydrogen storage capacity of 1.5 wt% under 5 MPa pressure and at room temperature (Tokarev et al., 2016). The same characteristic for O-doped boron nitride is a bit higher and equals 1.9 wt%.

5 Conclusion and perspectives

As can be seen from the literature analysis, both experimental and theoretical modeling data show the high potential of h-BN-based materials for effective hydrogen storage. In addition, theoretical modeling based on first-principles and DFT calculations demonstrates better results in hydrogen storage performance compared to the experimentally reproduced results. Nevertheless, it can be concluded that the best ways to improve the ability of h-BN materials to absorb hydrogen are to increase the effective specific surface area of the materials, correct the structure by making structural defects, possibly change the interplanar distance of layers, dope boron nitride with impurity elements (such as C and O), and form metal clusters on the surface (functionalization by Li, Ti, and others). Reviewed studies mention the hydrogen accumulation capabilities of h-BN-based materials in the range of 0.1–9.67 wt% at room temperature and increased pressure. Moreover, theoretical results are usually slightly overestimated compared to experimental ones. These numbers confirm that currently developed structures are suitable even for automotive applications. Thus, the best way to develop h-BN-based hydrogen storage systems with strong characteristics is to perform more experimental studies on the optimization of mass production of enhanced h-BN nanostructures. But to make the h-BN-based materials commercially attractive, further intensive research work devoted to the hydrogen release procedure and reuse of the materials should be proceed.

Author contributions

AK: Writing–original draft, Writing–review and editing. AMM: Writing–original draft, Writing–review and editing. PA: Writing–original draft, Writing–review and editing. ZP: Writing–original draft, Writing–review and editing. ATM: Writing–review and editing. AA-Q: Writing–review and editing.

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