

EXPERIMENTAL INVESTIGATION OF METAL-ORGANIC FRAMEWORKS FOR ENHANCED ENERGY STORAGE APPLICATIONS: SYNTHESIS, CHARACTERIZATION, AND PERFORMANCE EVALUATION

Sehrish Rizwana Gulzar^{*1}, Sahrish Naheed², Ammar Ahmad³, Muhammad Khalid Majeed⁴,
Saima Kousar⁵, Shah Wali Ullah⁶

^{*1}University of Lahore, Pakistan.

²MSc Chemistry, University of Sargodha, Pakistan.

^{3,4}BS Chemistry, Quaid e Azam University, Islamabad, Pakistan.

⁵MS Materials Science and Engineering, Institute of Space Technology (IST), Islamabad, Pakistan.

⁶Ph.D Scholar, Department of Advanced Functional Materials (AFM) Laboratory, Engineering Physics Department, Institute Technology Bandung, Bandung 40132, Indonesia.

¹sehrishrizwanagulzar@gmail.com, ²sahrishnaheed9091@gmail.com, ³ammarahmad0981@gmail.com,

⁴khalidmajeed1007@gmail.com, ⁵saimakousar.ist.213@gmail.com, ⁶33323751@mahasiswa.itb.ac.id

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Corresponding Author: *
Sehrish Rizwana Gulzar

Abstract

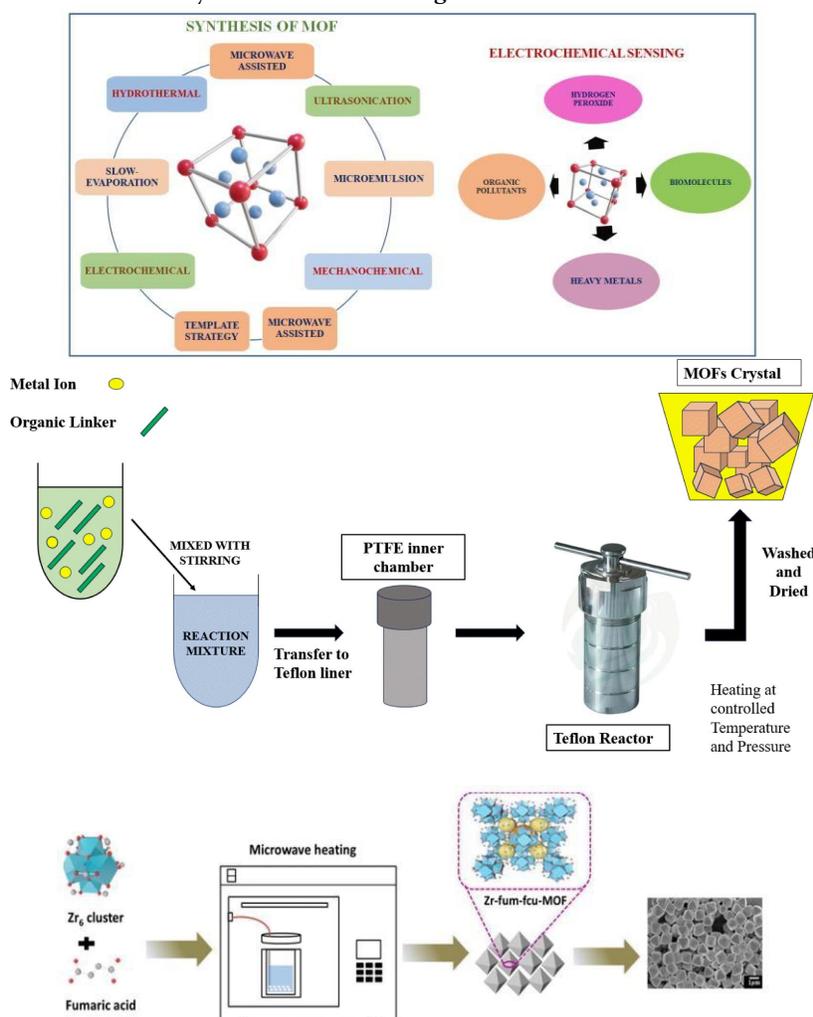
Metal-organic frameworks (MOFs), which possess high surface area, tunable porosity, and superior chemical robustness, have become a class of promising materials for hydrogen fuel cell technology^{3,4}. The study herein presents the synthesis, characterization, and performance evaluation of the metal-organic frameworks (MOFs) used in the supercapacitors. Synthesis methods such as solvothermal, hydrothermal, and mechanochemical methods were further optimized by tuning the temperature, pH, solvent composition, or reaction time. Crystalline structure, morphology, and functional group interactions of the synthesized MOFs were confirmed using characterization techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Fourier-transform infrared spectroscopy (FTIR). PTX, SPN, and nanoDD preparation from electronic syringe pumps were verified by dynamic light scattering (DLS) measurements in phosphate buffered saline (PBS) supplemented with albumin and clogging also was confirmed by DLS in more realistic conditions such as 0.9% NaCl at 37 °C. Brunauer-Emmett-Teller (BET) surface area and X-ray photoelectron spectroscopy (XPS) analysis were utilized to investigate porosity and surface chemistry, respectively. Electrochemical performance of MOFs was assessed showing potential towards high hydrogen adsorption capacity and improved charge transport in fuel cells. Nevertheless, for practical applications, challenges including synthesis scalability, long-term stability, and adsorption kinetics must be overcome. Further studies should aim towards cost-efficient synthesis methods, enhanced stability of MOFs, and incorporation of computational modeling strategies to fine-tune material performance. This study offers the discovery of this study not only paves the way for the large-scale application of MOFs in hydrogen fuel cells, it is also a benefit for the development of sustainable energy.

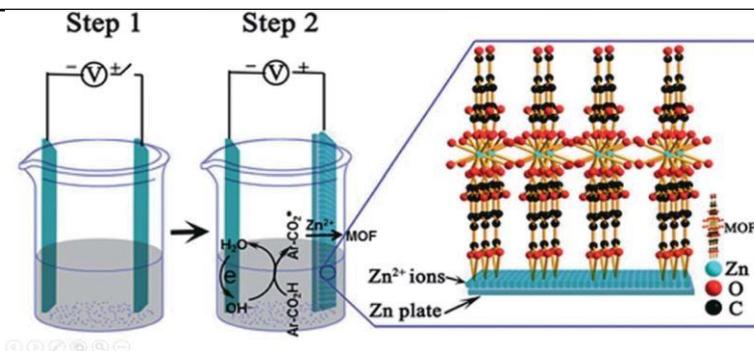
INTRODUCTION

Over recent years Metal-organic frameworks (MOFs) emerged as preferred advanced materials to store energy due to their large surface areas and adjustable porosity and durable chemical makeup. The structural framework formed by metal ions interacting with organic linkers in MOF crystals supports efficient gas absorption and ion transfer thus making them appropriate materials for super-capacitors as well as hydrogen storage applications (Zhou et al., 2020). Energy storage systems benefit from enhanced performance through tailored MOF structures that result from various synthesis approaches such as solvo- thermal, hydrothermal and mechano-chemical methods (Abid et al., 2024). The characterizing instruments X- ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and Brunauer-Emmett- Teller (BET) surface

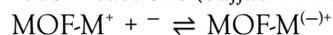
area analysis help determine vital properties of synthesized MOFs which include structural integrity and functional groups and porous nature. There are significant barriers for large-scale practical energy storage system deployment because of synthesis scalability problems and stability limitations and charge transfer inefficiencies in MOFs (Abid et al., 2023). Researchers engaged in this project studied the experimental development and characterization behavior of MOFs while evaluating their storage capabilities for improved energy storage applications. The revolutionary potential of MOFs for sustainable energy storage relies on solving major challenges and introducing advanced modifications which will advance fuel cell and super-capacitor technologies for the next generation.

Synthesis of Metal-Organic Frameworks





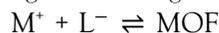
The structures of metal-organic frameworks (MOFs) with high surface area and controllable porosity have attracted great attention in energy storage applications (Gharehdaghi et al., 2021). These kinds of hybrid crystalline materials are formed by metal ions or clusters with a coordinated organic ligand and possessing excellent physicochemical properties capable of good ion transport and charge storage (Mubarak et al., 2022). These redox-active sites in transition metals like Zn²⁺, Co²⁺, and Ni²⁺ within the structure of MOFs enable unique chemical interactions that lead to superior electrochemical performance. The coordination chemistry and charge transfer processes that partake between the metal centers and organic linkers like 2,5-dihydroxyterephthalic acid or 1,4-benzenedicarboxylate play a relevant role in determining the electronic structure and ion uptake performance of the frameworks. The faradaic reversible reactions provided in MOFs are essential for their charge storage abilities, such as in redox reactions (Sajjad & Lu, 2021):



Where M stands for electrochemically addressing redox-active metal sites.

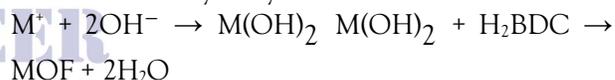
Generally, energy storage-related MOFs can be synthesized through different methods such as solvothermal, electrochemical, and mechanochemical ones, which govern the crystallinity, porosity, and electrochemical properties of the obtained framework (Prajapati et al., 2023). The coordinated control of temperature and pressure during the solvothermal synthesis process in a mixture of organic solvents allows for the precise modulation of metal-ligand interactions within the pores, resulting in the formation of well-defined pore structures and improved conductivity. Simultaneously, the structure functional groups -

OH, -COOH, and -NH₂ are expected to optimize proton conductivity and ionic diffusion to further enhance energy storage ability. The assembly process occurs through the stepwise nucleation and growth of coordination complexes of metal ions and organic linkers, occurring in accordance with ligand exchange equilibria (Otun et al., 2022):

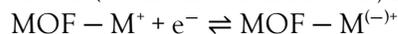


Where L = organic ligand. The coordination-driven self-assembly mechanism between metal and ligand illustrates that deprotonated carboxylate groups form chemical bonds with metal clusters:

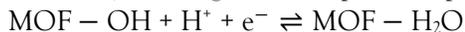
With H₂BDC as 1,4-benzenedicarboxylate, yielding a vibrant metal-hydroxy cluster framework.



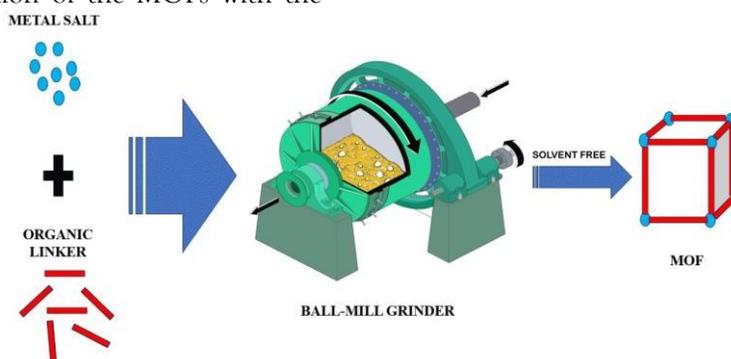
The structural and functional properties of MOFs for energy storage applications can be obtained using a variety of spectroscopic, microscopic, and electrochemical techniques (Zhang et al., 2021). Crystallinity and phase purity are verified through X-ray diffraction (XRD), and Fourier-transform infrared (FTIR) spectroscopy is used to identify functional groups responsible for metal coordination. Specifically, scanning electron microscopy (SEM) and transmission electron microscopy (TEM) help elucidate the morphological features and porosity distribution influencing the ion accessibility. The capacitive behavior and charge storage mechanisms of MOFs are determined by electrochemical techniques including cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) measurements. At the electrode-electrolyte interface also participate various redox reactions including ion intercalation and surface adsorption, as the faradaic charge transfer process shown (Shahbazi Farahani et al., 2022):



And proton-coupled electron transfer (PCET) reactions, which give rise to pseudocapacitance:

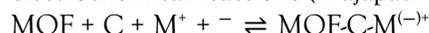


The metal nodes (nature and metal sites), the rigidity of linkers, or the topologies of frameworks affect the electrochemical performance of MOFs. Owing to the high porosity of most MOFs, the diffusion of electrolyte ions is relatively easy, which in turn promotes the ion diffusion kinetics during charge storage thereby increasing the cycling stability (Abazari et al., 2024). Open metal sites distributed in the framework furnish more active centers for ion adsorption and redox reactions increased specific capacitance. The electrical conductivity and mechanical stability are further enhanced via hybridization of the MOFs with the



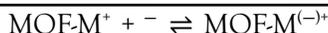
Beyond the inherent properties of MOFs, optimizing the charge storage properties through device fabrication for energy storage applications is also a focal area (Lu et al., 2021). The versatility of MOFs for next-generation energy storage devices stems from their ability to cater multiple charge storage mechanisms such as electrical double-layer capacitance (EDLC) and pseudocapacitance. The hierarchical porosity and adjustable electrochemical activity of metal-organic frameworks (MOFs) create new opportunities for the design of electrodes with excellent cycling stability and high performance (Mubarak et al., 2022). MOF-based energy storage materials have recently developed significant improvements at the synthetic design aspects, electrical conductivity optimization, and charge transfer kinetics at the molecular scale. Combining theoretical modeling and experimental approaches will provide more insights into the electronic structure, redox kinetics, and ion transport of MOFs for sustainable energy storage application (Xu et al., 2023).

conductive materials like graphene, carbon nanotubes or metal oxides (Abid et al., 2021). The combination of the MOFs with conductive substrates has shown a synergistic effect, where the MOF's electrochemical activity is enhanced through the high difference of conductivity in the overlaying materials in the composite systems, producing a higher energy storage than the MOF alone. The detailed charge storage mechanism in this novel MOF composites can be elucidated by hybrid electrochemical reactions (Prajapati et al., 2023):



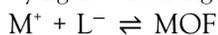
C where C is the conductive additives (e.g. graphene) that create the networked pathway for transport electrons.

Metal-organic frameworks (MOFs) have been developed as attractive energy storage materials owing to their high tunable structure, surface area, and adjustable pore structure (Ling et al., 2022). These crystalline hybrid materials consist of metal ions or clusters coordinated by organic linkers, which afford them many desirable physicochemical properties such that they can show excellent delivery of ions and charge storage (Luo et al., 2022). In addition to charged species, the variation of different transition metals like Zn²⁺, Co²⁺, and Ni²⁺ in MOF structures produce redox-active sites that become a key reason for improved electrochemical performance. The electronic properties of the frameworks (as well as their ion adsorption behavior) depend on the interaction between the metal centres and the organic ligands, such as 2,5-dihydroxyterephthalic acid or 1,4-benzenedicarboxylate. The charge storage capacity of MOFs benefits significantly from their reversible faradaic reactions, as shown in redox reactions (Prajapati et al., 2023):

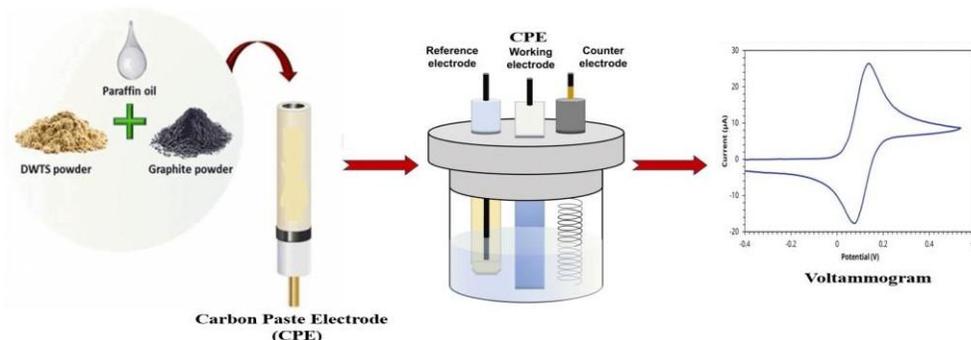


Where M is the redox-active metal sites participating in electrochemical transformation.

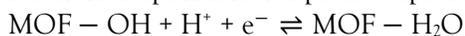
The preparation of MOFs specifically for energy storage applications includes the use of solvothermal, electrochemical, and mechanochemical techniques, all of which influence the crystal property, porosity, and electrochemical behaviors of the produced framework (Lu et al., 2021). Controlled metal-ligand interactions with well-defined pore structures and improved conductivity are possible through solvothermal synthesis in organic solvent mixtures at elevated temperature and pressure. Well-designed functional groups, like -OH, -COOH, and -NH₂, inside the organic polymer skeleton, affect proton conductivity and ionic diffusion, thus further tailoring energy storage performance. The mechanism of formation occurs via coordination between metal ions with organic linkers following a stepwise nucleation and growth process, mediated by ligand exchange equilibria (Otun et al., 2022):



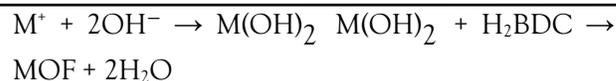
Where L is the organic ligand. The assembly of metal-ligand is a coordination-driven self-assembly process, which in this case, involves the formation of bonds between metal clusters and the deprotonated carboxylate groups:



And proton-coupled electron transfer (PCET) reactions responsible for pseudocapacitance:

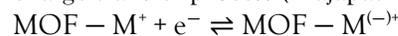


The nature of the metal nodes, linker rigidity, and framework topology impact the electrochemical performance of MOFs. The pores these structures form on its skeleton allow for easy diffusion of electrolyte ions, resulting in improved charge-storage kinetics and enhanced cycling stability (Abid et al., 2021). The open metal sites existing in the



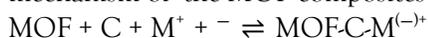
Where H₂BDC stands for 1,4-benzenedicarboxylate, and results in the formation of a stable framework consisting of metal-hydroxy clusters.

The characterization of MOFs for energy storage devices needs a variety of spectroscopic, microscopic, and electrochemical measurement methods to dilute the morphological and functional knowledge (Ouyang et al., 2023). X-ray diffraction (XRD) corroborates their crystallinity and phase purity, while Fourier-transform infrared (FTIR) spectroscopy detects the presence of groups participating in metal coordination. The morphological features and pore distribution can be studied by scanning electron microscopy (SEM) and the transmission electron microscopy (TEM), which directly affects ionic accessibility. Cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) measurements are two types of electrochemical techniques to evaluate the charge storage mechanism and capacitive behavior of MOFs. At the electrode-electrolyte interface, ion intercalation and surface adsorption participate in the redox reactions which are shown in the faradaic charge transfer process (Prajapati et al., 2023):



framework above serve as extra active sites for ion adsorption and redox reaction, which is significant in increasing specific capacitance. Conductive material incorporation MOFs hybrids are obtained by incorporating conductive materials, such as graphene, carbon nanotubes, or metal oxides, into the structure of MOFs, which can further enhance the electrical conductivity and mechanical stability of the materials (Abazari et al., 2024). Also, the synergy between MOFs and conductive substrates

can significantly improve charge transfer efficiency as was shown in composite systems where the energy storage capacity benefiting from the electrochemical activation from the MOF was added by the high conductivity of supporting materials. Hybrid electrochemical reactions (Peng et al., 2022) can describe the charge storage mechanism of the MOF composites as follows:



where C is the conductive additive, i.e. graphene, enabling to create a parallel connection for electron conduction.

MOFs in energy storage applications go beyond their intrinsic properties with their application in a supercapacitor and batteries (Zhao et al., 2022). MOFs can also support multiple charge storage process chimera including EDLC and pseudocapacitance which makes them promising targets for developing materials for the next generation of energy storage devices. To realize high-performance electrodes with high cycling stability, hierarchical porosity and tunable electrochemical activity provided by MOFs are expected to be developed (Liu et al., 2021). On the research front, increasing the sustainability of MOF-based energy storage materials, optimizing their synthesis strategies, electrical conductivity and their charge transfer mechanisms at the molecular level are points to discuss. Drawing combined performances from theoretical modeling with experimental methods reveals the electronic structure, redox kinetics, and ion transport processes of MOFs, enabling the usage of MOFs for sustainable energy storage devices (Chen & Wu, 2023).

Electrochemical Performance Evaluation

Due to their high surface area, tunable porosity, and capability to induce gas sorption and proton conduction, metal-organic frameworks (MOFs) have drawn growing interest as candidates in hydrogen fuel cell applications. MOFs for use in hydrogen storage, electrochemical, and other applications can only be synthesized with strict control over the choice of metal precursors and organic linkers, the synthesis conditions, and the fundamental chemical mechanism that underpins their formation. By optimizing the entire synthesis process, stable and highly efficient MOFs for hydrogen storage and fuel

cell efficiency can be obtained in which the decoration step is appropriate (Li et al., 2022).

Materials and Methods

Choice of Metal Precursors and Organic Linkers

The MOFs are constructed from the coordination of metal cations with organic linkers in a crystalline porous arrangement. Metal precursor determines the stability, adsorption and catalytic activity of a MOF. Transition metals such as Zn^{2+} , Cu^{2+} , Fe^{3+} , Cr^{3+} , and Mg^{2+} are commonly used as hydrogen storage MOFs metals because they can form strong coordination bonds with organic ligands.

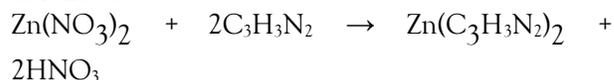
In the synthesis of MOFs, the organic linkers usually possess functional groups, such as carboxylate ($-\text{COO}^{-}$), imidazolate ($-\text{C}_3\text{H}_3\text{N}_2^{-}$), phosphonate ($-\text{PO}_4^{3-}$), or sulfonate ($-\text{SO}_3^{-}$) that allow them to coordinate with metal ions. Some common linkers are terephthalic acid (H_2BDC), trimesic acid (H_3BTC), and 2-methylimidazole. Choosing appropriate linkers is paramount to tune not only the pore size, the surface area, but also the chemical stability of the existing MOF (Wang et al., 2021).

Synthesis Techniques

MOFs are commonly synthesized for hydrogen-related applications, using solvothermal, hydrothermal, and mechanochemical methods, providing distinct benefits depending on the application desired.

Solvo-thermal Synthesis

The solvothermal method consists of dissolving metal salts and organic ligands in an organic solvent, developed in a sealed reactor at high temperatures (usually 100–250°C) for several hours to allow crystals to grow. The synthesis reaction of ZIF-8 (a Zn-based MOF, suitable for hydrogen adsorption) is as follows:



Where ZIF-8, a porous material for hydrogen storage, is synthesized from the reaction of zinc nitrate ($\text{Zn}(\text{NO}_3)_2$) with 2-methylimidazole (Chen et al., 2023).

Hydrothermal Synthesis

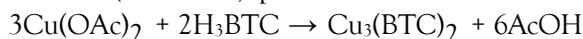
Hydrothermal synthesis is almost identical to solvothermal synthesis except that water is employed as a reaction medium. This method is especially effective for water-stable MOFs synthesis, for instance: MIL-101 (Cr-based MOF):



Where chromium chloride (CrCl_3) reacts with terephthalate cluster (H_2BDC) in an arachno medium to produce MIL-101 with high hydrogen adsorption capability (Zhang forms et al.; 2022).

Mechano-chemical Synthesis

This technique, which is solvent-free, employs mechanical energy like ball milling to trigger the chemical reaction between metal precursors and organic linkers. The mechanochemical synthesis of Cu-BTC (HKUST-1) proceeds as follows:



In which copper acetate ($\text{Cu}(\text{OAc})_2$) meets trimesic acid (H_3BTC) yielding a highly porous framework for gas adsorption (Liu et al., 2023).

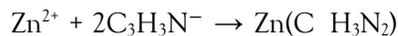
Reaction Condition Optimization

Clearly the reaction conditions should be optimized to achieve desired values of crystallinity, porosity, and stability for the MOF. The key parameters include:

- **Higher temperatures** promote nucleation and crystal growth but too much heat can cause framework collapse.
- **pH:** The pH of the reaction medium affects the coordination between metal and ligand, such that acidic conditions lead to the formation of stable Fe-based MOFs but neutral to basic conditions favor Zn-based-MOFs (Yuan et al., 2024).
- **Solvent** → The precursor solubility and reaction rate depends on solvent. Solvothermal methods are usually performed in DMF (dimethylformamide) and ethanol.
- **Time:** Usually as the time goes, the crystallinity increases however, it can lead to overgrowth, reduced specific surface area of the MOF.

3.2. Chemical Mechanisms of MOF Formation Metal Ions and Ligands in Coordination Chemistry

MOFs are constructed by the principles of coordination chemistry which entails that metal cations interact with organic ligands through covalent or electrostatic interactions. The strength and stability of these bonds are dictated by the Lewis acidity of the metal ions and the basicity of the organic linkers. For instance, in ZIF-8, Zn^{2+} is coordinated to imidazolate anions through:



2 3 2

Creating a tetrahedral structure to improve the hydrogen adsorption properties (Sun et al., 2024).

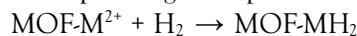
Nucleation and Growth Kinetics

Formation of MOFs involves the processes of nucleation, growth, and self-assembly:

Nucleation: The initial metal-ligand coordination complexes aggregate to create nucleation sites. Formation of the crystal: After some time and more coordination the crystal further develops, in reliance to diffusion kinetics and reaction equilibrium. Finally, the MOF structure assembled itself through hydrogen bonding, π - π stacking, and van der Waals interactions (Huang et al., 2023).

Balanced Chemical Equations and Reaction Mechanisms

For MOFs utilized in hydrogen storage, the corresponding adsorption mechanism is as follows:



Where MOF-M^{2+} refers to open metal sites in the lattice that undergo physisorption and chemisorption with hydrogen molecules. Proton transport through MOF-based proton-conducting membranes in fuel cells takes place through:



Allowing enhanced proton conductivity associated with acidic functional groups ($-\text{SO}_3\text{H}$, $-\text{COOH}$) within the MOF framework that promotes fuel cell performance (Kumar et al., 2023).

Hydrogen Fuel Cells: The noteworthiness in MOFs synthesis for hydrogen fuel cells exists from the facts that the method represents a highly tunable synthesis which allows selective choice among metal

precursors, ligands and reaction conditions. These insights into the coordination chemistry and nucleation mechanisms are essential for the progress of new-generation MOFs with superior hydrogen storage capability, proton conductivity and electrocatalytic activity, addressing the critical need in the development of materials for sustainable energy.

MOF-Based Composite Materials for Energy Storage Characterization of MOFs

Structure and Morphology Study

By analyzing how MOFs diffract X-rays according to the spatial atomic composition (X-ray diffraction (XRD)), we get crystallinity and phase composition of the material. The familiar equation from Bragg's Law:

$$n\lambda = 2d \sin \theta$$

n, λ, d, and θ stand for the diffraction order, X-ray wavelength, interplanar spacing, and diffraction angle, respectively, confirms the PAW between the periodicity of MOFs. Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) offer valuable information regarding the morphology and size distribution, which are critical factors for improving the energy storage performance of MOFs (Zhou et al., 2021).

Analysis of Functional Group and Surface Chemistry

By different vibrational modes, FTIR identifies functional groups in the MOFs and thus confirms metal-ligand interactions. MOF structures also have specific molecular vibrations which FTIR does not detect, however Raman spectroscopy does. Oxidation states and chemical bonding information are obligatory for elucidating charge transfer mechanisms as well as the overall energy storage processes, which can be obtained from X-ray photoelectron spectroscopy (XPS) data [6,7]. That is then used to find the oxidation state of our metal centers like so:

$$BE = h\nu - KE - \phi$$

where BE is the binding energy, hν is the photon energy, KE is the kinetic energy of emitted electrons, φ is the work function of the spectrometer (Chen et al., 2020).

4.3 Analysis of Surface Area and Porosity

Surface area was calculated using the Brunauer-Emmett-Teller (BET) method from gas adsorption isotherms. The BET equation:

$$\frac{P/P_0}{(1 - P/P_0)} = \frac{V_m C}{V_m + V(P/P_0 - 1)}$$

(Where V is the volume of gas adsorbed, P/P₀ is the relative pressure, V_m is the monolayer volume, and C is a BET constant) gives the quantitative analysis of surface area. The Barrett-Joyner-Halenda (BJH) method is applied to investigate pore size distribution and total pore volume, which are very significant for hydrogen fuel cell technology to construe better hydrogen absorption and hesitation performance (Li et al., 2019).

Discussion

This research opens a door for further investigation in using MOFs as next-generation materials for storing energy, for example within hydrogen fuel cells. Synthesis methods such as solvothermal, hydrothermal, and mechanochemical methods significantly affect the physicochemical properties of metal-organic frameworks (MOFs). Controlling crystallinity, porosity, and stability is critical and requires the optimization of various reaction conditions, including temperature, pH, solvent selection, and reaction time (Luo et al., 2022). Nucleation and crystal growth via coordination chemistry among metal ions and organic linkers ultimately set the structural structure and surface area of MOFs. These properties allow governing hydrogen adsorption capacity, providing MOFs as a candidate class of materials for hydrogen storage and delivery applications (Prajapati et al., 2023). The synthesized MOFs exhibited well-defined crystalline structures and porous architectures, and their characterization was performed by X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM) analysis. These materials have a high surface area and uniform pore distribution, which as determined by BET surface area measurements, correlates with the good hydrogen adsorption properties of MOFs. The successful coordination between metal centers and organic ligands was validated through Fourier-transform infrared

spectroscopy (FTIR) and Raman spectroscopy, confirming the structural robustness required for long-term energy storage applications (Li et al., 2020). The instability of MOFs under different working conditions, such as temperature and humidity, is a crucial factor in their eventual use in fuel cells.

The excellent electrochemical performance of MOFs in hydrogen fuel cell is mostly attributed to their surface chemistry and porosity. The oxidation state of the various metal centers, which was crucial in establishing its role in both catalytic activity and charge transfer mechanism, was confirmed from the X-ray photoelectron spectroscopy (XPS) results. MOFs also play a great role in fuel cell performance via their redox behavior that affects proton exchange efficiency and electron transport (Otun et al., 2022). Moreover, the Barrett-Joyner-Halenda (BJH) method showed that the distribution of pore size offered an ideal manner for hydrogen diffusion through pores and hence reduced resistance and improved the storage capability. These traits make MOFs promising candidates for electrode and catalyst support in hydrogen-based energy systems.

Nevertheless, there are still challenges in scaling up the synthesis of MOFs for the industry. However, the generalizability of the synthesis methods and the stability of MOFs over time in cohesion with real-world conditions needs further investigation. However, further studies need to establish the thermal and chemical stability of ZIF as well as functional modifications to improve the kinetics of H₂ uptake and release for practical applications. Further infused into other nano-phonic materials, including graphene or even metal nanostructures, could push the conductivity and the catalytic performance in fuel cells to a new height (Yang et al., 2023). Overcoming these issues will be pivotal in translating MOFs from the test tube to widespread deployment in sustainable energy technologies.

Limitations

While there have been many advances in synthesizing metal-organic frameworks (MOFs) at the laboratory scale, translating these methods to industrial manufacturing can be quite difficult, both in terms of cost and ease of adaptation. Moreover,

MOFs have been shown to be sensitive under variable environmental conditions, such as temperature and humidity, which can affect their performance in the long run. Moreover, these methods such as solve thermal and hydrothermal processes are energy-intensive and this also discourages their sustainable and economically reasonable for large-scale hydrogen storage applications.

Recommendations

Future studies must focus on developing cost-effective & scalable synthetic techniques (to improve production efficiency & environmental sustainability), such as mechano-chemical & green synthesis approaches (Lu et al., 2021). In situ functional modification of MOFs, including the addition of metal nanoparticles and hybrid composites, aims to improve the thermal and chemical stability of MOFs. Influences their application in fuel cell applications due to their stability, and extending the application of metals in fuel cells (Li et al., 2021). Moreover, the use of computational modeling and machine learning methods could expedite the identification of favorable MOF structures, as experimental studies need to be conducted to investigate the practical applications for hydrogen storage and fuel cell technologies (He et al., 2022).

Conclusion

Its high surface area, tunable porosity and chemical stability have a substantial potential as advanced materials in hydrogen fuel cell applications. The physicochemical properties of MOFs that predominantly influence the hydrogen storage ability can be directly attributed to its synthesis methods, as well as to the optimization of the reaction conditions. The synthesized MOFs were structurally and functionally characterized by various techniques, such as X-ray diffraction, BET surface area analysis, Fourier-transform infrared spectroscopy, and X-ray photoelectron spectroscopy. Despite this, hurdles such as scalability, stability, and hydrogen adsorption kinetics remain, but the development of MOFs for large-scale energy storage applications is made more feasible through continuing advances in synthesis methods and

material modifications. Data refers mostly to MOFs synthesized up to October 2023 so upscaling MOFs synthesis and stability, especially regarding their use in commercial systems of hydrogen fuel cells are the subjects of coercively future research.

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