PERSPECTIVE

Hydrogen Storage in ZSM-5: Advances and Challenges

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Abstract

ZSM-5 zeolite possesses a three-dimensional network of microporous channels formed by oxygen-linked Si and Al tetrahedra, which confers a high surface area, stability, and hydrophobic properties that increase with the Si/Al ratio. These characteristics make ZSM-5 a suitable material for the adsorption of gases such as hydrogen. In pure ZSM-5, hydrogen storage occurs primarily through physisorption in the micropores, exhibiting type I isotherms and an adsorption capacity that increases with pressure, especially at low temperatures. The relatively low adsorption energy indicates weak interactions that keep the hydrogen in a molecular state and allow for its reversible release. However, the storage capacity can be significantly modified by the incorporation of metals, which generate new active sites capable of activating or even dissociating hydrogen, partially altering the adsorption mechanism. Despite these advantages, the microporous nature of ZSM-5 can limit diffusion and mass transfer efficiency. Therefore, strategies such as the creation of hierarchical structures with mesopores, variation of composition and synthesis of the material represent key parameters of research to improve its performance in hydrogen storage applications.

Keywords: hydrogen storage, ZSM-5 zeolite, porous materials, modified zeolite.

1 Properties of ZSM-5

ZSM-5 is an MFI (Mobil-type five) zeolite, characterized by a three-dimensional cross-channel structure formed by silicon (Si) and aluminum (Al) tetrahedra joined by oxygen bridges [1, 2]. The porous structure of ZSM-5 gives it a high specific surface area [3]. It features two types of intersecting channels that form cavities approximately 9 Å in diameter, which allows the diffusion of relatively large molecules. ZSM-5 is highly thermally and chemically stable, and it resists high temperatures (up to 800 °C without significant structural degradation). Its stability and hydrophobicity increase with a higher Si/Al ratio [4], which favors the adsorption of organic compounds and limits the interference of water in adsorption and catalysis applications.

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2 Hydrogen Adsorption in ZSM-5

Due to its textural and structural properties, ZSM-5 zeolite is suitable for the adsorption of gases, including hydrogen, and for applications under high temperature conditions [5]. Furthermore, its hydrophobic nature and abundant active sites facilitate the selective adsorption of small molecules [6, 7].

2.1 Behavior and hydrogen adsorption mechanisms

Hydrogen adsorption in ZSM-5 increases almost linearly with pressure at various temperatures, with a rapid increase observed at 77 K (Langmuir) between 0.99 and 5.92 atm, which is typical of microporous materials and indicates monolayer adsorption and physisorption. Above this range, adsorption continues to increase slowly and reaches a maximum of approximately 2.89 wt.% at 12.16 atm. The adsorption isotherm is classified as type I, which indicates a strong adsorption at low pressures and a lower adsorption rate at higher temperatures due to the increase in Gibbs free energy [8, 9].

2.2 Adsorption energy and molecular hydrogen

The hydrogen adsorption energy on pure ZSM-5 is low, with a value of -0.27 eV in the most stable state. This indicates a weak interaction and favors hydrogen remaining in a molecular state and being able to easily leave the micropores of the zeolite. The low adsorption energy is related to the inability of pure ZSM-5 to provide enough electrons for strong adsorption, unlike metals, where adsorption is stronger and dissociation can occur [10].

2.3 Influence of composition and stability

The Si/Al ratio is a critical parameter that influences the hydrophobicity, adsorption capacity, and surface characteristics of ZSM-5. An increase in the Si/Al ratio increases hydrophobicity, which can affect the adsorption of polar molecules compared to nonpolar ones. In the case of hydrogen (a nonpolar molecule), greater hydrophobicity can facilitate adsorption by reducing competition with water molecules [11–14].

ZSM-5 maintains its porous structure and adsorption capacity up to 800 °C, with significant degradation occurring only above 1000 °C. This stability is advantageous for hydrogen adsorption applications that may involve temperature cycling [5].

3 Modification of ZSM-5

In pure ZSM-5, hydrogen adsorption is primarily physical and reversible, whereas in ZSM-5 modified with metals (such as Zn, Ni, Pd) additional mechanisms, such as heterolytic hydrogen dissociation and the formation of protonic acid sites or metal hydrides can occur, which is not characteristic of pure ZSM-5 [15, 16].

Modifying the surface of ZSM-5 can affect hydrogen adsorption. For example, incorporating disilane onto the surface of ZSM-5 significantly reduces hydrogen adsorption capacity (from 6.04 to 0.86 mg/g) due to partial blocking of the micropores. The modification creates kinetic traps and hysteresis loops between the adsorption-desorption isotherms. In this way, the slightly obstructed micropores allow hydrogen to enter, but hinder its release [17].

The incorporation of metals such as nickel or zinc within the pores of ZSM-5 can facilitate the activation and dissociation of hydrogen, thereby generating additional active sites and modifying the adsorption mechanism from physical to chemical. This is highly dependent on the temperature and the metal nature [18, 19].

The presence of copper in ZSM-5 (copper-exchanged ZSM-5) affects hydrogen adsorption, since the different copper species bind to H_2 with different affinities. Thus, the number and type of copper species depend on the Si/Al ratio and the degree of copper exchange, which influences the adsorption isotherms [20].

Hydrogen adsorption on ZSM-5 can be physical or chemical, depending on the temperature, the presence of metals, and the surface modification. At low temperatures, adsorption is predominantly physical, characterized by van der Waals interactions and the occupation of surface sites and micropores [8, 17].

4 Intrinsic Limitations of the ZSM-5 Structure

The microporous structure of ZSM-5 limits the diffusion of reactive species, especially large molecules, which can restrict hydrogen adsorption and storage efficiency. Furthermore, the presence of micropores can lead to rapid deactivation due to the deposition of pore-blocking compounds. This negatively impacts the adsorption capacity and the material regeneration [21–23].

On the other hand, slow transport within the pores can cause blockage and decrease mass transfer efficiency, which poses a challenge for hydrogen adsorption applications. Therefore, the introduction of mesoporous structures and the adjustment of pore

size can improve diffusion efficiency and adsorption performance [22, 24].

5 Challenges in the Modification of ZSM-5

The synthesis of hierarchical ZSM-5 using green materials (such as starch) has been shown to improve hydrothermal stability and hydrogen adsorption capacity due to the formation of intracrystalline mesopores. However, detailed characterization of textural properties and optimization of the synthesis remain areas of active research [24].

The incorporation of metals into ZSM-5 can modify hydrogen adsorption mechanisms by facilitating heterolytic dissociation and the formation of acidic and basic sites. However, stability, migration, and sintering of the metals within the structure remain challenges for maintaining long-term activity and adsorption capacity [18, 19], see Table 1.

Operational stability, regeneration efficiency, and resistance to fouling, such as the presence of contaminants or water vapor, are critical aspects that require further research for the industrial implementation of ZSM-5 in hydrogen storage [23, 25].

6 Future Perspectives and Research Areas

Systematic research is required to correlate synthesis parameters (such as Si/Al ratio, aging time, and material selection) with key material characteristics (porosity, active site density, structural stability) and their impact on hydrogen adsorption capacity and selectivity [25].

The development of scalable, cost-effective, and sustainable synthesis routes is essential for the practical application of ZSM-5 in hydrogen storage [24, 25].

Integrating ZSM-5 into multifunctional structures or designs, such as hybrid membranes or electrochemical reactors, could address complex gas mixtures and improve the efficiency and robustness of the hydrogen storage and release process [25].

Table 1. Key challenges for hydrogen storage in ZSM-5.

Challenge	Characteristics	References
Limited diffusion	Micropores restrict the access and diffusion of H_2	[21–23]
Hysteresis and kinetic traps	Blocking the micropores reduces adsorption capacity	[17]
Synthesis optimization	Lack of clear correlation between synthesis parameters and performance	[24, 25]
Stability and regeneration	Need to assess long-term stability and fouling resistance	[23, 25]
Scalability and sustainability	Synthesis methods must be economical and environmentally friendly	[24, 25]
Metal modification and doping	Adsorption is improved, but challenges arise regarding stability and metal migration	[18, 19]

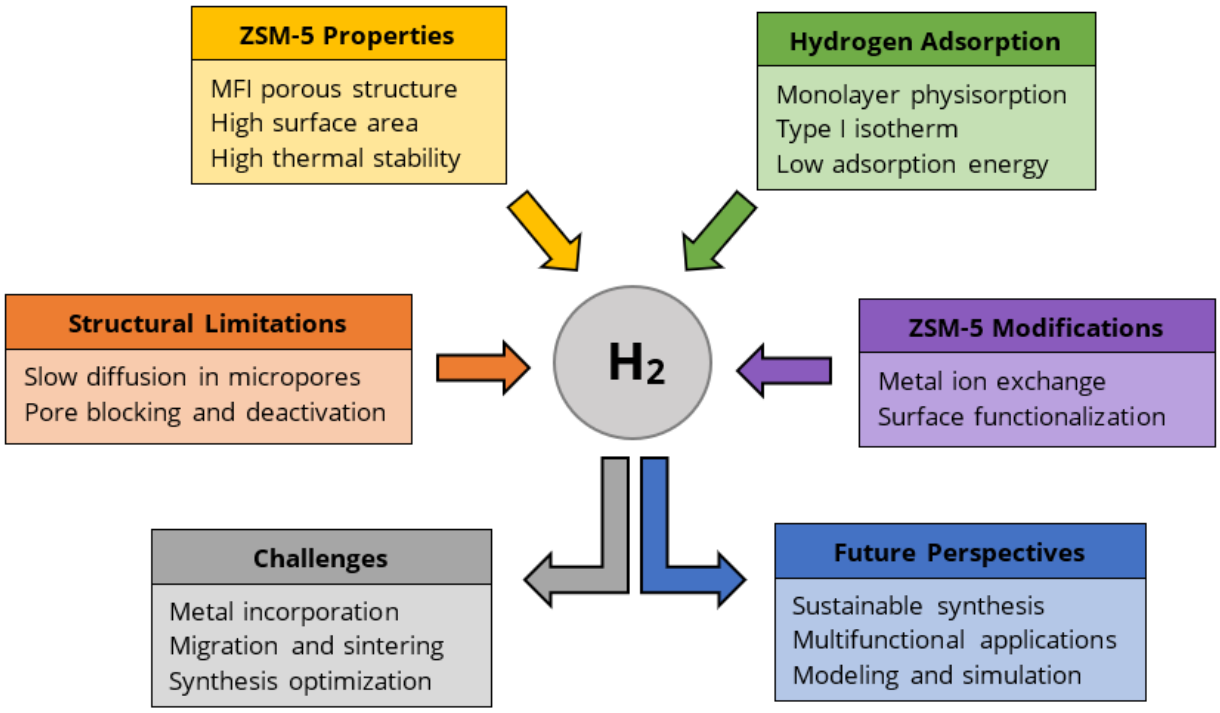

Figure 1. Characteristics of ZSM-5 and current challenges in hydrogen storage.

The use of simulations and adsorption isotherm models allows for predicting and optimizing hydrogen adsorption behavior based on active site energy and temperature, which facilitates the design of advanced materials [8, 26], see Figure 1.

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Conflicts of Interest

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Ethical Approval and Consent to Participate

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