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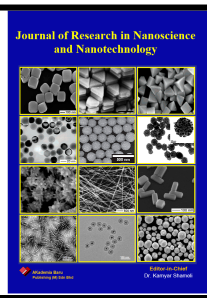


# Strategic Materials and Technological Pathways for Hydrogen Integration in the Net-Zero Transition

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**ABSTRACT**

The global transition to a net-zero economy by 2050 hinges on the integration of hydrogen as a clean energy vector. This report investigates the multifaceted role of hydrogen, from production through renewable-powered electrolysis to advanced storage solutions, with a focus on material innovations. We assess the technological challenges of hydrogen adoption, including the development of intermetallic hydrides for high-density storage. Specific examples, such as $LaMg_2Ni_9$-type alloys, demonstrate progress in substituting critical metals like nickel with sustainable alternatives (e.g., aluminum). Emerging mechanosynthesis techniques for nanostructured alloys are spotlighted as a breakthrough for immiscible-element systems. However, scaling hydrogen infrastructure faces barriers, including the energy-intensive extraction of rare-earth metals and unresolved recycling protocols. This work synthesizes current advancements and gaps to outline roadmap for hydrogen's sustainable deployment in energy grids and decarbonized transportation with expandable framework addressing industry constraint in depleted hydrogen storage materials.

*Keywords:*
Green hydrogen, intermetallic hydrides, net-zero transition, mechanosynthesis, rare-earth substitution, energy storage, sustainable aviation.

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## 1. General Introduction

The quest for decarbonization has elevated hydrogen from 18th-century scientific curiosity to a cornerstone of 21st-century energy strategies. Hydrogen has emerged as a critical pathway to net-zero emissions, offering versatility in storage and transport. However, its integration into global energy systems faces dual challenges: (1) scaling green hydrogen production via renewable-powered electrolysis, and (2) developing efficient storage materials to overcome the limitations of compressed/cryogenic methods.

Recent advances in intermetallic compounds demonstrate remarkable hydrogen absorption capacities, yet reliance on strategic metals like nickel and rare-earth elements raises sustainability concerns. Mechanosynthesis, a technique leveraging high-energy ball milling, enables concurrently the design of these novel alloys, bypassing traditional synthesis barriers. We try to bridge these material innovations with systemic challenges, from hydrogen-powered embedded systems to the geopolitical tensions of mineral supply chains. By critically assessing technological and socio-economic hurdles, we aim to chart a viable course for hydrogen's role in the 2050 energy landscape.

## 2. Hydrogen Revolution and Imperative Orientation for 2050 Net-Zero Transition

Hydrogen was first identified as distinct substance by English chemist Henry Cavendish in 1766 and was later named "flammable air". After, French chemist Antoine Lavoisier verified Cavendish's experiments in 1783 and named the molecule Dihydrogen $H_2$ [1]. Since the introduction of the Kyoto Protocol in the 1990s and the initiation of the annual climate conferences, a variety of socio-economic, industrial and stakeholder communities and actors have been debating the global energy strategy by 2050. Hydrogen storage is one of the key routes, as it's a clean fuel whose combustion produces only water [2]. There have been several discussions recently about integrating batteries having hydrogen tanks with solar panels installed in smart cities (Figure 1). This combination could provide a self-sufficient electricity supply without relying on national power grids [3-5].

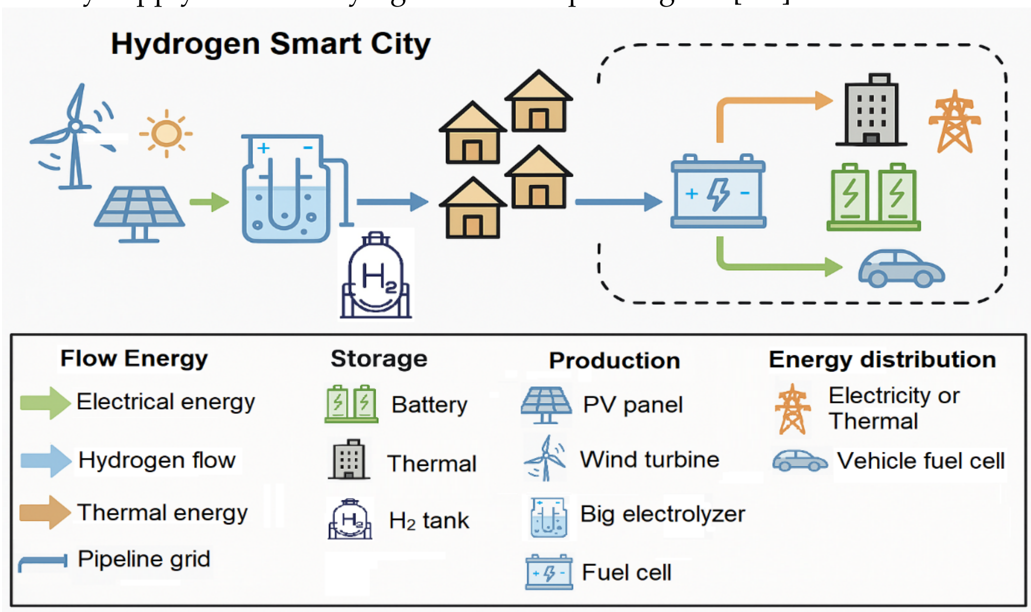


**Figure 1.** Structure of Hydrogen-based smart city [4].

A recent report on energy management estimates that the average cost of electricity per resident in a hydrogen-powered grid, designed for a city with 700,000 people, is around 0.3 $ per kilowatt-hour. This cost is mainly attributed to the initial investment required for solar or wind energy infrastructure at the beginning of the supply chain [4]. In this system, hydrogen acts both as a "carrier gas" (replacing traditional city gas) and as fuel for producing electricity. Meanwhile, the civil aviation industry is experiencing significant transformation, with intense competition among aircraft manufacturers to develop hydrogen-powered planes (Figure 2). This involves a substantial technological challenge: not only in replacing kerosene with the goal of achieving a decarbonized global aviation sector but also in redesigning aircraft and their propulsion systems [6-8].

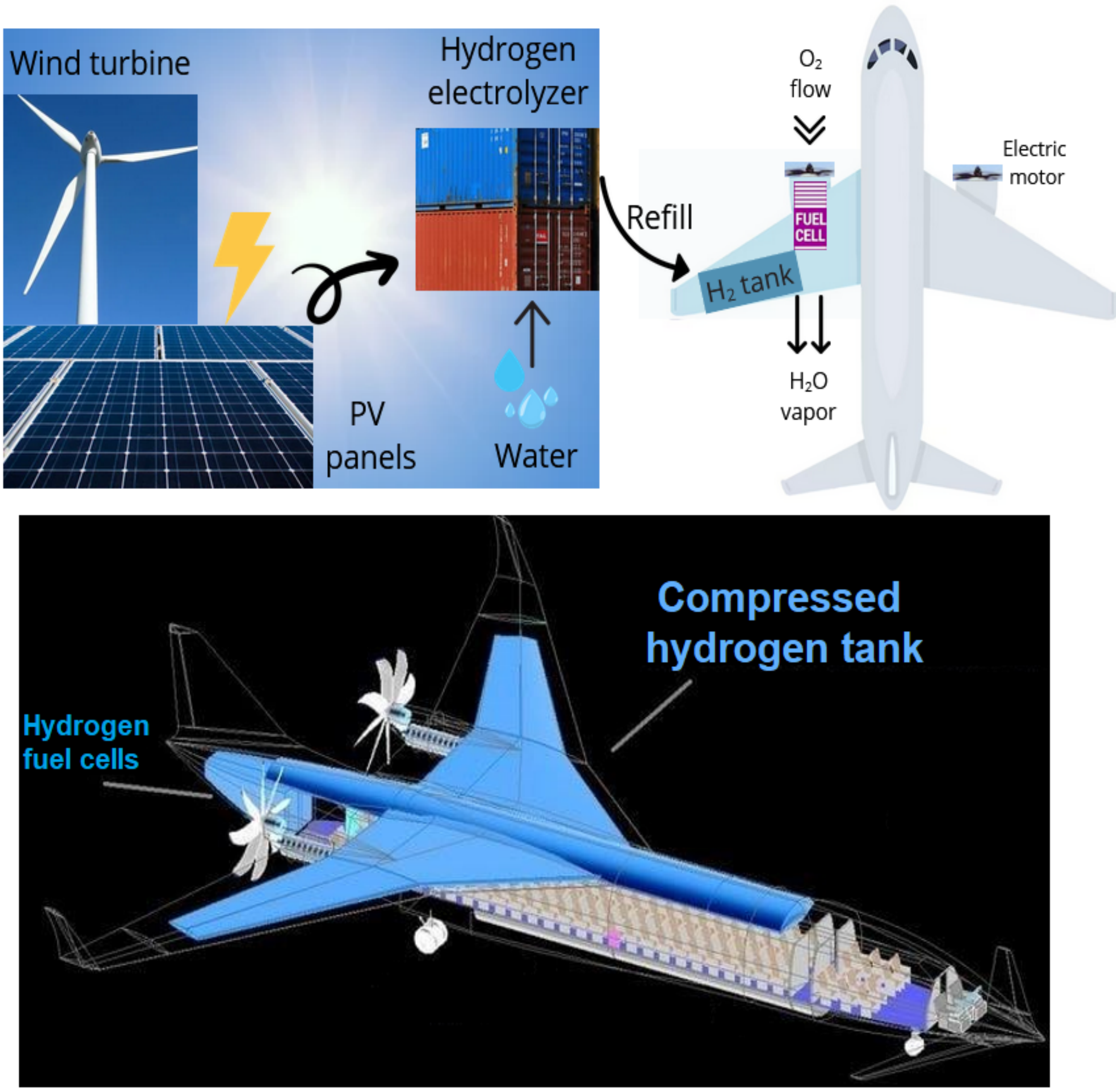


**Figure 2.** Onboard $H_2$ tank location in hydrogen-powered aircraft [6].

### 3. Emerging Materials and their Supply Challenges for Next-Generation

Hydrogen is considered a renewable energy source as it can be generated by splitting water molecules through electrochemical processes, using electricity from sources like solar panels or wind turbines [9-11].

An upscaling splitting prototype was recently showcased with effective method for separating hydrogen and oxygen through water electrolysis. In a laboratory setting, this method produced about 100 liters of pure hydrogen per day, which is roughly equivalent to 0.1 tons per day [12].
Looking ahead, plans are being developed for large-scale industrial production facilities aimed at providing clean hydrogen refueling infrastructure. This hydrogen, known as "Green Hydrogen," will be produced entirely from renewable energy sources, with a production capacity of more than 100 tons per day [13,14].

Hydrogen can be stored in several ways: as compressed gas, a cryogenic liquid (at low temperatures), or in solid form. Although storing hydrogen as a high-pressure gas or cryogenic liquid doesn't provide high enough storage densities, solid-state storage using materials like intermetallic hydrides presents a promising alternative [15,16].

Traditional storage methods have several disadvantages [17]:

- Systems with high mass containment, like heavy tanks, are prone to leakage, especially in compressed or cryogenic storage situations.
- Maintaining cryogenic conditions demands constant refrigeration, which consumes a significant amount of energy.

Nowadays, metal hydrides play a crucial role in paving the way for a future powered by hydrogen. They offer various benefits, including [18,19]:

- Improved safety relative to traditional storage techniques,
- High volumetric density, which means they are more compact,
- The ability to reversibly store hydrogen via cycles of absorption and release.

Hydrogen can be reversibly absorbed into the interstitial sites within the crystal structure of a metal or alloy. This process offers a compact and reliable storage option, providing volumetric capacities substantially superior to those of liquid hydrogen. Various intermetallic compounds have been explored for their potential in hydrogen storage, with the most prevalent being $AB_2$ type $ZrNi_2$ compounds and $AB_5$ type $LaNi_5$ compounds. Among these, $LaNi_5$-based alloys have seen considerable commercial outcome, particularly in their application in Nickel-Metal Hydride (Ni-MH) batteries. However, the absorption/desorption isotherm indicates that the formed hydride, $LaNi_5H_6$, is associated with a relatively high equilibrium pressure plateau, measuring near 2 atm at 25 °C, which is above atmospheric pressure [20,21].

Recent breakthrough in hydrogen storage materials include compounds from the $AB_3$ or $AA'_2B_9$ family, such as $LaMg_2Ni_9$. These materials consistently show better absorption capacities and thermodynamic behavior compared to conventional alloy types [22,23].

To create these new compounds having typical hydrides with near-ambient equilibrium pressures at 25°C, research scientists should combine $LaNi_5$ with specific $AB_2$-type compounds (which $AB_2$-hydrides opt-in low equilibrium pressure at room temperature).

To meet growing global demand for renewable energy technologies (electric vehicles, batteries, fuel cells, wind turbines and solar panels), a massive supply of high-value materials will be important in the long term. However, the dark side of this green revolution reveals an escalating conflict: a polluting rush to extract rare earth metals and critical minerals (with end-of-life recycling remain unresolved challenge).

## 4. Strategic Alloy Design for Sustainable Hydrogen Storage

Forthcoming exploration trends concern partial substitutions within $LaMg_2Ni_9$-type alloys and their corresponding solid-gas hydrogen reactions. Critical status of nickel, among strategic metals, urges advanced development to reduce its concentration in alloying composition. Aluminum is a promising substitution alternative despite intrinsic conductivity, its modern production methods utilizing ceramic anodes (carbon-free, emitting only $O_2$) present significant environmental advantages over nickel's energy-intensive extraction process. Nickel industry relies on high-pressure sulfuric acid leaching (250 °C) followed by costly pyrometallurgical refinement. Future research directions may explore complete rare-earth element substitution in these intermetallic alloys, such as replacing lanthanum with more abundant alternatives like calcium, to further enhance sustainability and cost-efficiency.

In this perspective, mechanosynthesis (reactive ball milling) is a pioneering approach and remains a widely utilized technique for developing novel intermetallic compounds. The resulting alloys typically adopt $AA'_2B_5B'_4$ or $A_3B_9$ ($AB_3$-type) structures.
First employed in the 1980s, this synthesis method overcomes limitations of conventional approaches, particularly for producing nanomaterials and intermetallics from immiscible elements [24]. The process mechanism, during mechanosynthesis, comes down essentially that powder particles undergo repeated high-energy impacts from metallic ball movement. These collisions induce severe mechanical deformation, atomic-level mixing via fracture/welding cycles and enhanced solid-state diffusion. The key point is that this procedure enables production of complex intermetallic alloys with unique nanostructured configuration relying on mechanical concepts rather than thermal processes.

## 5. General Conclusion

Hydrogen stands at a pivotal juncture: its potential to decarbonize energy grids, industry, and aviation is undeniable, yet its success depends on overcoming material and infrastructural challenges. The development of intermetallic hydrides (e.g., $LaMg_2Ni_9$, $AB_2/AB_5$ alloys) and nickel-aluminum substitutions illustrates progress toward sustainable storage, while mechanosynthesis unlocks nanostructured alloys with tailored properties. However, the "green revolution" must confront the environmental costs of mineral extraction and the urgent need for circular economy frameworks.

To bridge these technical advances with real-world deployment, policymakers and industry must align incentives with material innovation. Key priorities include:

(1) Scale electrolyzer technologies to reduce green hydrogen costs,
(2) Standardize recycling protocols for rare-earth-containing alloys,
(3) Foster international collaboration to mitigate supply-chain vulnerabilities.

As hydrogen transitions from labs to cities, interdisciplinary synergy-materials science, policy, and engineering will dictate its viability.
The path to 2050 demands not just innovation, but solutions that achieve lower hydrogen production costs while reducing rare-earth dependency—a benchmark for true sustainability.

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