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A Comparative Study of Carbon Nanotubes and Boron Nitride Nanotubes as Nanomaterial for Hydrogen Storage

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A B S T R A C T

In this study the potential of nanomaterial, specifically carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs), for efficient hydrogen storage, addressing challenges associated with current methods are reviewed. Emphasizing the need for systematic approaches, the study traces the historical evolution of CNTs and BNNTs, highlighting their unique properties and applications. While CNTs initially garnered attention, limitations in their binding strength at room temperature shifted focus towards BNNTs, which exhibit superior hydrogen storage capacities. Experimental evidence, theoretical investigations using computational methods, and studies on carbon doped BNNTs underscore BNNTs' enhanced performance, especially at ambient temperature. The results affirm BNNTs as crucial contributors to advancing clean energy applications, positioning them favorably over CNTs for efficient hydrogen storage.

Keywords: hydrogen storage, boron nitride nanotubes (BNNTs), carbon nanotubes (CNTs), nanomaterial

Introduction

Hydrogen (H_2) is known as an abundant, clean, and renewable energy carrier. When utilized as a fuel, it produces no air pollution or greenhouse gas emissions. Hence, it is pioneering in ongoing effort to find and implement solutions for sustainable energy. However, its realization as a mainstream fuel source must overcome a critical challenge, which is efficient hydrogen storage [1]. Presently, prototype hydrogen-fueled vehicles rely on compressed gas or liquid hydrogen, but these methods come with inherent technical challenges. Issues such as unwieldy tank size, safety concerns, and additional energy requirements for liquidation pose significant obstacles, particularly in the context of commercial hydrogen storage. To address these challenges, more robust and systematic approaches are imperative in the quest for efficient hydrogen storage media. A crucial element in this pursuit is gaining an atomistic understanding of how hydrogen sorption occurs on various materials, as it is believed to play a pivotal role in advancing these processes [2]. In the constant search for answers, the scientific community has turned its attention towards nanomaterial. Nanostructured systems, with their specific characteristics, including surface-to-bulk ratio, offer a hopeful and viable way to revolutionize hydrogen storage [3][4] .

Among the nanostructured materials under scrutiny, carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs) have emerged as focal points on scientific investigations [5]. Carbon, long a subject of hydrogen storage research, has faced limitations in achieving the desired storage capacity. The exploration of specific carbon nanostructures, such as mechanically milled graphite and defective nanostructured graphite, has provided insights into enhanced hydrogen adsorption capabilities [3].

Researchers are also drawn to boron nitride nanotubes (BNNTs) due to their intriguing characteristics and structural similarities to carbon nanotubes. While carbon nanotubes have long been in the spotlight for hydrogen storage, recent insights suggest that BNNTs could surpass their carbon counterparts. Experimental evidence indicates a superior hydrogen storage capacity in BNNTs, presenting an enticing opportunity to overcome the limitations associated with pure carbon-based materials [6].

Theoretical investigations into the interaction between hydrogen and nanostructures have further deepened our understanding. While chemisorption and physisorption have been explored in both carbon and boron nitride nanostructures, the specific mechanisms governing hydrogen storage in these materials remain a subject of ongoing study. This paper undertakes a thorough investigation of nanostructured hydrogen storage materials, concentrating on the special characteristics and behaviors of both carbon and boron nitride nanomaterial, in an effort to close the gap between theory and experiment.

As we dive into the details of how hydrogen adheres to nanomaterial, our aim is to learn about which one of them is the best at storing hydrogen. We want to understand the unique features and behaviors of these nanomaterial, both carbon and boron nitride. By figuring out how these materials interact with hydrogen, we hope to bring us a step closer to making hydrogen storage more efficient and practical.

Nomenclature

Boron nitride nanotubes (BNNTs)

Carbon nanotubes (CNTs)

Density functional theory (DFT),

Evolution of nanotubes: from carbon to boron nitride

The historical development of carbon and boron nitride nanotubes is a fascinating topic that spans the early 1990s. CNTs, discovered in 1991 by Sumio Iijima, a Japanese physicist, are cylindrical structures made of carbon atoms. Renowned for their exceptional properties such as high strength, flexibility, and electrical conductivity, carbon nanotubes have become promising materials for applications in nanotechnology [7]**.** In parallel, BNNTs were first synthesized in 1995 by researchers at the University of California, Berkeley. Composed of boron and nitrogen atoms arranged in a hexagonal lattice structure similar to carbon nanotubes, BNNTs exhibit excellent thermal and chemical stability, along with high mechanical strength, making them attractive for high-temperature applications and as reinforcements in composite materials [8], [9]**.**

The development of both carbon and boron nitride nanotubes has opened up new possibilities in materials science and nanotechnology. CNTs have found applications in diverse fields, such as electronic devices, hydrogen storage, and field emitters, owing to their unique properties [6]. Simultaneously, ongoing research explores the potential applications of BNNTs in high-temperature settings and as reinforcements in composite materials. This dynamic interplay between theoretical predictions, experimental validations, and technological applications continues to drive advancements in the field, promising innovative solutions for future challenges in nanotechnology and materials science.

The idea of using nanomaterial in H storage

Nanotubes are becoming popular for storing hydrogen, offering a step forward in cleaner and more efficient energy options. Hydrogen, seen as a clean fuel, faces storage challenges with traditional methods like compressed gas or liquid hydrogen, which have issues like bulky tanks and safety concerns [3]. Various research has been conducted to explore nanotube structures and compositions and to predict their hydrogen adsorption capacities and desorption temperatures. This systematic approach streamlines the search for a suitable nanomaterial with desirable storage characteristics. CNTs and BNNTs are being explored as potential candidates to overcome these challenges and improve hydrogen storage.

Utilizing nanomaterial for hydrogen storage presents a range of advantages that address existing challenges in conventional storage methods. One significant benefit lies in the enhanced surface area offered by nanomaterial, particularly nanotubes like CNTs and BNNTs. These materials exhibit a high surface-to-volume ratio, providing more sites for hydrogen molecules to attach. This increased surface area enhances the overall storage capacity of hydrogen, offering a potential solution to the limitations of traditional storage materials [6], [7].

Physisorption, a physical bonding mechanism prevalent in nanomaterial, is another advantageous feature for hydrogen storage. This mechanism relies on weak van der Waals forces, allowing hydrogen molecules to adhere to the surface without undergoing chemical reactions. Unlike some conventional methods, physisorption does not necessitate high pressures or low temperatures, making it a practical and energy-efficient approach [10].

Nanomaterial show promise in achieving room temperature hydrogen storage, a notable advantage compared to some conventional methods that require extreme conditions for effective hydrogen releasing. The problem with storing hydrogen lies in its weak attachment to solid surfaces, requiring either high pressure or low temperature. The potential for storing and releasing hydrogen in conditions closer to ambient temperatures enhances the practicality and safety of hydrogen storage for diverse applications. Nanotubes, with their unique structures, seem promising. Therefore, one major reason CNTs and BNNTs are being studied for hydrogen storage is due to their unique structures. Challenges of weak hydrogen bonds find solutions in nanotubes with their high surface area, unique shapes, and friendly interactions. Several research projects are conducted to understand and find the most suitable nanomaterial for efficient hydrogen storage, pushing us closer to cleaner and sustainable energy technologies [5], [11].

CNTs and BNNTs in hydrogen storage advancements

CNTs and BNNTs have been subjects of extensive research for their potential in hydrogen storage, offering distinct features and findings. Initially, CNTs garnered attention as a potential solution to the storage challenges faced by hydrogen due to their unique structures. However, research findings indicated limitations, particularly in terms of their weak binding strength at room temperature, posing obstacles to achieving efficient hydrogen storage. This propelled a shift in focus towards alternative nanomaterial, including BNNTs, which exhibit intriguing properties like partial ionic bonds and a distinct surface structure [5], [6], [10].

When examining the properties of CNTs, it becomes apparent that they possess a hydrogen storage capacity of approximately 0.2 wt%, emphasizing the challenges associated with their weaker binding strength. BNNTs present a more promising scenario, with storage capacities reaching up to 3 wt% and 4.2 wt% for collapsed BNNTs. BNNTs differentiate themselves from CNTs as they consistently maintain a semiconductor nature, characterized by a band gap around 5.5 eV. This, combined with the partial ionic B-N bonds and a distinctive surface structure featuring a slight buckling effect, contributes to a more favorable interaction between hydrogen molecules and the surface of BNNTs compared to CNTs [3].

Computational methods, along with DFT, have played a crucial role in understanding the hydrogen adsorption properties of both CNTs and BNNTs. Studies on CNTs revealed weak binding of hydrogen at room temperature, prompting further exploration. On the other hand, research delving into BNNTs showed that they could potentially achieve high hydrogen storage capacity at temperatures suitable for practical applications. The bonds in BNNTs emerged as a key factor influencing the binding energy of hydrogen, leading to a slightly polarized hydrogen molecule and a stronger interaction with BNNTs compared to CNTs [10], [12].

In essence, while both CNTs and BNNTs are nanostructured materials with high surface-to-bulk ratios, BNNTs, with their unique electronic and structural properties, demonstrate superior potential for efficient hydrogen storage. The contrast in their binding strengths, storage capacities, and the nature of their chemical bonds highlights BNNTs as more promising candidates for advancing hydrogen storage technologies.

According to Koswattage et.al the ab initio calculations conducted on carbon-doped boron nitride nanotubes (BNNTs) reveal enhanced hydrogen binding energies compared to clean BNNTs, aligning with experimental findings. Unlike the adsorption of atomic hydrogen, hydrogen molecules undergo physisorption on BNNTs. The binding energies for hydrogen on carbon doped BNNTs fall within the optimal range for serving as a hydrogen storage medium. Defects introduced by carbon doping influence donor or acceptor defect levels based on the carbon atom's site in the boron or nitrogen position. These factors highlight the preference of BNNTs over carbon nanotubes (CNTs) for hydrogen storage [10].

Further, activated BNNTs exhibit promise as effective hydrogen storage media at room temperature. The introduction of oxidized pores enhances hydrogen diffusion inside the tube, increasing available adsorption sites and, consequently, storage capacity. Quantum mechanical simulations demonstrate that severe chemical treatments, like peroxidation, drastically elevate hydrogen binding energy on nanotubes, presenting a potential avenue for designing room temperature hydrogen storage [10].

Comparatively, defective nanostructured hexagonal boron nitride (h-BN) achieved through mechanical milling under a hydrogen atmosphere displays distinct characteristics. The hydrogen concentration in h-BN, resulting from chemical absorption during milling, differs significantly from graphite due to variations in local electronic structures. Hydrogen trapped by B and N dangling bonds formed during milling is partially desorbed as molecular hydrogen over a wide temperature range. The absence of hydriding/dehydriding reversibility emphasizes the role of energy conditions provided by mechanical milling in achieving chemical absorption in the h-BN-H system. Despite heating to 1173 K, some hydrogen remains trapped, underscoring h-BN's ability to retain its defective nanostructure. Overall, these findings contribute valuable insights into the potential of BNNTs and hydrogen-absorbing materials for clean energy applications [10].

Discussion

This review tried to explore the potential of nanomaterial, particularly carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs), for efficient hydrogen storage. Hydrogen is recognized as a clean and renewable energy carrier, but the challenge lies in developing effective storage methods. The review tried to emphasize the need for systematic approaches to address the limitations of current storage techniques, such as compressed gas or liquid hydrogen, which face issues like bulky tanks, safety concerns, and additional energy requirements [7], [13].

The historical evolution of both CNTs and BNNTs is traced, highlighting their unique properties and applications in nanotechnology. While CNTs initially garnered attention, limitations in their binding strength at room temperature prompted researchers to explore alternative nanomaterial, leading to the rise of BNNTs [14]. Experimental evidence indicates that BNNTs exhibit superior hydrogen storage capacities, making them more promising for overcoming the challenges associated with pure carbon-based materials.

There are experimental as well as theoretical investigations using computational methods like density functional theory (DFT) to understand the hydrogen adsorption properties of both CNTs and BNNTs. It discusses how CNTs, despite their unique structures, face challenges with weak binding at room temperature, steering the focus towards BNNTs, which demonstrate better storage capacities, distinct surface structures, and semiconducting properties.

The studies are expanded to include carbon doped BNNTs, which exhibit higher hydrogen binding energies, especially when hydrogen molecules are physisorbated. At room temperature, activated BNNTs show promise as hydrogen storage materials because their oxidized pores improve the transport of hydrogen. According to simulations using quantum mechanics, chemical processes such as peroxidation can greatly increase the hydrogen binding energy. This indicates that BNNTs have a greater potential for storing hydrogen at ambient temperature than CNTs [5], [10].

The unique properties of BNNTs are further highlighted through a comparative analysis with defective nanostructured h-BN produced by mechanical milling in a hydrogen environment. The studies underscore the significance of energy conditions in achieving chemical absorption in the h-BN-H system, even without hydriding/dehydriding reversibility. Overall, the results affirm the improved performance of BNNTs and hydrogen-absorbing materials, establishing BNNTs as important contributors to the advancement of clean energy applications.

Summary

When exploring the potential of nanomaterial, specifically CNTs and BNNTs, for efficient hydrogen storage, addressing challenges associated with current methods it seemed that while CNTs initially attracted attention, limitations in their binding strength at room temperature redirected focus towards BNNTs, which exhibit superior hydrogen storage capacities, distinct surface structures, and semiconducting properties. Theoretical investigations, employing computational methods like density functional theory (DFT), reveal the challenges faced by CNTs and the promising characteristics of BNNTs,

particularly when carbon doped. Activated BNNTs at room temperature demonstrate potential as effective hydrogen storage materials due to improved hydrogen transport through oxidized pores. It can be said that BNNTs shows a greater potential for storing hydrogen at ambient temperature compared to CNTs.

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