International Journal of Hydrogen Energy 59 (2024) 1434–1458

Contents lists available at ScienceDirect

International Journal of Hydrogen Energy

journal homepage: www.elsevier.com/locate/he

Role of metal-organic framework in hydrogen gas storage: A critical review

A.R. Yuvaraj [a,*], A. Jayarama [b,**], Deepali Sharma [c], Sanjog S. Nagarkar [c], Siddhartha P. Duttagupta [d], Richard Pinto [e]

[a] *Department of PG Studies in Chemistry, Alva's College, Moodbidri, Karnataka, 574227, India*
[b] *Department of Physics, Alva's Institute of Engineering and Technology, Mijar, Moodbidri, D.K, Karnataka, 574225, India*
[c] *Department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India*
[d] *Department of Electrical Engineering, Indian Institute of Technology Bombay, Mumbai, India*
[e] *Department of Electronics and Communication Engineering, Alva's Institute of Engineering and Technology, Mijar, Moodbidri, D.K., Karnataka, 574225, India*

A R T I C L E I N F O

Handling Editor: Dr A Bhatnagar

Keywords:
Hydrogen storage
Metal-organic frameworks
Fluorinated MOFs
Nanocomposites
Supramolecular building layers
Pillaring design
Physisorption
Chemisorption and DFT calculations

A B S T R A C T

Hydrogen gas, well-known for its remarkable energy density (0.0107 MJ/m^3 at STP), is gaining recognition as a potential substitute fuel due to its positive environmental impact. However, the significant hurdle of secure and effective storage of H_2 continues to be a pressing issue. Investigating this challenge, we delve into the potential of metal-organic frameworks (MOFs) as a compelling solution, subjecting them to a thorough analysis. We begin by underscoring the significance of H_2 as an energy carrier, necessitating effective storage. We explore H_2 adsorption on MOFs, highlighting their unique properties and potential for enhanced storage capacity. This review encompasses MOF structure, synthesis, and characterization techniques. It probes MOF-based on carboxylates, nanocomposites, and metal cluster-building components, emphasizing tunable properties and performance in H_2 storage. Design strategies involving supramolecular Building Layers and MOF Pillaring Design are explored, showcasing their ability to enhance H_2 adsorption properties. Additionally, we highlight fluorine-containing and carbon-based MOFs, renowned for their remarkable H_2 storage capabilities, achieved through tailored structures and expansive surface areas. This review explores the application of activated carbon derived from nanoporous polymers for hydrogen adsorption, emphasizing the crucial involvement of carbon-based materials in physisorption methods. To enhance the comprehension of MOFs, we integrate calculations using Density Functional Theory (DFT), Molecular Dynamics simulations, and Grand Canonical Monte Carlo (GCMC) simulations. This all-encompassing examination serves as a valuable reference for scientists and engineers, delivering profound insights and notable progress in the field of MOFs for hydrogen gas storage. Despite tremendous advancements in the field of MOF-based hydrogen storage, a significant gap remains for practical applications due to safety concerns. Further, storing H_2 at 77 K is not very practical due to the requirement of liquid nitrogen. The preferred storage condition would be at 10–100 bar and near room temperature (298 K). Nevertheless, some outstanding results obtained with she-MOF-1 demonstrate exceptional H_2 adsorption with a high storage capacity of 12.60 wt % at temperature 77 K and pressure 100 bars, making it promising for applications requiring substantial H_2 storage. Additionally, MOF-5's remarkable BET (Brunauer-Emmett-Teller) surface area of 3512 m^2/g positions it advantageously in adsorption-driven processes. Analysing H_2 adsorption properties of fluorinated (Co-FINA-1 and Co-FINA-2) and non-fluorinated (Co-INA-1 and Co-INA-2) MOFs reveals that fluorination significantly increases H_2 storage capacities, with Co-FINA-1 exhibiting the highest storage at 1.97 wt % at 77 K and 1 bar pressure, highlighting the positive impact of fluorination on H_2 adsorption. The review highlights promising materials for hydrogen storage, such as she-MOF-1 with exceptional 12.60 wt % adsorption, MOF-5's remarkable BET surface area and the positive impact of fluorination on storage capacities, underscoring their potential for sustainable and economically viable H_2 storage systems.

* Corresponding author.
** Corresponding author.
E-mail addresses: yuvaraj.chem123@gmail.com (A.R. Yuvaraj), jrmarasalike@gmail.com (A. Jayarama).

https://doi.org/10.1016/j.ijhydene.2024.02.060
Received 2 November 2023; Received in revised form 19 January 2024; Accepted 5 February 2024
Available online 16 February 2024