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# Mechanical Strain as an Emerging Design Parameter for Next-Generation Hydrogen Storage Materials

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**Abstract:** Hydrogen storage remains a major obstacle for the implementation of hydrogen-based energy systems, which challenges the material science to search for materials with improved capacity, thermodynamics, and kinetics. Mechanical strain has emerged as a promising yet unexplored design parameter for tuning hydrogen-material interactions at the atomic scale. This paper reviews hydrogen storage materials from a strain-engineering perspective, examining how tensile and compressive strain influence adsorption energies, diffusion behaviour, and structural stability. Most studied material classes, including metal hydrides, metal–organic frameworks, carbon-based systems, and low-dimensional materials, are discussed alongside representative case studies demonstrating enhanced performance under strain. By consolidating recent insights and identifying critical challenges, this work highlights mechanical strain as a viable and scalable strategy for the design of next-generation hydrogen storage materials.

**Keywords:** Hydrogen storage; Mechanical strain; Strain engineering; Energy materials; Adsorption kinetics.

## Introduction

The upcoming climate change is demanding innovative solutions for clean energy and environmental remediation (Jayabal, 2024; Østergaard et al., 2023). Hydrogen have been brought into focus due to the global issues of energy scarcity and environmental pollution (Tang et al., 2023). The researchers and industries worldwide got attracted significant interest on hydrogen energy technologies. Advancing hydrogen storage solution is a key step in achieving sustainable and environmentally-friendly energy system for the system for future. Hydrogen, a tasteless, colourless, odorless, and nontoxic molecule, is valued for its high energy density, zero pollution emissions, and compatibility with green energy systems. Various methods can produce hydrogen, from burning fossil fuels to utilizing biomass or organic waste, electrolysis, steam methane reforming (SMR), or thermochemical processes. Owning to its potential, the global demand for hydrogen is on a steady rise and is projected to surge by nearly 74 EJ by the year 2050(*Https://Www.Irena.Org/Energy-Transition/Policy/Policies-for-Green-Hydrogen#:~:Text=Green%20hydrogen%20value%20chain&text=Under%20IRENA's%201.5%C2%B0C,Of%20global%20electricity%20consumption%20today.*, n.d.).

Variety of methods are developed for the hydrogen production. Electrolysis is a process in which electricity is used to split water into hydrogen and oxygen, enabling the production of green hydrogen when powered by renewable energy sources(Lee et al., 2025). Although the process is highly sustainable, its large-scale application is constrained by high electricity costs and energy demands. Steam methane reforming (SMR) is a widely used method in which natural gas reacts with steam to produce hydrogen and carbon dioxide(Abe et al., 2024; Sikiru et al., 2024). This process results in *grey hydrogen,* or *blue hydrogen* when carbon capture technologies are applied. Thermochemical processes (*Https://Www.Energy.Gov/Eere/Fuelcells/Hydrogen-Production-Thermochemical-Water-Splitting*, n.d.), such as solar thermochemical water splitting, use high temperatures to decompose water and offer a low-carbon route for hydrogen production, but these methods are still in the experimental stage. Hydrogen stands out as a promising clean energy carrier, but being the lightest element its practical uses relies heavily on its storage. Advancing hydrogen storage solutions is a key step in achieving sustainable and environmentally, friendly energy system for future.

## Most Studied Materials

A wide range of materials has been explored for hydrogen storage, each with its own advantages and limitations.

- **Metal hydrides(Klopčič et al., 2023)** such as $MgH_2$ and $NaAlH_4$ offer high volumetric hydrogen densities, but they require high desorption temperatures, show slow kinetics, and often have poor reversibility during repeated charging and discharging cycles. Complex hydrides like ammonia borane ($NH_3BH_3$) and metal borohydrides (e.g., $LiBH_4$, $Mg(BH_4)_2$) have high gravimetric hydrogen capacities; however, they often decompose irreversibly and release impurities, making regeneration difficult.

- **Carbon-based materials(Assyl et al., 2025)** such as activated carbon, carbon nanotubes, and graphene provide lightweight structures with large surface areas that support physisorption, but weak hydrogen binding results in very low storage capacities under ambient conditions, often requiring cryogenic temperatures to be effective.
- **Metal–organic frameworks (MOFs)** and **covalent organic frameworks (COFs)(Han et al., 2008; Sutton et al., 2024)** exhibit ultrahigh surface areas and tunable pore structures that enhance hydrogen adsorption at low temperatures, but their storage capacity decreases significantly at room temperature and many suffer from moisture sensitivity and high synthesis costs.
- **Liquid and chemical hydrogen carriers** (e.g., ammonia, methanol, formic acid)(Daud et al., 2025; Kim & Yang, 2024) offer convenient transport and storage, yet face issues of toxicity, carbon emissions, and high energy demands for hydrogen release and regeneration. Recently**, two-dimensional (2D) materials** such as graphene, transition metal dichalcogenides ($MoS_2$, $WS_2$), MXenes ($Ti_2C$, $Ti_2N$), borophene, and phosphorene have emerged as promising candidates due to their high surface-to-volume ratio and tunable structures that can enhance hydrogen adsorption. However, challenges such as weak or overly strong hydrogen binding, material instability (e.g., oxidation of phosphorene), and difficulties in large-scale synthesis still constrain practical applications. Overcoming these barriers through doping, surface modification, hybrid composites, and design guided by computational modeling is essential for developing efficient, safe, and cost-effective hydrogen storage technologies.

### Hydrogen Storage Using Two-dimensional (2D) materials (Ghotia et al., 2025)

Two-dimensional (2D) materials have emerged as promising hydrogen storage media through mechanisms such as physisorption, spillover, and chemisorption. Experimental studies on graphene-based hybrids, MXenes, and boron nitride nanosheets demonstrate measurable hydrogen uptake under practical conditions. Defects, dopants, and surface functionalization further enhance active sites and optimize hydrogen binding energies. Materials such as graphene, transition metal dichalcogenides, borophene, phosphorene, and MXenes combine lightweight structures, mechanical flexibility, and chemical stability, making them promising for next-generation energy storage.

Reduced graphene oxide multilaminates confining Mg nanocrystals achieve reversible storage of ~6.5 wt% while enhancing kinetics and oxidation resistance(Cho et al., 2016). Pd-decorated MXenes(Phuong Doan et al., 2021) exhibit hydrogen adsorption at room and cryogenic temperatures due to catalytic dissociation and spillover effects. Defect-engineered or oxygen-doped hexagonal boron nitride nanosheets show multi-wt% hydrogen uptake near ambient conditions(Lei et al., 2014). Theoretical studies further predict high storage capacities in metal-decorated or super-alkali-functionalized 2D materials such as graphene, borophene, phosphorene, and MXenes via Kubas-type interactions. Despite these advances, challenges related to reversibility, material stability, dopant clustering, and scalable fabrication remain, motivating continued efforts in defect engineering and 2D–hydride hybrid design.

## Effects of strain on hydrogen storage:

Strain engineering (Dewangan et al., 2023; Myrzakhmetov et al., 2025) is widely recognized as a promising strategy for enhancing hydrogen storage performance, especially in low-dimensional and nanostructured materials. Owing to their mechanical flexibility, 2D lattices can sustain large uniaxial or biaxial strain. The application of tensile or compressive strain changes lattice parameters and bond lengths, which results in continuous modulation of band structure, charge distribution, hydrogen adsorption energies and storage capacity. Tensile strain often enhances hydrogen adsorption(Zhou et al., 2010) by improving charge transfer and orbital interactions between hydrogen and surface atoms, while compressive strain can either weaken or optimize hydrogen binding depending on the material. Appropriate strain levels can activate additional adsorption sites, lower energy barriers for hydrogen adsorption and desorption, and improve reversibility under practical conditions.

Defect engineering (Dewangan et al., 2023; Liu & Fan, 2023; Myrzakhmetov et al., 2025) provides powerful tools to tailor the electronic structure and adsorption energetics of 2D materials beyond pristine limits. Defects introduce localized electronic states and catalytic sites, while their interaction with strain further tunes defect stability and reactivity. Together, strain-defect coupling offers a rational strategy to enhance hydrogen adsorption, diffusion, and reversibility, opening new pathways for efficient hydrogen storage and energy-related applications.

## Case studies for hydrogen storage:

Several materials have shown improved hydrogen storage performance through strain engineering. For example, DFT studies indicate that **compressive strain on graphene increases hydrogen adsorption energy and uptake**, achieving ~9.4 wt% $H_2$ at ~6% strain compared to negligible uptake in the unstrained case. In 2D holey graphyne(Vaidyanathan et al., 2025), moderate biaxial strain enhances hydrogen affinity and results in significant storage capacity (~5.88 wt %), surpassing many theoretical targets. Similarly, **$Mg_2NiH_4$ hydride under tensile and compressive strain** exhibits improved ionic conductivity and kinetics, reducing energy barriers for hydrogen diffusion and improving storage behavior(Mahamiya et al., 2022). Strain combined with defects also increases hydrogen uptake in graphene-based systems, and strain-induced effects on functionalized graphane derivatives yield high theoretical storage capacities, highlighting how strain tuning can optimize hydrogen storage performance in diverse material classes.

## Conclusion

This review focuses on mechanical strain and defects as a highly effective and flexible parameter for the atomic-scale design of hydrogen storage materials. In various material systems, including metal hydrides, porous frameworks, carbon materials, and particularly two-dimensional materials, strain has been demonstrated to influence adsorption energies, diffusion barriers, and reversibility. The combination of strain effects with defect engineering and surface functionalization can further enhance hydrogen adsorption capacities and rates. Although significant theoretical and experimental progress has been made, there are still challenges in strain engineering, material stability, and scalability. These problems will have to be overcome by combined computational and experimental approaches to enable the successful application of strain-engineered hydrogen storage materials in energy-related technologies.

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