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Review Paper on Hydrogen Storage using MXenes

Madhu Yadav[1,2*]
[1]*Department of Physics, University of Rajasthan Jaipur, JLN Marg, Jaipur-302004 Rajasthan, India*
[2] *Centre for Non-Conventional Energy Resources, University of Rajasthan Jaipur, JLN Marg Jaipur 302004 Rajasthan, India*
**Corresponding author: madhurao3259@gmail.com*

Abstract: Hydrogen is a renewable energy source that has the potential to transform the energy industry. However, efficient hydrogen storage remains a major hurdle. MXenes, a class of two-dimensional transition metal carbides, nitrides, and carbonitrides, have been identified as viable hydrogen storage materials. This review looks at the structure, synthesis, characteristics, and hydrogen storage processes of MXenes, emphasizing recent advances, current obstacles, and future prospects in the sector.

Key Words: Hydrogen, MXene, Storage, transition metal, MAX phase, Capacity

1. Introduction.

The shift to a hydrogen-based economy provides a long-term answer to the world's energy crisis and environmental degradation. Hydrogen has a high energy density and produces merely water when combusted. However, storage presents substantial technical hurdles. MXenes, a new class of two-dimensional (2D) materials, have showed tremendous promise in addressing these difficulties due to their distinct characteristics. This study presents a complete overview of current MXene research for hydrogen storage applications.

2. Structure and Synthesis of MXenes.

2.1 Structure of MXenes

MXenes are generated from the MAX phases, which are ternary carbides, nitrides, or carbonitrides with the general formula: $M\ n+1\ \boldsymbol{M}\ X\ n$ M n+1AX n(n = 1, 2, 3). In this formula, M is an early transition metal, A is an element from group 13 or 14, and X is carbon or nitrogen. MXenes are created by selectively etching the A element from the MAX phases, resulting in a layered structure with the formula $M\ n+1\ X\ n\ T\ x$ M n+1X nT x, where $T\ x$ T xspecifies surface terminations such as -OH, -O, and -F.

2.2 Synthesis Methods.

2.2.1 Etching Process.

The most popular approach for producing MXenes is to selectively etch the A element from the MAX phases with hydrofluoric acid

(HF) or a combination of lithium fluoride (LiF) and hydrochloric acid (HCl). This method typically includes the following steps:

MAX Phase Synthesis: The MAX phase precursor is produced using high-temperature solid-state processes.
Etching: The A layer is selectively removed with HF or a combination of LiF and HCl, resulting in multilayered MXene.
Delamination: Sonication or intercalation procedures are used to exfoliate multilayered MXenes into single or few-layer MXenes.

2.2.2 Alternative Methods.
To reduce the usage of harmful chemicals, alternate synthesis methods such molten salt etching and electrochemical etching have been investigated. These technologies aim to provide a safer and more environmentally responsible way to produce MXene.

2.3 Properties of MXene
MXenes have numerous distinguishing characteristics that make them ideal for hydrogen storage:
High Surface Area: The 2D shape offers a huge surface area for hydrogen adsorption.
Surface Functional Groups: Termination groups like -OH, -O, and -F increase chemical reactivity and functionalization.
Metallic Conductivity: Many MXenes have strong electrical conductivity, which is useful for catalysis and energy storage.
Mechanical Strength: MXenes have high mechanical strength and flexibility.

3. Hydrogen Storage Mechanisms
MXenes can store hydrogen by a variety of processes, such as physisorption and chemisorption and hydrogen spillover.

3.1 Physical adsorption
Physisorption involves weak van der Waals interactions between hydrogen molecules and the MXene surface. This process is reversible and normally takes place at low temperatures. MXenes' high surface area boosts their hydrogen physisorption ability.

3.2 Chemisorption.
Chemisorption is the creation of strong chemical connections between hydrogen atoms and the MXene surface. This reaction is normally irreversible at ambient temperature, and higher temperatures are required for hydrogen emission. Surface terminations like -OH and -O can improve chemisorption by providing active locations for hydrogen binding.

3.3 Hydrogen Spill Over
Hydrogen spillover occurs when hydrogen molecules dissociate into atoms on a catalytic surface and migrate to the MXene support. When paired with suitable catalysts, this technique has the potential to dramatically increase MXenes' hydrogen storage capacity.

4. Recent Developments in MXene-Based Hydrogen Storage

4.1 Experimental Studies

Recent experiments have shown that certain MXenes have the capacity to store hydrogen. Ti_3C_2Tx MXene, for example, has a high surface area and variable surface chemistry, which contributes to its significant hydrogen uptake capability. Other MXenes, such as V_2CTx and Nb_2CTx, have also been studied, yielding encouraging results in hydrogen adsorption and desorption experiments.

4.2 Theoretical Studies

DFT simulations have been widely utilized to forecast the hydrogen storage capacity of MXenes. This research provides information about hydrogen adsorption sites, binding energies, and diffusion paths on MXene surfaces. Theoretical models imply that functionalizing MXenes with particular groups improves their hydrogen storage ability.

5. Challenges and Future Directions.

5.1 Challenges.

Despite the apparent promise, numerous problems must be overcome before the practical deployment of MXenes in hydrogen storage:

Stability: MXenes are susceptible to oxidation, which can reduce their hydrogen storage capability.

Scalability: The synthesis of MXenes requires toxic chemicals and sophisticated methods, which make large-scale manufacture difficult.

Optimization: To acquire larger hydrogen storage capacities, MXene composition and surface functionalization must be further optimized.

5.2 Future Directions.

Future study should center on:

Developing Eco-Friendly Synthesis Methods: Making MXene manufacturing more sustainable.

Enhancing Stability: By creating protective coatings or encapsulating techniques.

Exploring new MXene compositions: To identify materials with high hydrogen storage capacity.

Combining MXenes with Catalysts: Using the hydrogen spillover effect to improve storage.

6. Conclusion.

MXenes are a promising family of materials for hydrogen storage due to their distinct structural and chemical characteristics. While substantial work has been made in understanding and improving their hydrogen storage capabilities, additional study is required to overcome current limitations and fully realize their potential in practical applications. MXenes have the potential to play a critical role in the development of efficient and sustainable hydrogen storage systems as technology advances.

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