



ORIGINAL ARTICLE

Modern Materials For Hydrogen Storage: Comparative Analysis Of Carbon Nanotubes And LaNi₅H₆ Metal Hydrides

Ilolov A.M. ^{1,*}, Akimkhojaev T. ²

¹ International University of Tourism and Entrepreneurship of Tajikistan, Dushanbe, Tajikistan; Email: ilolov2@gmail.com

² Center for Innovative Development of Science and Digital Technologies, National Academy of Sciences of Tajikistan, Dushanbe, Tajikistan; Email: Tura3010@gmail.com

*Corresponding Author: A. M. Ilolov (Email: ilolov2@gmail.com)

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ABSTRACT

Hydrogen energy is widely recognized as a key component of future sustainable energy systems due to its high energy density and environmentally friendly nature. However, efficient, safe, and cost-effective hydrogen storage remains a major technological challenge. This study presents a comprehensive comparative analysis of carbon nanotubes (CNTs) and LaNi₅H₆ metal hydrides as hydrogen storage materials. The mechanisms of hydrogen storage, including physisorption and chemisorption, are discussed in detail. The influence of structural properties, temperature, pressure, and material modification on hydrogen storage performance is analyzed. The results indicate that CNTs provide high surface area and fast adsorption kinetics but exhibit limited storage capacity under ambient conditions. In contrast, LaNi₅H₆ metal hydrides demonstrate stable, reversible, and efficient hydrogen storage. The potential of hybrid systems combining nanostructured carbon materials and metal hydrides is identified as a promising direction for future research.

Keywords: Hydrogen storage; Carbon nanotubes; Metal hydrides; LaNi₅H₆; Adsorption; Renewable energy; Nanomaterials.

1 | INTRODUCTION

The global shift toward sustainable and low-carbon energy systems has significantly increased interest in hydrogen as a clean and efficient energy carrier. Hydrogen offers a high gravimetric energy density and produces only water as a by-product during combustion or electrochemical conversion. Despite these advantages, the development of efficient hydrogen storage technologies remains a major obstacle to the widespread adoption of hydrogen energy systems. Conventional methods of hydrogen storage, including compressed gas and liquefied hydrogen, suffer from several drawbacks such as high energy consumption, safety concerns, and low volumetric density. As a result, material-based hydrogen storage has emerged as a promising alternative. Among various materials, carbon nanostructures and metal hydrides have received considerable attention. Carbon nanotubes (CNTs), due to their high surface area and unique electronic properties, have been proposed as potential hydrogen storage materials. Early studies reported hydrogen storage capacities up to 4.2 wt% in CNTs; however, subsequent investigations revealed significant discrepancies and limitations under practical conditions. Metal hydrides, particularly LaNi₅H₆, are well-established materials capable of reversibly storing hydrogen through chemical bonding. They offer stable storage and controlled hydrogen release, making them suitable for practical

applications. Progress in storage materials is closely tied to parallel developments on the production side of the hydrogen value chain: regional assessments of green hydrogen production technologies and renewable resource potential, including recent studies conducted in Tajikistan and the wider Central Asian region, highlight the growing relevance of an integrated approach that combines efficient generation and storage [12–13, 16].

This study aims to provide a comprehensive comparison of CNTs and LaNi₅H₆ metal hydrides, highlighting their advantages, limitations, and potential for future hydrogen storage systems.

2 | HYDROGEN STORAGE MECHANISMS

Hydrogen storage in advanced materials is governed by physicochemical interactions that depend on the structure, surface properties, and thermodynamic behavior of the material.

Physisorption is based on weak van der Waals interactions between hydrogen molecules and the surface of materials. This mechanism is reversible and does not involve dissociation of hydrogen molecules. The adsorption energy typically ranges from 0.02 to 0.1 eV. In carbon nanotubes, hydrogen molecules are adsorbed on both the outer and inner surfaces. However, due to the weak interaction energy, hydrogen is easily desorbed at room temperature, which limits storage efficiency.

Chemisorption involves the formation of chemical bonds between hydrogen atoms and the host material. This mechanism is typical for metal hydrides, including LaNi₅H₆. In this process, hydrogen molecules dissociate into atoms, which occupy interstitial positions within the metal lattice. This results in stable hydrogen storage with higher binding energy compared to physisorption. The thermodynamic behavior of metal hydrides is described by pressure–composition isotherms, which exhibit characteristic plateau regions corresponding to phase transitions.

Figure 1 illustrates the fundamental difference between hydrogen storage mechanisms in carbon nanotubes and metal hydrides. In CNTs, hydrogen is adsorbed on the surface through weak van der Waals interactions without dissociation, which limits storage stability at ambient conditions.

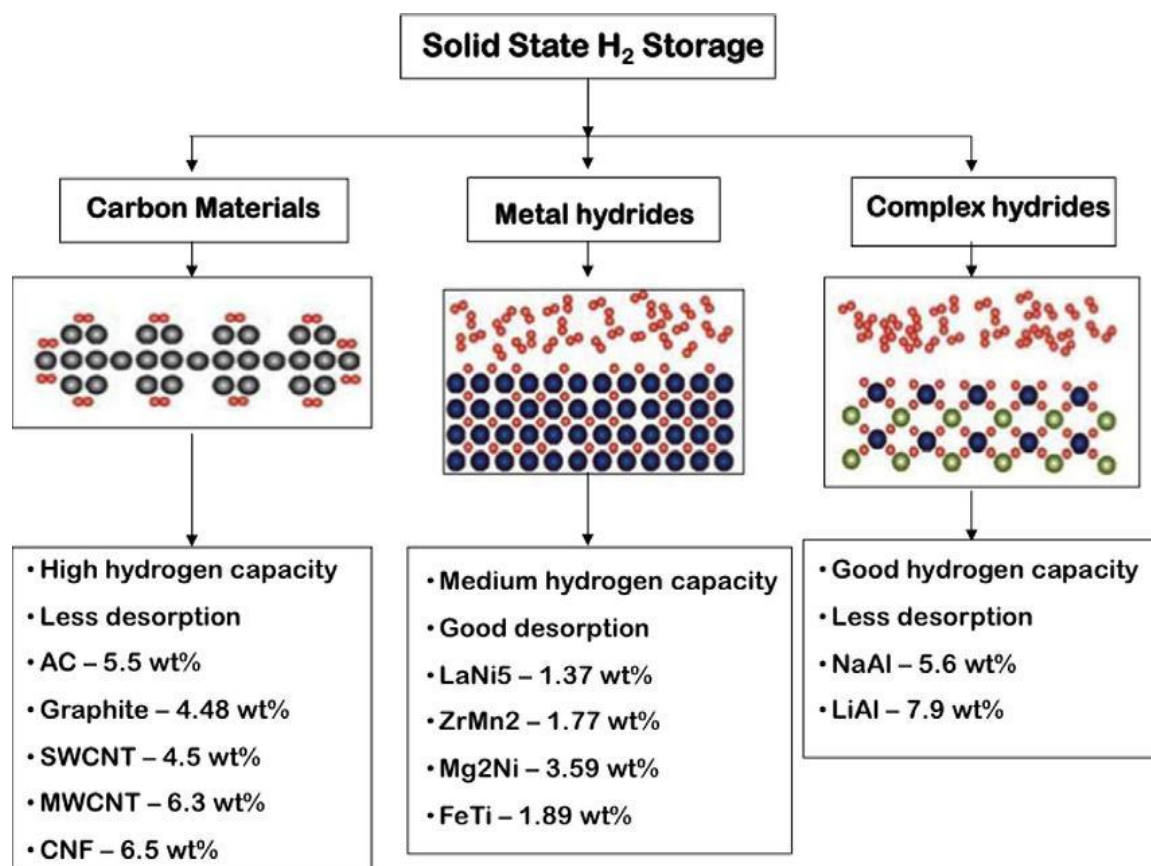


Figure 1. Schematic representation of hydrogen storage mechanisms in carbon nanotubes (physisorption) and LaNi₅H₆ metal hydrides (chemisorption).

In contrast, LaNi₅H₆ stores hydrogen through chemisorption, where hydrogen molecules dissociate into atoms and occupy interstitial lattice sites. This results in significantly stronger bonding and improved storage stability.

3 | CARBON NANOTUBES FOR HYDROGEN STORAGE

Carbon nanotubes are cylindrical nanostructures formed by rolling graphene sheets. They are classified as single-walled and multi-walled nanotubes. Their structure provides high specific surface area and internal cavities suitable for hydrogen storage. Experimental studies show that hydrogen storage in CNTs is strongly dependent on temperature and pressure. At ambient conditions, storage capacity is typically below 1 wt%. At low temperatures and high pressures, adsorption increases due to reduced thermal motion and increased interaction.

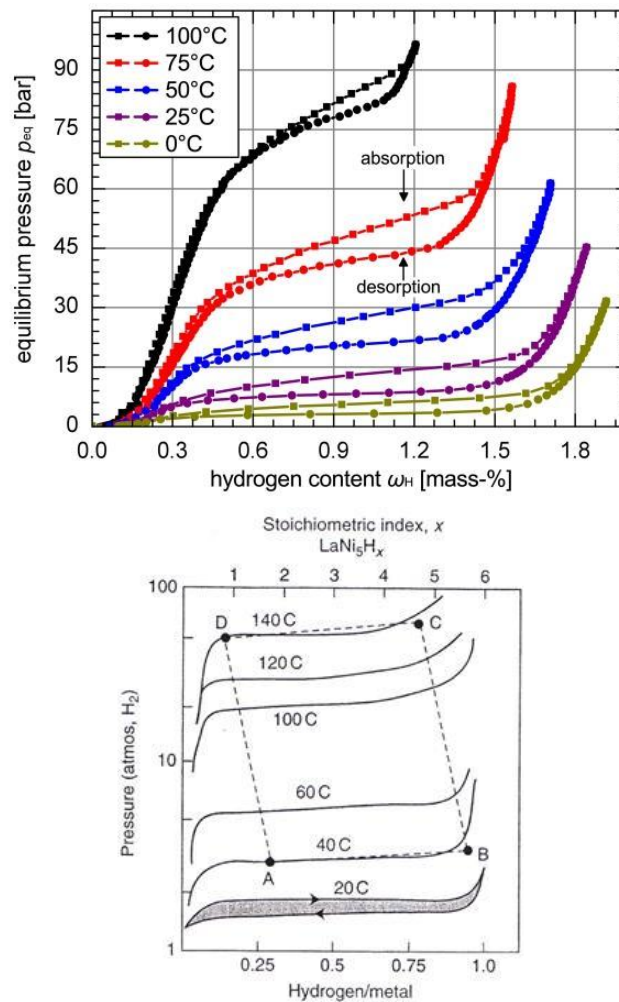


Figure 2. Pressure–composition isotherm of LaNi₅H₆ showing hydrogen absorption behavior.

Figure 2 presents the characteristic pressure–composition isotherm of LaNi₅H₆. The plateau region corresponds to equilibrium between hydrogen absorption and desorption phases. This behavior confirms the ability of metal hydrides to store hydrogen reversibly under controlled thermodynamic conditions. The flat plateau indicates stable hydrogen storage over a range of pressures, which is essential for practical applications. Carbon nanotubes have been widely studied as potential hydrogen storage materials due to their unique structural and electronic properties. Their cylindrical geometry provides a large specific surface area, and their hollow interior offers additional space for hydrogen adsorption. However, experimental studies have revealed that hydrogen storage in pristine CNTs is limited under ambient conditions. The weak interaction between hydrogen molecules and the carbon surface results in low adsorption capacity, typically below 1 wt% at room temperature. To overcome this limitation, various modification strategies have been proposed. Metal doping is

one of the most effective approaches. Transition metals such as titanium and iron can enhance hydrogen adsorption by providing active sites for dissociation. Once dissociated, hydrogen atoms can bind more strongly to the surface, increasing storage capacity. Another approach involves the introduction of structural defects. Defects such as vacancies and functional groups increase the number of active sites and enhance interaction with hydrogen. However, excessive defect formation may compromise the structural integrity of nanotubes. Additionally, the use of alkali metals such as sodium and potassium has shown promising results in theoretical studies. These elements can donate electrons to the CNT structure, increasing the binding energy of hydrogen molecules. Despite these advances, practical implementation of CNT-based hydrogen storage systems remains challenging due to issues related to scalability, reproducibility, and long-term stability.

4 | METAL HYDRIDES

Metal hydrides represent one of the most mature and reliable technologies for hydrogen storage. Among them, LaNi₅H₆ has been extensively studied due to its favorable thermodynamic and kinetic properties. The hydrogen absorption process in LaNi₅ involves the dissociation of hydrogen molecules on the metal surface, followed by diffusion of hydrogen atoms into the lattice. The formation of the hydride phase is reversible, allowing repeated hydrogen absorption and desorption cycles without significant degradation. One of the key advantages of LaNi₅H₆ is its plateau pressure behavior, which enables controlled hydrogen release. The equilibrium pressure depends on temperature and follows the Van't Hoff equation. This allows tuning of operating conditions for specific applications. Furthermore, LaNi₅-based hydrides exhibit fast kinetics due to the catalytic activity of nickel. This ensures rapid hydrogen uptake and release, which is essential for practical energy systems. However, metal hydrides also have limitations, including relatively high weight and sensitivity to impurities. Surface oxidation and contamination can reduce hydrogen absorption efficiency over time.

A comparative analysis of CNTs and LaNi₅H₆ highlights key differences between these materials. CNTs offer higher theoretical storage capacity when modified, but their performance under ambient conditions remains limited. In contrast, LaNi₅H₆ provides stable and predictable hydrogen storage. Furthermore, the temperature dependence confirms that CNTs are less suitable for practical applications without modification.

Hybrid systems combining CNTs and metal hydrides represent a promising approach for improving hydrogen storage performance. CNTs can provide rapid hydrogen adsorption due to their high surface area, while LaNi₅H₆ ensures stable storage through chemisorption. The integration of these materials allows combining fast kinetics with reliable storage capacity.

5 | DISCUSSION

The comparative analysis of carbon nanotubes (CNTs) and LaNi₅H₆ metal hydrides reveals fundamental differences in hydrogen storage mechanisms, performance, and practical applicability. One of the key findings of this study is the strong dependence of hydrogen storage efficiency in CNTs on external conditions. Hydrogen adsorption decreases significantly with increasing temperature. This behavior is directly related to the weak van der Waals interactions governing physisorption. At elevated temperatures, thermal energy overcomes these weak interactions, resulting in rapid desorption of hydrogen molecules. Consequently, CNT-based storage systems exhibit limited performance under ambient conditions. Furthermore, pristine CNTs provide very low hydrogen storage capacity, typically below 1 wt%. This value is insufficient for practical hydrogen storage applications. Although modified CNTs exhibit improved performance, the enhancement is highly dependent on the type of modification and remains difficult to reproduce consistently. The effect of doping highlights the importance of material engineering. Transition metals such as Fe and Ti introduce active sites that facilitate hydrogen dissociation and stronger binding. Similarly, alkali metals modify the electronic structure of CNTs, increasing hydrogen adsorption energy. However, these modifications introduce additional complexity, including potential instability, clustering of dopants, and degradation over multiple cycles. In contrast, metal hydrides such as LaNi₅H₆ demonstrate significantly more stable and predictable hydrogen storage behavior. The pressure–composition isotherm exhibits a well-defined plateau region, indicating equilibrium between hydrogen absorption and desorption phases. This plateau behavior is a key advantage, as it enables controlled hydrogen

release under predictable thermodynamic conditions. Another important aspect is the difference in storage mechanisms. CNTs rely on surface adsorption, while LaNi₅H₆ stores hydrogen within its crystal lattice. This fundamental difference explains why metal hydrides provide higher stability and reliability. Chemisorption ensures stronger bonding and reduces hydrogen loss under normal conditions. From a practical perspective, CNTs offer advantages in terms of lightweight structure and high surface area, which may be beneficial for mobile or portable energy systems. However, their low storage capacity and sensitivity to temperature limit their current applicability. On the other hand, LaNi₅H₆ metal hydrides are already used in industrial applications due to their robustness and reliability. Their main limitations include relatively high weight and heat management requirements during hydrogen absorption and desorption processes. The concept of hybrid systems provides a promising pathway to overcome the limitations of individual materials. By combining CNTs and metal hydrides, it is possible to integrate fast adsorption kinetics with stable storage capacity. CNTs can serve as a conductive and high-surface-area matrix, improving heat transfer and reaction rates in metal hydrides. Such hybrid systems may also address one of the critical challenges in hydrogen storage—balancing gravimetric and volumetric efficiency. CNTs contribute to lightweight structure, while metal hydrides provide high storage density. It should also be noted that the overall efficiency of a hydrogen energy system depends not only on storage materials but also on the performance of upstream production units such as proton exchange membrane electrolyzers, whose numerical efficiency analysis has been addressed in recent studies [14–15]. Overall, the results of this study suggest that neither CNTs nor metal hydrides alone fully meet the requirements for next-generation hydrogen storage systems. Instead, the future lies in the development of advanced nanocomposite materials that combine the advantages of both approaches.

6 | CONCLUSION

This study presents a comprehensive comparative analysis of carbon nanotubes (CNTs) and LaNi₅H₆ metal hydrides as materials for hydrogen storage, focusing on their mechanisms, performance characteristics, and practical applicability. The results confirm that CNTs, despite their high specific surface area and promising theoretical potential, exhibit limited hydrogen storage capacity under ambient conditions. Hydrogen adsorption in CNTs is strongly dependent on temperature and surface modification. The weak van der Waals interactions responsible for physisorption lead to rapid desorption at elevated temperatures, which significantly limits their practical use. Although doping and defect engineering can enhance storage capacity, these approaches introduce additional complexity and do not fully resolve the fundamental limitations of CNT-based systems.

In contrast, LaNi₅H₆ metal hydrides demonstrate stable and efficient hydrogen storage through chemisorption. The presence of a well-defined plateau region in the pressure–composition isotherm confirms their ability to reversibly store hydrogen under controlled thermodynamic conditions. The strong bonding of hydrogen within the metal lattice ensures high stability and reliability, making LaNi₅H₆ suitable for real-world applications. The fundamental difference in storage mechanisms explains the observed performance gap between CNTs and metal hydrides. While CNTs rely on surface adsorption, metal hydrides store hydrogen within their bulk structure, resulting in significantly improved stability.

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AUTHOR CONTRIBUTION

Conceptualization, A.M.I. and T.A.; Methodology, A.M.I.; Software, A.M.I.; Validation, A.M.I., T.A.; Formal Analysis, A.M.I.; Investigation, A.M.I.; Resources, A.M.I.; Data Maintenance, A.M.I.; Writing - Original Draft Preparation, A.M.I.; Writing Review & Editing, T.A.; Visualization, A.M.I.; Supervision, T.A.; Project Administration, T.A. All authors have read and agreed to the published version of the manuscript.

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DATA AVAILABILITY

The datasets generated and analyzed during the current study are available from the corresponding author on reasonable request.

CONFLICTS OF INTEREST

The authors declare no conflict of interest.

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REFERENCES

1. Liu, C., Fan, Y. Y., Liu, M., Cong, H. T., Cheng, H. M., & Dresselhaus, M. S. (1999). Hydrogen storage in carbon nanotubes. *Science*, 286(5442), 1127–1129.
2. Dillon, A. C., Jones, K. M., Bekkedahl, T. A., Kiang, C. H., Bethune, D. S., & Heben, M. J. (1997). Storage of hydrogen in single-walled carbon nanotubes. *Nature*, 386(6623), 377–379.
3. Schlappbach, L., & Züttel, A. (2001). Hydrogen-storage materials for mobile applications. *Nature*, 414(6861), 353–358.
4. Sandrock, G. (1999). A panoramic overview of hydrogen storage alloys from a gas reaction point of view. *Journal of Alloys and Compounds*, 293–295, 877–888.
5. Lyu, J., et al. (2020). Recent progress in carbon nanotubes for hydrogen storage. *Nanomaterials*, 10(2), 123.
6. Darkrim, F. L., Malbrunot, P., & Tartaglia, G. P. (2002). Review of hydrogen storage by adsorption in carbon nanotubes. *International Journal of Hydrogen Energy*, 27(2), 193–202.
7. Züttel, A. (2003). Materials for hydrogen storage. *Materials Today*, 6(9), 24–33.
8. Orimo, S. I., Nakamori, Y., Eliseo, J. R., Züttel, A., & Jensen, C. M. (2007). Complex hydrides for hydrogen storage. *Chemical Reviews*, 107(10), 4111–4132.
9. Broom, D. P. (2011). *Hydrogen storage materials: The characterisation of their storage properties*. Springer.
10. Ilolov, M., Rakhmatov, J., Kabirov, S., & Inagaki, F. (2024). Maximum Power Point Tracking Using Adaptive Neuro-Fuzzy Inference Systems for the Photovoltaic Modules.
11. Soldatov, A., et al. (2023). Synthesis of graphdiyne and study of hydrogen adsorption. *Journal of Physical Chemistry*, 97(10), 3456–3462.
12. Ilolov, M., Kabirov, Sh.O., Rasulov, S., Rahmatov, J.Sh., & Yusufbekov, N.Sh. (2023). On the choice of green hydrogen production technology in Tajikistan. *Bulletin of the National Academy of Sciences of Tajikistan*, 3(192), 124–131.
13. Ilolov, M., Kabirov, Sh.O., Rasulov, S., Rahmatov, J.Sh., & Yusufbekov, N.Sh. (2023). On the potential energy resources of solar energy and green hydrogen production in the area of Lake Karakul (Eastern Pamir). *Bulletin of the National Academy of Sciences of Tajikistan*, 4(193), 147–156.
14. Ilolov, M., Kabir, Sh.O., Ilolov, A.M., Rahmatov, J.Sh., & Rasulov, S. (2025). On the efficiency of proton exchange membrane electrolyzer: Numerical analysis. *Journal of Applied Data Analysis and Modern Stochastic Modelling*, 2(1), 6–16.
15. Ilolov, M., Kabir, S.O., Ilolov, A.M., Rahmatov, J.S., & Rasulov, S. (2025). On the efficiency of proton exchange membrane electrolyzer: Numerical analysis. In *2025 IEEE International Conference on Manipulation, Manufacturing and Measurement on the Nanoscale (3M-NANO)* (pp. 480–484). Changchun, China. <https://doi.org/10.1109/3M-NANO65639.2025.11261023>
16. Jumaev, D.Sh., Ilolov, M., Rasulov, S., & Rahmatov, J.Sh. (2026). Key factors for establishing a green hydrogen production cluster on the shore of Lake Khovarkul (Karakul), Eastern Pamir. *Reports of the National Academy of Sciences of Tajikistan*, 69(7–8), 436–442.