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Journal of Engineering Science and Technology Management

| ISSN (Online) 2828 -7886 |



Article

Advancements in Metal Organic Frameworks for Energy Storage Applications: A Review of Current Research and Future Directions

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DOI: 10.31004/jestm.v6i3.291

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ARTICLE INFORMATION

Volume 6 Issue 3

Received: 03 October 2025

Accepted: 20 March 2026

Publish Online: 23 October 2026

Online: at <https://JESTM.org>

Keywords

Absorption,
Carbon Dioxide,
Jet Bubble Column,
Kinetics,
Potassium Carbonate

ABSTRACT

Growing energy demand and environmental pressures require storage materials that combine reversible capacity, efficient transport, and durability. Metal-organic frameworks (MOFs) offer tunable metal nodes, organic linkers, and pore structures, enabling their use as active frameworks, composite components, and precursors to derived materials. This review examines their application in lithium-ion, sodium-ion, lithium-sulfur, and zinc batteries, supercapacitors, and hydrogen storage, together with computational and artificial intelligence approaches to material design. Representative results include 2305 mAh g⁻¹ after 500 cycles at 0.1 A g⁻¹ for a MOF-derived lithium-storage electrode and 97.9% capacity retention after 1000 cycles at 1 A g⁻¹ for a SnPS3@C sodium-storage electrode. These benchmarks arise from different chemistries and test conditions and do not establish a universal performance ranking. The review relates reported improvements to conductive networks, accessible reaction sites, and accommodation of structural change, while examining low conductivity, instability, and limitations in performance normalization. Hydrogen adsorption is assessed by distinguishing material uptake from complete-system storage requirements. Computational screening is considered alongside synthetic accessibility, model uncertainty, and experimental validation. Future research should prioritize application-specific hybrid architectures, matched-condition comparisons, scalable preparation, and device-level assessment to establish which MOF design principles remain effective beyond laboratory demonstrations

1. Introduction

Increasing energy demand and variable renewable generation require reliable storage. Metal–organic frameworks (MOFs) provide tunable chemistry and porosity for addressing transport and storage limitations (H. Zhang et al., 2017; Liang et al., 2018). This review connects their structure and synthesis with application-specific performance and practical constraints.

1.1 Scope and Objectives of the Review

This narrative review covers MOFs and their derivatives in lithium-ion, sodium-ion, lithium–sulfur, and zinc batteries, supercapacitors, and hydrogen storage, including computational and AI-assisted design. It provides a qualitative synthesis rather than exhaustive coverage or statistical pooling.

The contribution is a cross-application analysis of framework chemistry, conductive integration, and structural accommodation. Pristine MOFs, composites, and derived phases are distinguished because their operating structures and failure mechanisms differ. Performance is interpreted with test conditions and normalization, linking computational predictions to experimental feasibility without implying direct comparability across chemistries.

2 Literature Review

2.1 Framework Structure and Tunable Properties

MOFs are crystalline coordination networks assembled from inorganic metal ions or clusters and organic linkers (Cai et al., 2021; Figure 1a). Their topological diversity, accessible porosity, and tunable components enable control of adsorption and

electrochemical behavior (Sandhu et al., 2024; Figure 1b). High electronic conductivity, however, is not an inherent property of all MOFs.

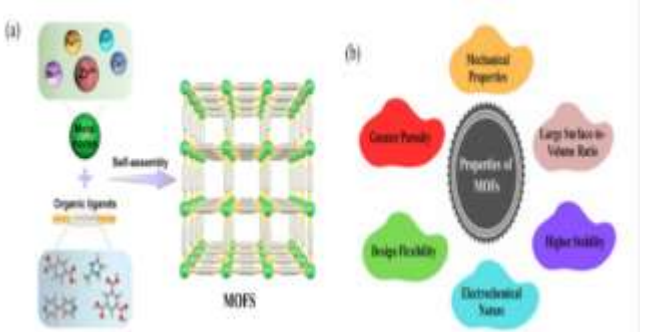


Figure 1: (a)Schematic Illustration of Self-Assembly of MOFs (W. Wang, Chen, et al., 2024) (b) Distinguishing properties of MOFs (Sandhu et al., 2024)

Building-block selection enables control of pore dimensions, functional groups, and redox-active sites. This modularity connects metal and ligand chemistry to storage requirements, while conductive guests or supports can improve electronic access (L. Kong et al., 2020; Saha & Gómez García, 2024). Framework design must therefore balance accessible sites with conductivity and stability.

2.2 Synthesis Strategies

Solvothermal/hydrothermal, microwave-assisted, electrochemical, and mechanochemical routes offer different trade-offs in crystal quality, reaction time, solvent demand, and scalability (Table 1). Temperature, metal source, linker, concentration, and pH control morphology and porosity (H. Lin et al., 2022). High-quality crystal growth does not necessarily translate into efficient electrode manufacture.

Table 1: Comparison of MOF Synthesis Methods

Synthesis Method	Key Characteristics	Advantages	Limitations	Ref
Solvothermal/ Hydrothermal	Electrical heating in sealed vessels (60-300°C, high pressure); long reaction times (hours to days)	Produces high-quality single crystals for structural analysis; stable for carboxylate linkers	Small scale; long reaction times; low space-time yields; challenges for industrial scale-up; often uses expensive organic solvents	(Banerjee et al., 2008; McKinstry et al., 2016)

Microwave-Irradiation	Rapid, uniform heating via microwave irradiation; short reaction times (minutes to hours)	Fast crystallization and nucleation; phase selectivity; narrow particle size distribution; facile morphology control; improved MOF properties (stability, conductivity, porosity); reduced/avoided toxic solvents	Potential for reduced crystal quality if conditions are not optimal (Cho et al., 2012)
Electrochemical	Anodic dissolution of bulk metal plates to supply metal ions; ambient conditions	Simple, easy, and faster synthesis; eliminates metal salts; high linker utilization (Faraday efficiencies); continuous process potential	Rarely reported method for synthesis of MOFs. (Lalawmpuia et al., 2024; Martinez Joaristi et al., 2012)
Mechanochemical	Grinding/milling (ball milling) with little/no solvent; room temperature	"Green" (solvent-free); quantitative yields; short reaction times (10-60 min); uses metal oxides (water as byproduct); can accelerate reactions (LAG/ILAG)	Limited understanding of mechanisms; difficult to obtain large product quantities; limited to specific MOF types (Klimakow et al., 2010)

2.3 Importance of MOFs in Energy Storage

MOFs provide active frameworks, composite components, and precursors to porous derivatives for storage and conversion (H. B. Wu & Lou, 2017). Their value depends on how structure resolves the transport and stability limitations of each application.

Porosity can expose reaction sites and facilitate electrolyte transport, but performance also requires connected pores, electrolyte compatibility, and electronic access. Surface area alone does not establish energy density or cycle life (L. Kong et al., 2020). Gas storage likewise depends on pressure, temperature, and usable capacity rather than maximum uptake alone (Shanmugam et al., 2023).

Composites and converted phases address the low conductivity and limited structural persistence of many pristine MOFs (Sandhu et al., 2024). Benefits must be assigned to the operating phase and conductive additives. Environmental advantages require evidence on synthesis, activation, resource use, and service life rather than inference from porosity.

3. Research Methodology

3.1 Review Design and Scope

A narrative review qualitatively synthesizes selected literature on pristine MOFs, composites, and derived materials across the applications defined in Section 1.1. Computational design is considered alongside experimental implementation; no quantitative meta-analysis is performed.

3.2 Basis of Comparison

Studies are organized by application and material function, comparing composition, preparation, structure, mechanism, and performance. Battery results are interpreted with current, cycling, and voltage; supercapacitor capacitance and charge measures are distinguished; hydrogen uptake is assessed with pressure, temperature, and system boundaries.

3.3 Analytical Approach and Limitations

The analysis relates outcomes to electronic connectivity, ion accessibility, structural accommodation, and interfacial stability. Different configurations and normalization bases restrict cross-study rankings. No reproducible database-search protocol, formal screening, or risk-of-bias assessment is reported, limiting claims of exhaustive coverage and practical transferability.

4. Results and Discussion

4.1 MOFs for Battery Applications

MOFs function as active electrodes, porous precursors, and electrolyte or separator components. Their porosity and chemical tunability can improve transport and reaction-site access, provided the operating structure remains conductive and stable (Sandhu et al., 2024).

4.1.1 MOFs in Lithium-Ion Batteries

Lithium-ion batteries operate through ion transfer between separated electrodes; voltage reflects their electrochemical-potential difference, while usable energy depends on capacity and complete-cell mass (Figures 2a,b). This distinction underlies evaluation of MOF-based active phases and derived electrodes.

MOF pores can improve electrolyte access and accommodate reaction-associated expansion, but electronic connectivity and structural persistence remain necessary (Dubal et al., 2019). Thermal conversion produces distinct inorganic/carbon phases, so improvements should be assigned to the operating material rather than automatically to the precursor.

Fang et al. (2016) obtained binder-free Co_3O_4 nanosheets on 3D nickel foam, reporting cycling to 2000 cycles and high-rate operation at 25 A g^{-1} . Porous sheets shorten transport distances and buffer expansion, while the foam maintains electrical contact. Co_3O_4 hollow spheres also reached 7000 cycles at 5 A g^{-1} , although with low capacity (J.-K. Sun & Xu, 2014), showing why cycle count alone cannot establish electrode quality.

Hollow carbon shells protected CoSe nanoparticles and provided transport pathways, supporting 91.6% capacity retention (H. Hu et al., 2016). Redox-active frameworks offer another route: $\text{Cu}(2,7\text{-AQDC})$, with active metal nodes and anthraquinone ligands, delivered an initial 147 mAh g^{-1} and approximately 105 mAh g^{-1} after 50 cycles (Z. Zhang et al., 2014; Figures 2c–f). Ligand activity therefore expands storage opportunities but does not eliminate fading.

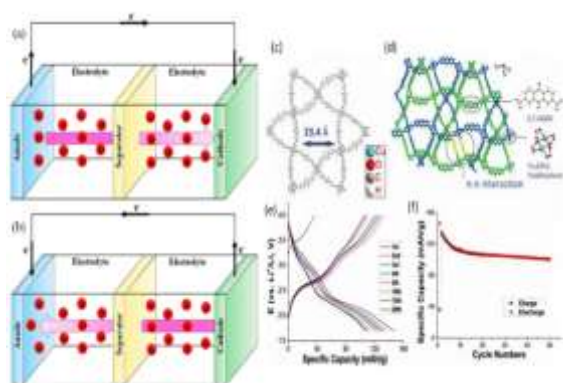


Figure 2:(a) The general mechanism of lithium-ion batteries for discharging and (b) charging processes (Luo et al., 2022). (c) The single Kagome layer of $\text{Cu}(2,7\text{-AQDC})$ in a battery. (d) The indication picture of the glided adjacent layers. (e) Charge–discharge profiles of the 10 wt% MOF battery. (f) Cycle performances of the battery for 50 cycles (Z. Zhang et al., 2014)

The binder-free CNWs/CZCOZ/CF architecture combines MOF-derived Cu-Zn-Co oxides with copper nanowires and foam. It delivered 2305 mAh g^{-1} after 500 cycles at 0.1 A g^{-1} and recovered much of its low-rate capacity following operation at 10 A g^{-1} (X. Lin et al., 2020; Figures 3a,b). Conductive scaffolding and internal pores support transport and accommodate expansion. The proposed electron-sharing mechanism is illustrated in Figure 3c.

A related C/N-containing $\text{Cu}_{0.39}\text{Zn}_{0.14}\text{Co}_{2.47}\text{O}_4\text{-CuO/CNT}$ electrode on copper foam delivered 1282 mAh g^{-1} over 1000 cycles at 5 A g^{-1} (J. Lin et al., 2019). Figures 3d,e show elemental distribution and the proposed interfacial storage mechanism. Its performance cannot be ranked directly against CNWs/CZCOZ/CF because the currents differ. Both designs illustrate conductive integration and strain accommodation, but fragmentation, contact loss, and repeated interphase formation require post-cycling verification. Practical assessment also requires areal loading, support-mass normalization, and lithium-limited full cells.

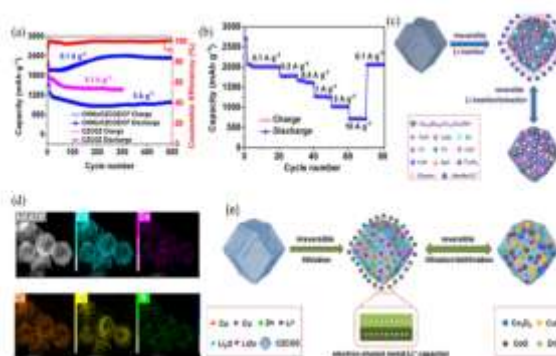


Figure 3 a-c Key characteristics of CNWs/CZCOZ/CF: (a) Cycling stability and coulombic performance efficiency, (b) rate capability at different current densities, and (c) schematic representation of the "electron sharing" model for charge/discharge operations (X. Lin et al., 2020) (d) (d) EDS elemental pictures, (e) synergistic effect of CZCOC@CNTs/CF during the lithiation/delithiation process (J. Lin et al., 2019).

4.1.2 MOFs in Sodium-Ion Batteries

Sodium-ion batteries motivate architectures that accommodate insertion and conversion-related

expansion. Dong et al. (2017) used ZIF-8 templating, sulfurization, cation exchange, and a resorcinol–formaldehyde-derived carbon layer to produce $\text{ZnS-Sb}_2\text{S}_3@\text{C}$ core–double-shell polyhedra (Figure 4a). The ZnS core, Sb_2S_3 shell, and protective carbon exterior combine structural accommodation with electrical connectivity (Figure 4b), supporting the cycling and rate behavior in Figures 4c,d.

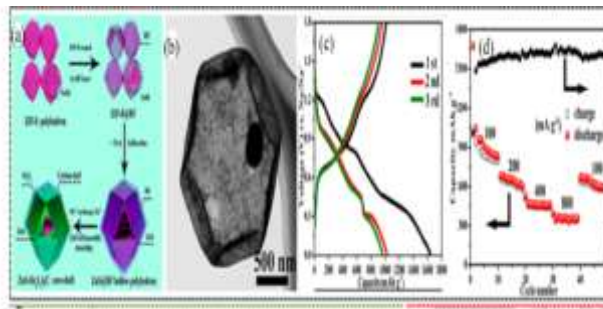


Figure 4. a) Synthesis of $\text{ZnS-Sb}_2\text{S}_3@\text{C}$ Core-Double Shell Polyhedron Composites. b) TEM of core double shell c,d) charge/discharge curve and rate capabilities at a current density of 100 mA/g¹ (Dong et al., 2017)

Yue et al. (2024) phosphor-sulfurized coated tin-MOF cubes to form porous $\text{SnPS}_3@\text{C}$ (Figure 5a). Internal voids accommodate conversion–alloying strain, while carbon improves electrical access and limits polarization. Structural characterization and electrochemical profiles support the proposed storage mechanism

(Figures 5b–d). Reported capacities were 1342.4 mAh g^{−1} at 0.1 A g^{−1} and 731.1 mAh g^{−1} at 4 A g^{−1}, with 97.9% retention after 1000 cycles at 1 A g^{−1}. These rate and retention results describe separate tests; the low-rate capacity is not the capacity necessarily maintained during long-term cycling.

L. Wang et al. (2022) converted nickelic MOFs into carbon-encapsulated yolk–shell $\text{Ni}_2\text{P/C}$, NiS_2/C , and NiSe_2/C through phosphorization, sulfuration, or selenation (Figures 5i–l). $\text{Ni}_2\text{P/C}$ showed lower polarization and faster kinetics, with an initial discharge/charge pair of 3222.1/1979.3 mAh g^{−1} and 765.4 mAh g^{−1} after 110 cycles at 0.1 A g^{−1}, compared with 706.4 and 735.8 mAh g^{−1} for the sulfide and selenide (Figures 5m–p). The initial mismatch indicates substantial irreversible storage. Together, these studies link phase chemistry, void space, and carbon connectivity to performance; matched loading, voltage, and full-cell sodium inventory remain necessary for comparison.

4.1.3 MOFs in Lithium-Sulfur Batteries

Lithium–sulfur batteries face low sulfur-phase conductivity, volume changes, and soluble-polysulfide shuttling. MOF hosts combine physical confinement with polar metal/ligand interactions, while conductive integration permits retained intermediates to remain electrochemically accessible (Z. Zhao et al., 2014). Effective design must balance adsorption, transport, and conversion rather than maximize binding alone.

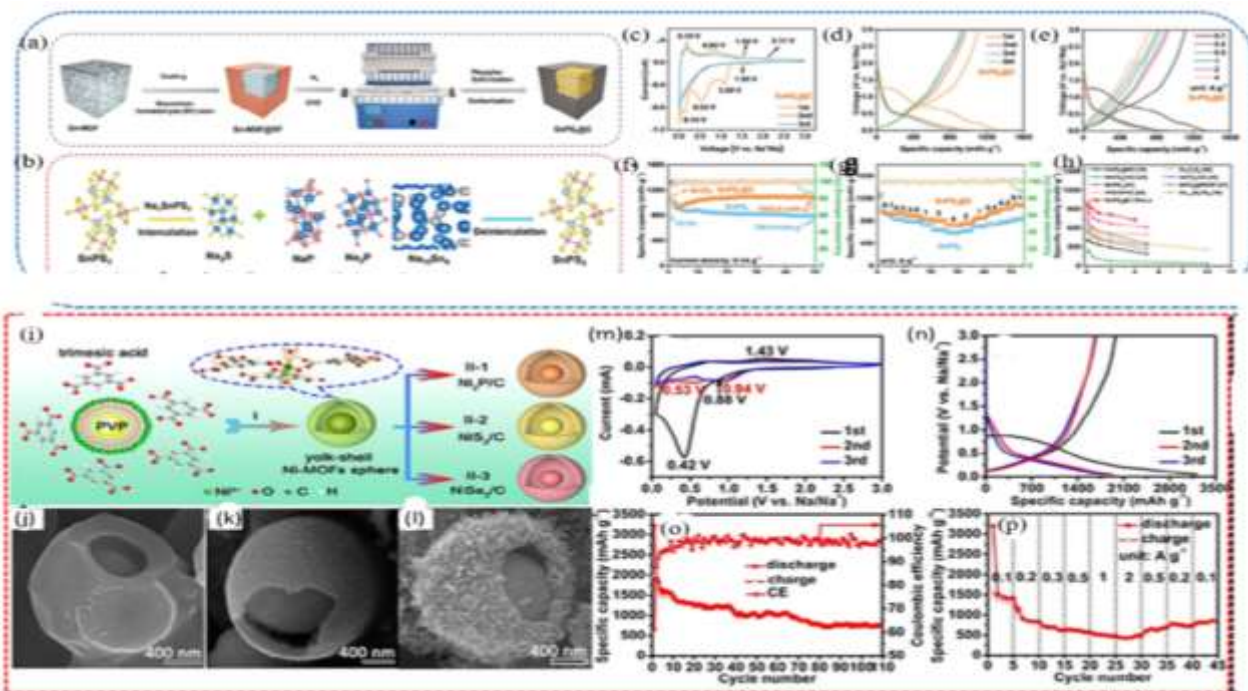


Figure 5: a) Design of Porus core shell structure of SnPS₃@C b) Sodium storage mechanism in the SnPS₃@C electrode. Initial CV curves for SnPS₃@C electrode. GCD curves for SnPS₃@C electrodes at 0.1 A g⁻¹ current density and varied current densities. f) Cycling performance of SnPS₃ and SnPS₃@C electrodes at 0.1 A/g. g) SnPS₃ and SnPS₃@C electrode performance. h) Comparison of SnPS₃@C electrode rate performance with MTP-based SIB anodes (Yue et al., 2024) i) Schematic depicting the manufacture of carbon-encapsulated yolk-shell nickelic spheres: (I) hydrothermal method, (II-1) phosphorization, (II-2) sulfuration, and (II-3) selenation reaction. j-l) SEM pictures of Ni₂P/C, NiS₂/C, and NiSe₂/C. m) The first three CV curves at 0.1 mVs⁻¹. n) The corresponding cycle curves. o) Cycle performance at 0.1 Ag⁻¹. p) Rate capabilities with varied current densities of 0.1-2 Ag⁻¹ (L. Wang et al., 2022).

MIL-47-derived V₂O₃@C hollow microcuboids combine transport channels, carbon confinement, and chemical adsorption to limit polysulfide loss (Yang et al., 2020; Figures 6a,b). DFT also predicts favorable polysulfide interactions in porphyrin-like V-MOFs (D. Chen et al., 2022), although adsorption predictions alone do not demonstrate device performance. MnNi-MIL-100@S retained approximately 708.8 mAh g⁻¹ after 200 cycles (W. Li et al., 2021; Figures 6c,d), illustrating the potential of bimetallic host chemistry. Smaller Cu-MOF particles improved utilization where limited

conductivity restricted reactions to accessible surfaces (Hong et al., 2018). Table 2 compares reported Li-S results, which depend on sulfur fraction, current, cycle count, and voltage. Excessive binding can impede conversion; sulfur-normalized capacity does not establish device energy density without areal loading, electrolyte-to-sulfur ratio, and lithium inventory. Adsorption evidence must also be distinguished from catalytic conversion.

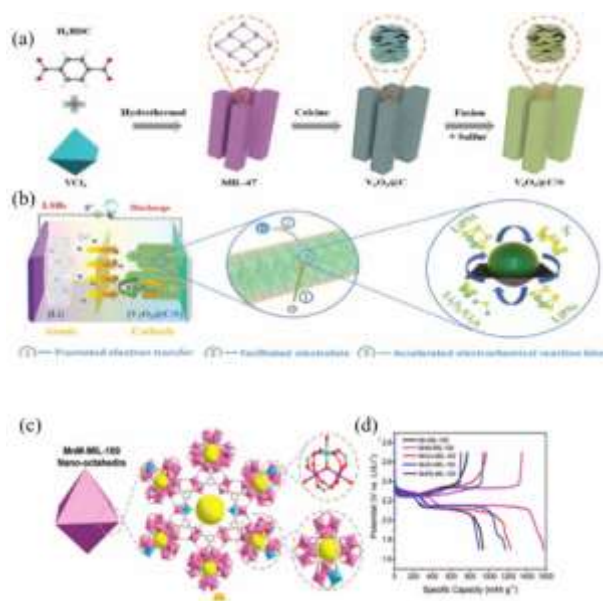


Figure 6: (a) Three main properties of the $V_2O_3@C/S$ electrode material; (b) fabrication process of the $V_2O_3@C/S$ (Yang et al., 2020). (c) Preparation of $MnM-MIL-100$ and (d) GCD profiles at a current density of 0.1C. (W. Li et al., 2021).

Table 2: Performance Metrics of Selected MOF-Based Materials in Lithium-Sulfur Batteries

MOF Used	S Loading (wt%)	Current Density (C)	Cycle Number	Voltage vs. Li/Li ⁺ (V)	Specific Capacity (mAh g ⁻¹)	Reference
ZIF-8	54	0.2	1000	1.4–3.0	≈170	Bai et al. (2016)
MIL-100(Cr)	48	0.1	60	1.0–3.0	≈410	Demir-Cakan et al. (2011)
ZIF-8	30	0.1	100	1.0–3.0	≈510	Z. Wang et al. (2014)
ZIF-8	50	0.5	300	1.8–2.8	553	Zhou et al. (2014)
HKUST-1	50	0.5	300	1.8–2.8	286	Zhou et al. (2014)
NH ₂ -MIL-53	50	0.5	300	1.8–2.8	332	Zhou et al. (2014)
MIL-53	50	0.5	300	1.8–2.8	347	Zhou et al. (2014)
MIL-101(Cr)	50	0.2	50	1.5–3.0	650	Bao et al. (2014)
Ni ₆ (BTB) ₄ (BP) ₃	60	0.1	100	1.5–3.0	611	Park et al. (2016)
MIL-101(Cr)	58.8	0.8	134	1.0–3.0	809	Z. Zhao et al. (2014)
MOF-525	50	0.5	200	1.5–3.0	700	Zhou et al. (2015)

4.1.4 MOFs in Zinc Batteries

Zinc offers a redox potential of -0.763 V versus SHE and theoretical capacities of 819 mAh g⁻¹ and 5854 mAh cm⁻³, motivating aqueous zinc-ion and zinc-air systems (Bhambri & Mandal, 2023). Their requirements differ: zinc-ion cells depend on reversible cathode storage, whereas zinc-air cells require durable oxygen electrocatalysis. Neither system avoids zinc-anode instability merely by selecting a high-capacity cathode.

Aqueous Zn-salt electrolytes provide ion transport but also govern electrode stability (Wei et al., 2024). Zinc-air systems face zinc-anode instability and limited durable bifunctional air-

cathode sites (X. Hu et al., 2018). Figures 7a,b distinguish the zinc-air architecture from aqueous zinc-ion operation; theoretical energy estimates should not be equated with measured rechargeable-device performance.

MOF metal sites and derived phases can promote oxygen reduction and evolution, while coordinated ligands and porous supports influence accessibility and intermediate stabilization (S. Li et al., 2021). These catalytic functions must be evaluated separately from Zn-ion storage and from corrosion or plating instability at the zinc anode.

The V-MOF-48@CNTF example illustrates morphology and electrode integration in a fiber-shaped zinc-ion device (He et al., 2019). Growth-dependent

structure, SEM morphology, and comparison of synthesis durations appear in Figures 7c–e. The Zn/PVA/CNTF assembly and current-dependent charge–discharge and capacity results (Figures 7f–h) connect hierarchical porosity with device architecture. These observations support evaluation of transport and rate response without independently identifying the degradation mechanism.

Table 3 summarizes zinc-ion metrics. Capacity and reversibility must be assessed with dissolution, electrolyte reactions, material identity, and normalization. Oxygen-catalyst improvements cannot establish enhanced Zn-ion insertion or resolution of zinc-anode failure, and unmatched test conditions preclude a universal ranking.

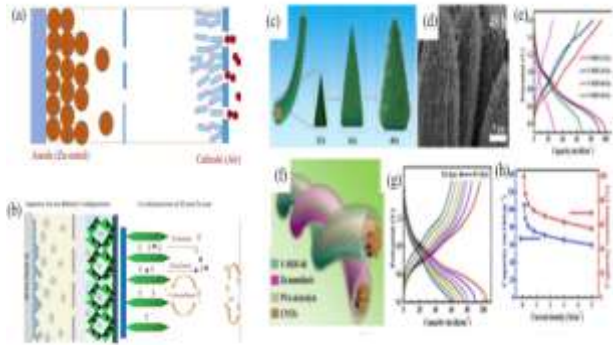


Figure 7: (a) Zn-air battery schematic representation (b) Mechanism of aqueous Zinc-ion battery (Y. A. Kumar et al., 2024). (c) A diagram of the process for producing the Vanadium-MOF@CNTF, which has a nanowire structure. (d) SEM picture of vanadium-MOF 48. (e) V-MOF-60//Zn, V-MOF-48//Zn, V-MOF-24//Zn, and V-MOF-12//Zn galvanostatic charge-discharge curves measured at 0.1A/cm. (f) Illustration of the all-solid-state fiber-shaped V-MOF-48/Zn battery. (g) The galvanostatic charge-discharge curves, and (h) fiber-shaped V-MOF-48//Zn battery specific capacities determined at various current densities (He et al., 2019).

Table 3: Performance Metrics of Selected MOF-Based Materials in Zinc-Ion Batteries

Electrode	Capacity (mAh g ⁻¹)	Cycling stability	Current density (A g ⁻¹)	Voltage window (V)	Reference
Mn-H ₃ BTC-MOF-4	138	93.5% after 1,000 cycles at 3 A g ⁻¹	0.1	1.0–1.9	Yin et al. (2021)
Mn ₃ O ₄ @C	331.5	141% after 1,900 cycles at 3 A g ⁻¹	0.2	0.8–1.8	Alzard et al. (2024)
CoMn-PBA HSs	128.6	75.4% after 1,000 cycles at 1 A g ⁻¹	0.05	0.4–1.8	Raja et al. (2022)
MnO _x @N-C	203	105% after 1,600 cycles at 2 A g ⁻¹	0.1	0.8–1.8	Fu et al. (2018)
Cu ₃ (HHTP) ₂	228	75% after 500 cycles at 4 A g ⁻¹	0.05	0.5–1.3	Nam et al. (2019)
VHCF	176	92.9% after 1,000 cycles at 5 A g ⁻¹	0.2	0.2–2.0	S. Zhang et al. (2022)
Mn ₂ O ₃ /Al ₂ O ₃	90	57.1% after 1,100 cycles at 1.5 A g ⁻¹	0.3	1.0–1.8	Gou et al. (2020)
Mn-Co-O@C	306	94.7% after 2,000 cycles at 2 A g ⁻¹	0.5	0.8–1.9	Dhilip et al. (2022)
CoFe(CN) ₆	173.4	100% after 2,200 cycles at 3 A g ⁻¹	0.3	0.7–2.0	L. Ma et al. (2019)
KMHCF	123.8	90% after 500 cycles at 0.25 A g ⁻¹	0.05	1.0–2.0	Ni et al. (2022)

4.2 MOFs for Supercapacitor Applications

Supercapacitors provide rapid charge–discharge and high power through electric-double-layer storage, pseudocapacitive redox, or battery-type reactions (Figure 8). These mechanisms require different interpretations of capacitance and capacity. MOF porosity and redox-active sites can improve electrolyte access, but low conductivity and coordination instability limit utilization. Conductive frameworks, carbon-supported

composites, and derived inorganic phases address these limitations through distinct mechanisms (Augustyn et al., 2014; Qiu et al., 2020; Sanati et al., 2021).

Conductive integration and structural support explain the representative architectures in Figure 9. NiCo-LDH@C uses a MOF-derived carbon scaffold; ultrathin NiCo-MOF nanobelts shorten transport distances; and Fe-MOF-derived Ni–Fe–OH@PCNFs combine accessible hydroxide sites with a conductive network (J. Yuan et al., 2023; Panda et al., 2023;

Acharya et al., 2023). The latter delivers 1528 F g⁻¹ at 1 A g⁻¹ with 86.7% retention after 10,000 cycles. These are separate performance conditions and should not be merged into an unsupported claim about retained low-rate capacitance.

The (CuCo)Se/NC and NiFe2O4-QD/Ni-MOF examples further combine active phases with conductive or dispersing supports (P. Sun et al., 2021; Xu et al., 2023). Graphene, polyaniline, and intrinsically conductive MOFs offer complementary routes to electrical connectivity (Rahmanifar et al., 2018; Srinivasan et al., 2020; Sheberla et al., 2017; Figure 10). Their benefit must be balanced against pore blockage, inactive mass, restacking, and polymer swelling.

Table 4 preserves the reported material comparisons. Values in F g⁻¹, C g⁻¹, and areal units are not interchangeable: charge in C g⁻¹ converts to mAh g⁻¹ by division by 3.6, whereas conversion to average capacitance requires a specified voltage interval. Single-electrode measurements also differ from two-electrode device results. Loading, electrolyte, voltage window, and mass normalization must therefore accompany claims of superior performance.

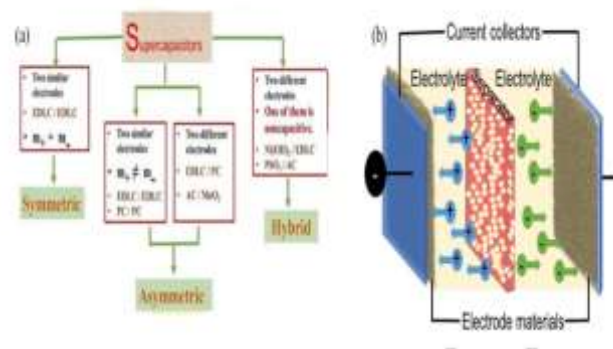


Table 4: Performance Metrics of Selected MOF-Based Supercapacitors

Electrode	Morphology	Electrolyte	Potential window (V)	Cs	Cyclic stability	Method of Synthesis	Ref.
Ni-MOFs	Hollow nanosphere	3 M KOH	0–0.45	473 @ 0.5 A/g	94 % 3000	Solvothermal	(M.-K. Wu et al., 2018)
(CuCo)Se/NC	Polyhedral	2 M KOH	0–0.4	121.4C/g @ 1 A/g	130 % 1200	Selenization	(P. Sun et al., 2021)
ZnMn2O4/C	Nanorods	1 M Na2SO4	0–1.2	589 @ 1 A/g	98 % 2000	Facile	(Zhu et al., 2018)

Figure 8 Supercapacitor electrode assembly and component configurations (Attia et al., 2022; Sanati et al., 2021).

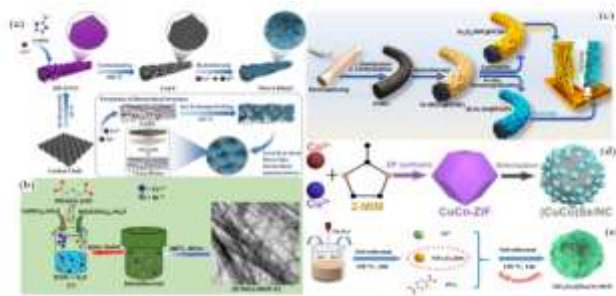


Figure 9 Preparation of (a) NiCo-LDH@C, (b) NiCo-MOF nanobelts, (c) Ni–Fe–OH@PCNFs, (d) (CuCo)Se/NC, and (e) NiFe2O4-QDs/Ni-MOF composites (J. Yuan et al., 2023; Panda et al., 2023; Acharya et al., 2023; P. Sun et al., 2021; Xu et al., 2023).

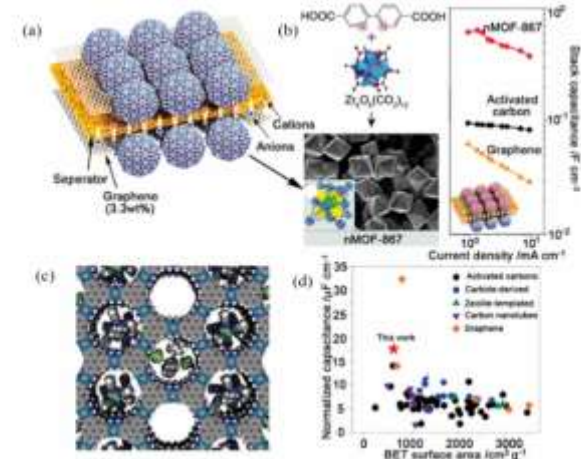


Figure 10 MOF supercapacitor architectures, nanocrystal topology, and comparative capacitive behavior (Choi et al., 2014; Gu et al., 2020).

Co-MOFs	Nanorod	3 M KOH	0–0.4	958 @ 2 A/g	92 % 3000	Hydrothermal	(Ramachandran et al., 2018)
Ni/Co-MOFs-rGO	Particles distributed on Nanosheets	6 M KOH	0–0.6	860 @ 1 A/g	91.6 % 6000	One pot Co-Synthesis	(Rahmanifar et al., 2018)
NiMOFs@NCS/NF	3D porous network	2 M KOH	0–0.6	8.7C cm ² @ 1 mA cm ²	89.7 % 5000	Hydrothermal	(Pan et al., 2021)
Ni-MOFs	Microsphere	6 M KOH	0–0.6	1498 @ 1 A/g	Nil	Hydrothermal	(Manikandan et al., 2021)
rGO-NiCo₂S₄ MOFs	Nanoflakes and sheets	6 M KOH	-0.1–0.45	972 @ 1 A/g	70.5 %	Hydrothermal	(S. Kumar et al., 2021)
Ni/Co-MOFs/rGO	Spherical and rod	1 M KOH	0–0.5	958 @ 1 A/g	109 % 5000	Chemical	(Kumaraguru et al., 2020)
Ni-Co-S/ACC-MOFs	Nanosheet & Hollow	6 M KOH	0–0.5	2392 @ 1 A/g	85 % 10,000	Hydrothermal	(W. Zhao et al., 2019)
NiO-MOFs	Cauliflower	2 M KOH	0–0.5	1863 @ 0.5 A/g	82 % 5000	Explosion-Thermolysis	(Meng et al., 2020)
Co₂-Ni-MOFs	Flower	6 M KOH	0–0.6	1300 @ 1 A/g	71 % 3000	Hydrothermal	(J. Wang et al., 2019)
CoNi-MOFs	Vertically oriented sheets	1 M KOH	-0.2–0.5	1044 @ 2 A/g	94 % 5000	Electrodeposition	(Deng et al., 2018)
Ni-MOF@PEDOT	Nanosheet	0.5 M Na ₂ SO ₄	-	1401 F/g at 0.5 A/g	80.6 % 1000	In-situ deposition	(L. Shi et al., 2022)
CeO₂@ ZIF-8		-	-	132 F/g at 1 A/g	90 % 5000	Wet chemical strategy	(Rabani et al., 2021)

4.3 MOFs for Hydrogen Storage

MOFs store molecular hydrogen by reversible adsorption, with capacity governed by pore geometry, binding sites, pressure, and temperature. MOF-5 established the importance of framework preparation, while MOF-210 demonstrated high cryogenic uptake (Rosi et al., 2003; Kaye et al., 2007; Furukawa et al., 2010). Figures 11 and 12 relate pore topology and metal/linker environments to adsorption. Neither high surface area nor strong binding alone guarantees high deliverable capacity because density and residual loading at discharge also matter (Han et al., 2007; Z. Chen et al., 2022).

NPF-200 exhibits a volumetric working capacity of 37.2 g L⁻¹ between 100 and 5 bar at 77 K (X. Zhang et al., 2020). The DOE 2025 benchmarks discussed in the reviewed literature are 5.5 wt% and 40 g L⁻¹ for usable hydrogen in a complete onboard system (Z. Chen et al., 2022). The NPF-200 result is

material-level and cryogenic, so it does not establish compliance. Packing, vessel mass, insulation, thermal management, and operating efficiency must be included in system assessment.

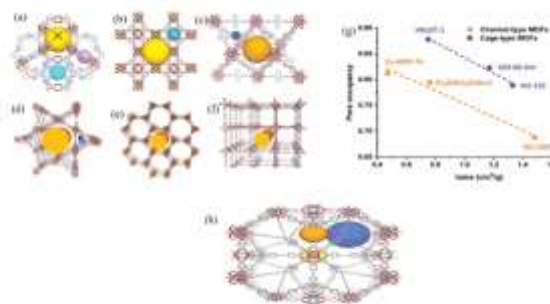


Figure 11 Representative MOF topologies, pore occupancy, and NPF-200 cage structures for hydrogen adsorption (X. Zhang et al., 2020).

The relative contribution of metal clusters and organic linkers changes with loading and framework architecture. This mechanistic distinction supports optimizing a defined charge–discharge window rather

than maximum uptake at a single pressure (Han et al., 2007).

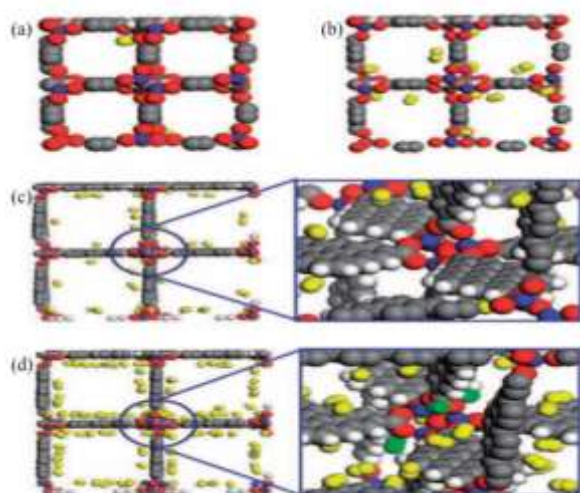


Figure 12 Hydrogen adsorption in Zn-MOF-C6 and Zn-MOF-C30 at the pressures indicated in the original panels (Han et al., 2007).

4.4 Computational and AI-Assisted MOF Design

High-throughput screening and machine learning prioritize MOFs by linking composition and topology to target properties. DFT examines redox and host–guest interactions, GCMC predicts adsorption, and molecular dynamics probes transport (Q. Ma et al., 2025; Z. Shi et al., 2020; Chafiq et al., 2024). Their roles are complementary, but an ideal-crystal prediction is not proof of a feasible storage device.

Synthetic accessibility, activation damage, defects, and residual guests create a gap between prediction and measurement. Adsorption results depend on force fields and charges; electrochemical models may omit reconstruction and interphase formation. Machine-learning validation should test transfer across structural families and quantify uncertainty. Screening is most useful when synthesis constraints and experimental feedback, including unsuccessful outcomes, guide subsequent selection.

4.5 Current Challenges and Future Perspectives

Application-specific hybrids should address verified failure mechanisms. Battery derivatives require connected conductive networks, strain accommodation, and high initial efficiency; Li–S hosts require sulfur utilization under limited electrolyte; zinc electrodes require aqueous stability; and supercapacitors require device-level validation. MOF–graphene and MOF–polymer combinations are supported by the reviewed examples, while MOF–MXene remains a candidate for further testing (Rahmanifar et al., 2018; Srinivasan et al., 2020).

Translation requires reproducible phase composition, controlled activation, practical loading, and consistent normalization. Solvent recovery, linker availability, conversion energy, and production yield should inform scalability and sustainability assessments. Operando or post-cycling measurements are needed to distinguish stable architectures from reconstructed active phases and to connect computational targets with observed degradation.

5. Conclusion

MOFs support energy storage as active frameworks, composite components, porous precursors, and adsorbents. Accessible sites, connected transport pathways, and structural accommodation explain their promise in batteries and supercapacitors; pore geometry and binding environments govern hydrogen adsorption. Benefits remain conditional on conductivity, chemical persistence, and operating conditions. Capacity and cycle life require interpretation with current, normalization, and device configuration, while material-level hydrogen uptake must be separated from complete-system storage. Progress depends on application-specific design, reproducible synthesis, mechanistic characterization, and computational screening linked to experimental feasibility.

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