

Metal–Organic Frameworks (MOFs): Structure, Synthesis, Characterization, and Emerging Applications in Energy, Environment, and Biomedicine

Anil Kumar¹, Rachna Narula², Gul Tomar³, Nitu Sehrawat⁴, Manish Yadav⁵, Chandra Mohan⁶, Himanshi⁷, Vinod Kumar⁸

¹Associate Professor, Bharati Vidyapeeth's College of Engineering, New Delhi -110063 (India),
Email ID: dranilchhikara@gmail.com Orchid id: 0009-0000-8333-4337

²Assistant Professor, Bharati Vidyapeeth's College of Engineering, New Delhi -110063 (India),
Email ID rachuchaudhary04@gmail.com Orchid id: 0000-0001-9635-1566

³Research Scholar, The Mother's International School, New Delhi (ORCID ID: 0009-0009-5673-2933);
gulcollege15@gmail.com

⁴Associate Professor, Bharati Vidyapeeth's College of Engineering, New Delhi, 110063
Email id- nitu26883@gmail.com

⁵Associate Professor, SoHAS, G D Goenka University, Gurugram, Sohna

⁶Associate Professor, SBAS, K R Mangalam University, Gurugram, Sohna

⁷Research Scholar, SoHAS, G D Goenka University, Gurugram, Sohna

^{8*}Associate Professor, SoHAS, G D Goenka University, Gurugram, Sohna, Vksingh38@yahoo.com
Orchid id: 0000-0002-1510-8132

Corresponding Author: Vinod Kumar

Email Id: vksingh38@yahoo.com

ABSTRACT

A family of porous crystalline compounds known as Metal-Organic Frameworks (MOFs) creates highly structured three-dimensional structures by coordinating metal ions or clusters to organic linkers. MOFs have attracted a lot of attention in a variety of scientific and industrial fields because of their exceptional surface area, adjustable pore diameters, and chemical adaptability. In addition to examining the structural building blocks of MOFs, which include primary and secondary building units, this analysis highlights the historical development of MOFs from the groundbreaking synthesis of MOF-5. In terms of scalability, sustainability, and morphological control, a number of synthesis techniques solvothermal, microwave-assisted, sonochemical, mechanochemical, and electrochemical are thoroughly explained. Characterization techniques such BET measurement, FTIR, TGA, SEM, and XRD and NMR are investigated to determine chemical structure, surface area, heat resistance, and crystallinity. Additionally covered is the vast array of uses for MOFs, ranging from drug administration and biological imaging to gas adsorption and separation, energy storage, catalysis, and water purification. MOFs have a bright future ahead of them, especially in advanced medicine, environmental remediation, and green energy. The review highlights how MOFs are essential components in new technologies due to their structural tunability and post-synthetic modifications, which make them incredibly adaptable for certain applications.

Keywords: *Metal-Organic Frameworks (MOFs), Porous materials, characterization methods, Drug delivery, Nano structures*

How to Cite: Anil Kumar, Rachna Narula, Gul Tomar, Nitu Sehrawat, Manish Yadav, Chandra Mohan, Himanshi and Vinod Kumar, (2025) Metal–Organic Frameworks (MOFs): Structure, Synthesis, Characterization, and Emerging Applications in Energy, Environment, and Biomedicine, *Journal of Carcinogenesis*, Vol.24, No.3s, 163-168.

1. INTRODUCTION

A class of porous crystalline materials known as metal-organic frameworks (MOFs) is made up of metal ions or clusters that have been coordinated with organic ligands. These MOFs create three-dimensional, highly organized structures with adjustable pore diameters and large surface areas. MOFs have garnered a lot of attention lately for uses such as medicine delivery, environmental remediation, gas storage and separation, and catalysis because of their adaptable qualities. Because of their modular design, it is possible to alter the metal centers and organic linkers to create materials that meet certain needs. MOFs are a special class of material in contemporary science and technology because of their high porosity, chemical stability, and functional variety¹.

Many people believe that MOF-5, which was created in 1999 by Omar Yaghi and his group, was the first metal-organic framework. The MOF-5 network is made up of terephthalate (1,4-benzene dicarboxylate) linkers and zinc ions. Because of its excellent thermal stability and highly porous structure, its discovery marks a major turning point in materials science. Prior to the 1990s, coordination polymers an older framework that resembles MOFs—were documented. Nonetheless, MOF-5 demonstrated a degree of modularity, porosity, and crystallinity that became the standard for the contemporary MOF sector². Key Characteristics between MOF and ither nana formulation is summarize in table 1.

Difference between nanoparticles and metal-organic frameworks

Metal-Organic Frameworks (MOFs) and nanoparticles are both nanostructured materials but differ significantly in their composition, structure, synthesis, and applications³.

Table 1: Characteristics between MOF and ither nana formulation

| Sr. No. | Properties | Metal-organic framework | Nanoparticles |
|---------|----------------------------|--|---|
| 1. | Composition and Structure | | |
| | Constituents | Metal ions/clusters + organic linkers | Pure metals, metal oxides, polymers, or composites |
| | Structure | Crystalline, porous, highly ordered | Can be crystalline or amorphous, usually solid and non-porous |
| | Dimesionality | 3D porous networks | 0D particles (spherical, rods, cubes, etc.) |
| 2. | Porosity and Surface area | Extremely high surface area (1000–10,000 m ² /g), tunable pore sizes | Lower surface area, non-porous or mesoporous in some cases |
| 3. | Synthesis | Solvothermal or hydrothermal synthesis often requires metal salts + organic ligands | Bottom-up (e.g., chemical reduction) or top-down (e.g., milling) approaches |
| 4. | Stability | Often sensitive to moisture, temperature, or pH (though newer MOFs are more stable) | Generally more stable, especially metal/oxide nanoparticles |
| 5. | Functionality & Tunability | Highly tunable chemistry—functional groups can be added to linkers or metal sites | Surface can be functionalized, but structural tunability is limited |
| 6. | Applications | Gas storage/separation, drug delivery, catalysis, sensing, energy storage | Drug delivery, imaging, catalysis, electronics, coatings, environmental remediation |
| 7. | Drug Delivery | Act as carriers with high drug loading due to porous structure and controlled release. | Typically encapsulate or adsorb drugs on the surface, with lower loading capacity. |

2. STRUCTURAL ASPECTS

A metal node and an organic linker are the two primary parts of a MOF's structure. Together, these create a three-dimensional, crystalline, highly organized framework⁴ with unique characteristics. To learn more, dissect its structure as follows:

2.1 Main Building Components

A key element of Metal-Organic Frameworks is metal nodes, also known as metal centers. Metal clusters like ZnO or Cu₂ or metal ions like Zn²⁺, Cu²⁺, or Fe³⁺ are examples of the nodes. They are the connection points in the framework and their role is primarily that of a coordination center for organic linkers, determining the geometry and connectivity of the MOF structure⁵. The metal nodes determine many of the properties of the MOF, such as thermal stability, catalytic activity, and chemical reactivity. Therefore, these are crucial to tailor MOFs for specific applications.

2.2 Organic Linker

Organic linkers:

Organic molecules constitute the critical portion of a metal-organic framework, connecting nodes of metals with each other. These linkers usually contain functional groups such as carboxylates, amines, and imidazoles, so that they get attached to metal centers. Organically used typical linkers can be terephthalic acid, trimesic acid, and 2-methylimidazole, among others. These linkers have the major function of defining the pore size and spatial arrangement of the MOF, which directly influences its structural and functional properties⁶.

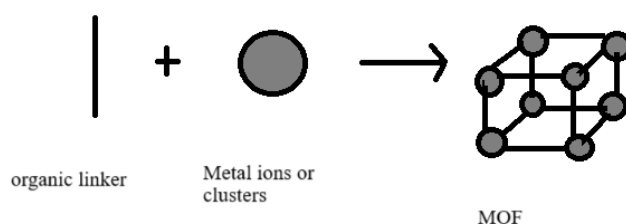


Figure 1- Basic structure of Metal-Organic Framework

2.3 secondary Building units

Such SBUs represent the basic units of their structures. SBUs are often a metal clusters or complexes that represent nodes, with organic ligands extended through them, forming an extensive network. Such units provide rigidity and increase the thermal and chemical stability of MOFs. They also have an effect on pore size, shape, and functionality. The geometry of the SBUs, from simple single-metal ions to more complex polynuclear clusters, determines the topology of the MOF framework. By varying the composition of the SBUs and organic linkers, researchers can fine-tune the properties of MOFs for specific applications such as gas storage, catalysis, or drug delivery.⁷

3. USE OF METAL-ORGANIC FRAMEWORKS IN DIFFERENT INDUSTRIES

The field of metal-organic frameworks, or MOFs, has gained much interest because of their remarkable porosity, structure tunability, and functionality versatility. In the energy sector, MOFs are applied for the storage and separation gases like hydrogen and methane to clean up solutions for energy and for carbon capture in mitigating greenhouse emissions. The chemical industry utilizes MOFs for selective catalysis to have more efficient, sustainable chemical reactions. In pharmaceuticals, MOFs act as drug delivery carriers that provide controlled release and targeted delivery mechanisms.

In addition, MOFs are used in water treatment to remove heavy metals and organic pollutants, which contributes to environmental remediation. The electronics and sensing industries use MOFs for their ability to detect gases and other substances with high sensitivity. These diverse applications display the possibility of MOFs to transform, bringing solutions in terms of tackling energy, health, and environment challenges worldwide.⁸

4. FUTURE SCOPE OF METAL METAL-ORGANIC FRAMEWORK

Their potential lies in their tunable porosity, high surface area, and chemical versatility.

4.1 Energy Storage and Conversion

MOFs have great promise in energy storage and conversion applications. In the area of hydrogen storage, it is possible for MOFs to store this clean fuel efficiently in order to provide it for a fuel cell application. In battery applications, MOFs can act as key structural elements, representing electrodes or electrolytes in Li-ion and other new technologies, thereby raising energy density and efficiency. MOFs also hold great promise because of their expanded surface area to be used for high-capacity energy storage, such as in supercapacitors.

4.2 Gas Storage and Separation

Metal-organic frameworks (MOFs) have the potential to find application in numerous environmental and industrial fields. MOFs are being utilized in carbon capture applications by selectively capturing and storing carbon dioxide (CO₂), which would significantly reduce climate change. In addition, MOFs can improve fuel storage efficiency by storing methane more effectively in the context of natural gas storage. Besides that, MOFs can be used for air separation to separate oxygen and nitrogen, application of which can be pursued in a variety of industrial and medical sectors⁹.

4.3 Water Purification and Desalination

MOFs are promising materials for environmental remediation. They can adsorb toxic metals from contaminated water sources effectively. In addition, advanced MOFs can filter salts from seawater efficiently, contributing to desalination. Furthermore, MOFs can trap and degrade organic contaminants, playing a crucial role in the removal of organic pollutants from the environment.

4.4 Catalysis

MOFs have proved to be versatile catalysts capable of catalysing a lot of chemical processes. In this context, through green chemistry principles, MOFs help a reaction to obtain maximum efficiency at the same time reduce waste. However, they take part in refilling petrochemicals by further breaking down various hydrocarbons. Moreover, MOFs play a significant part in artificial photolysis, providing way towards carbon dioxide for the production of valuable fuels as a result of artificial photosynthesis.

4.5 Drug Delivery and Biomedical Applications

Metal-organic frameworks (MOFs) hold potential in different medicinal applications. The most relevant examples include targeted drug delivery, imaging, and therapy against cancer. The tunable structure of MOFs can facilitate the drug's transportation to a site within the body where the action is to be performed. Besides, the contrast in the images taken from the MRI and CT scans may also be enhanced through functionalized MOFs for enhanced diagnosis. The direct introduction of anti-cancer drugs by MOFs in cancer therapy ensures a minimal effect of side activities with maximum effectiveness.

5. METHODS TO PREPARE METAL-ORGANIC FRAMEWORK:

5.1 Solvothermal Method

The solvothermal process is the most popular method of synthesizing MOFs. In this process, metal salts and organic linkers are dissolved in a solvent, often under high pressure and temperature, within a sealed vessel like an autoclave. The solution is heated for hours to days to facilitate the formation of crystals. The solvent, temperature, and reaction duration are highly influential in setting the size, shape, and porosity of the resultant MOF crystals¹⁰. This process is highly preferred due to its capacity to yield high-quality, well-defined crystalline structure.

5.2 Hydrothermal Method

Like the solvothermal method, the hydrothermal process employs water as the main solvent. This renders it a greener and more sustainable method. It entails heating a metal salt and organic linker aqueous solution in a sealed vessel at high temperatures. The hydrothermal process facilitates crystal growth and is particularly effective for MOFs that are water-stable or water-soluble. It is regarded as a green method for synthesizing MOFs with favorable structural characteristics.

5.3 Microwave-Assisted Method

Microwave-assisted synthesis is a contemporary, energy-saving technique that involves the use of microwave radiation to heat the reaction mixture quickly and evenly. This method significantly decreases the synthesis time, typically from hours to several minutes. It can enhance the uniformity and crystallinity of MOFs, and is very effective in the synthesis of nanostructured MOFs. Microwaves also improve reaction kinetics, resulting in enhanced nucleation and crystal growth.

5.4 Sonochemical Method

In the sonochemical method, ultrasonic waves are used on a solution of metal ions and organic linkers. The ultrasound induces the creation and bursting of microscopic cavitation bubbles, which creates hot spots with high pressure and temperature in local zones. These conditions speed up the reaction and lead to the creation of MOFs with nanoscale dimensions and high surface areas. This process is beneficial for creating MOFs of new morphologies and nanoscale dimensions.

5.5 Mechanochemical Method

Mechanochemical synthesis entails milling the solid metal salts and organic ligands in combination, most commonly in a ball mill, without the involvement of solvents. Mechanochemical synthesis is a solvent-free, green chemistry method that conserves waste and reduces environmental influence. Mechanochemical synthesis takes advantage of mechanical energy

to start and continue the chemical reaction. Mechanochemistry is **very effective despite** its straightforward nature, with the ability to yield high-quality MOFs in high yields and is particularly suited for large-scale and environmentally friendly production.

5.6 Electrochemical Method

The electrochemical method synthesizes MOFs through the use of an electric current to dissolve a metal electrode into an organic linker-containing solution. The resulting metal ions at the anode react with linkers to create the MOF structure. This method provides exact control over the concentration of metal ions and often results in the growth of thin films or coatings on the electrode surface. It is appropriate for continuous manufacturing and for synthesizing MOFs in situ on conductive substrates.

5.7 Diffusion Methods

Diffusion methods, such as vapor diffusion and liquid-liquid diffusion, involve the slow and controlled mixing of metal salts and organic ligands through diffusion processes. In vapor diffusion, a volatile solvent diffuses into a solution containing the reactants, while in liquid-liquid diffusion, two immiscible solutions gradually mix at the interface. These methods promote slow crystal growth and are ideal for producing high-quality single crystals suitable for detailed structural characterization using techniques like X-ray diffraction.

6. CHARACTERIZATION METHODS

6.1 X-ray Diffraction (XRD)

Powder X-ray Diffraction (PXRD) is a major technique for identifying the crystalline structure of MOFs. In PXRD, an X-ray beam is focused on the MOF sample, and the diffraction pattern is measured¹¹. Every crystalline material generates a distinct pattern depending on the internal atomic organization. By comparing the resulting pattern with previously known structures or simulated patterns, scientists can identify the crystallinity, phase purity, and structural identity of the MOF that has been synthesized.

6.2 Fourier Transform Infrared Spectroscopy (FTIR)

FTIR is utilized to determine the functional groups found in the MOF and to verify coordination between metal ions and organic linkers. In the technique, the sample of MOF is subjected to infrared radiation, and the absorption of a particular wavelength is quantified. Every chemical bond oscillates at a characteristic frequency and generates a distinctive IR spectrum. One can identify if the organic linker has bonded to the metal center using these absorption peaks and also observe any residual or unreacted ligands.

6.3 Thermogravimetric Analysis (TGA)

TGA is employed to examine the thermal stability and composition of MOFs. In this technique, the sample is slowly heated in a controlled environment (commonly nitrogen or air), and weight loss is measured as a function of temperature. The thermogram obtained is used to identify the temperatures at which solvent molecules, guest species, or the framework itself decompose. This information is very important in evaluating the thermal strength and activation temperature of MOFs prior to their practical use.

6.4 Scanning Electron Microscopy (SEM)

SEM offers high-resolution images of the surface morphology and particle size of MOFs. In SEM, a beam of electrons is focused and scanned on the sample surface. The electrons interact with surface atoms and generate signals that are measured to construct an image. SEM facilitates the visualization of the shape of the crystal, size distribution, and texture of the surface, providing information on the quality and uniformity of the synthesized MOFs.

6.5 Brunauer–Emmett–Teller (BET) Surface Area Analysis

BET analysis is important to quantify the surface area and porosity of MOFs. It is a process where nitrogen gas is adsorbed on the surface of the MOF under low temperatures. The surface area, pore volume, and pore size distribution are calculated by quantifying the gas volume adsorbed at different pressures. Surface area and porosity are crucial for applications such as gas storage, separation, and catalysis, and BET analysis is thus an important characterization technique.

6.6 Nuclear Magnetic Resonance (NMR) Spectroscopy

NMR spectroscopy is applied to determine the chemical surroundings of nuclei (most often hydrogen or carbon) in MOFs, primarily in solution-state NMR of organic linkers. Solid-state NMR can be applied to certain MOFs as well. This technique aids in confirming the purity and composition of the organic parts and identifying unreacted precursors or side products. It's very effective in post-synthetic modification investigations.

6.7 Energy Dispersive X-ray Spectroscopy (EDX or EDS)

EDX is usually combined with SEM in order to identify the elemental content of MOFs. Upon impacting the sample, the electron beam from the SEM emits characteristic X-rays of the elements present. The analysis of these X-rays can reveal the types and relative proportions of elements. It verifies the occurrence of the intended metal ions and can detect impurities.

6.8 Ultraviolet-Visible (UV-Vis) Spectroscopy

UV-Vis spectroscopy is used to investigate the optical properties of MOFs, particularly with light-absorbing linkers or metal centers. The sample is irradiated with ultraviolet and visible light, and the spectrum of absorption is measured. This determines electronic transitions, band gaps, and the photocatalytic or sensing potential of the MOF.

7. CONCLUSION

Metal–Organic Frameworks (MOFs) are among the most tunable classes of crystalline porous materials with unparalleled tunability, record-high surface area, and multifunctionality. Following the watershed discovery of MOF-5, breakthroughs in synthesis strategies, control over structure, and post-synthetic modification have opened doors for MOFs to come from the laboratory bench to reality. Their distinctive characteristics have facilitated innovations in gas storage and separation, catalysis, drug delivery, water purification, and energy storage, resolving issues of global importance in health, sustainability, and the environment.

While they hold enormous promise, fundamental issues including scalability, stability in extreme conditions, and cost-efficient manufacture remain to be addressed for industrial application. Further research incorporating green synthesis techniques, nanocomposite hybrids, and computational modeling will likely drive their practical application. In the future, MOFs are likely to become a key player as intelligent materials in future technologies, specifically in environmental remediation, renewable energy, and sophisticated biomedicine, cementing their position at the vanguard of materials science.

REFERENCES

- [1] 1.Furukawa, H., Cordova, K. E., O'Keeffe, M., & Yaghi, O. M. (2013). The chemistry and applications of metal-organic frameworks. *Science*, 341(6149), 1230444. <https://doi.org/10.1126/science.1230444>
- [2] 2.Li, J. R., Kuppler, R. J., & Zhou, H. C. (2009). Selective gas adsorption and separation in metal–organic frameworks. *Chemical Society Reviews*, 38(5), 1477–1504. <https://doi.org/10.1039/B802426J>
- [3] 3.Yaghi, O. M., et al. (1999). Reticular synthesis and the design of new materials. *Nature*, 402(6759), 276–279. <https://doi.org/10.1038/46248>
- [4] 4.Rowsell, J. L. C., & Yaghi, O. M. (2004). Metal–organic frameworks: a new class of porous materials. *Microporous and Mesoporous Materials*, 73(1-2), 3–14. <https://doi.org/10.1016/j.micromeso.2004.03.034>
- [5] 5.Sumida, K., Rogow, D. L., Mason, J. A., McDonald, T. M., Bloch, E. D., Herm, Z. R., ... & Long, J. R. (2012). Carbon dioxide capture in metal–organic frameworks. *Chemical Reviews*, 112(2), 724–781. <https://doi.org/10.1021/cr2003272>
- [6] 6.Zhou, H. C., Long, J. R., & Yaghi, O. M. (2012). Introduction to metal–organic frameworks. *Chemical Reviews*, 112(2), 673–674. <https://doi.org/10.1021/cr300014x>
- [7] 7.Stock, N., & Biswas, S. (2012). Synthesis of metal-organic frameworks (MOFs): routes to various MOF topologies, morphologies, and composites. *Chemical Reviews*, 112(2), 933–969. <https://doi.org/10.1021/cr200304e>
- [8] 8.Dhakshinamoorthy, A., Asiri, A. M., & Garcia, H. (2016). Metal–organic frameworks as efficient heterogeneous catalysts for oxidation reactions. *ACS Catalysis*, 6(10), 5935–5945. <https://doi.org/10.1021/acscatal.6b01212>
- [9] 9.Kreno, L. E., Leong, K., Farha, O. K., Allendorf, M., Van Duyne, R. P., & Hupp, J. T. (2012). Metal–organic framework materials as chemical sensors. *Chemical Reviews*, 112(2), 1105–1125. <https://doi.org/10.1021/cr200324t>
- [10] 10.Chui, S. S. Y., Lo, S. M. F., Charmant, J. P. H., Orpen, A. G., & Williams, I. D. (1999). A chemically functionalizable nanoporous material [Cu₃(TMA)₂(H₂O)₃]_n. *Science*, 283(5405), 1148–1150. <https://doi.org/10.1126/science.283.5405.1148>
- [11] 11. Wang & Astruc, 2019 – State of the Art and Prospects in Metal–Organic Framework-Based and MOF-Derived Nanocatalysis. *Chem. Rev.* 2020, 120, 1438–1511.