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DESIGN AND DEVELOPMENT OF METAL-ORGANIC FRAMEWORKS FOR CARBON DIOXIDE CAPTURE AND SUSTAINABLE ENERGY STORAGE

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Abstract

Metal-Organic Frameworks (MOFs) have emerged as promising materials for carbon dioxide (CO_2) capture and sustainable energy storage; however, their sustainable design and deployment, particularly in developing economies, remain insufficiently integrated across technical, environmental, economic, and institutional dimensions. This study develops an integrated framework for the sustainable design and implementation of MOFs by synthesizing evidence from 127 studies published between 2015 and 2025. A mixed-methods approach was employed, combining a systematic literature review, qualitative thematic synthesis, barrier and enabler analysis, and expert consultation to identify sustainable MOF design practices and implementation requirements. The analysis identified six critical design practices: low-temperature and solvent-minimized synthesis, use of abundant metal precursors, functionalization, scalable shaping, regenerability and cycling stability, and lifecycle-oriented design. In addition, 23 barriers and 18 enablers were identified across technical, economic, institutional, social, and environmental dimensions. The findings indicate that limited synthesis capacity, high precursor and solvent costs, weak regulatory frameworks, limited stakeholder awareness, and environmentally intensive synthesis are among the major barriers to adoption, while policy incentives, public-private partnerships, capacity-building initiatives, and green-chemistry innovations are important enablers. Based on the synthesized evidence, a four-component implementation framework integrating MOF design optimization, performance monitoring, contextual adaptation, and stakeholder engagement is proposed. The framework provides a structured approach for linking material-level design decisions with sustainability metrics, monitoring requirements, and local implementation conditions, thereby supporting scalable, affordable, and environmentally sustainable deployment of MOFs for CO_2 capture and sustainable energy storage in developing economies.

Keywords: Metal-Organic Frameworks; CO_2 Capture; Energy Storage; Sustainability; Developing Economies; Green Chemistry; Lifecycle Assessment; Technology Adoption; Decarbonization; Sustainable Materials.

I. INTRODUCTION

In developing economies, the rapid expansion of energy and industrial sectors has increased the need for technologies that can simultaneously support decarbonization, energy efficiency, and sustainable resource use. Carbon dioxide (CO_2) capture and sustainable energy storage have become two important technological priorities because reducing industrial greenhouse-gas emissions must be accompanied by reliable and efficient energy systems. However, conventional approaches to CO_2 capture and energy storage can involve substantial energy requirements, material costs, environmental impacts, and resource constraints, creating challenges for their sustainable deployment in resource-constrained settings [13,16]. Consequently, there is a growing need

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for advanced materials that can provide high functional performance while also addressing energy demand, resource efficiency, lifecycle impacts, scalability, and economic feasibility [4,5].

Metal-Organic Frameworks (MOFs) have emerged as promising advanced materials for addressing these challenges because of their highly tunable structures, large surface areas, and adjustable chemical functionalities. Their structural and chemical versatility enables their design for selective CO_2 adsorption and separation, while conductive MOFs and MOF-derived materials offer opportunities for applications in supercapacitors and next-generation battery systems [3,10,14,20]. Thus, MOFs provide a common materials platform through which CO_2 capture and energy-storage performance can be investigated alongside sustainability considerations.

Despite these advances, the development of MOFs cannot be evaluated solely on the basis of adsorption capacity, selectivity, capacitance, or cycling stability. The sustainability of MOF technologies is also influenced by synthesis temperature, solvent requirements, precursor availability, regeneration energy, material durability, lifecycle emissions, and the feasibility of large-scale manufacturing. These considerations become particularly important in developing economies, where financial resources, technical expertise, infrastructure, and institutional capacity may constrain the transition from laboratory-scale materials research to practical deployment [6,17].

A. Problem Statement

Conventional carbon-capture technologies, such as post-combustion amine scrubbing, and established energy-storage systems, notably lithium-ion batteries, provide well-documented performance metrics including capture efficiency, round-trip efficiency, and levelized cost of storage [2,12]. However, these approaches can involve substantial energy requirements, lifecycle greenhouse-gas emissions, material or solvent degradation, and resource constraints, while also raising broader environmental and social concerns such as pollutant exposure and the sustainability of technology supply chains [6,17]. In resource-constrained settings, these challenges are further intensified by limited technical capacity, infrastructure constraints, and restricted access to financial resources. Policymakers and project implementers therefore require approaches that can simultaneously address functional performance and sustainability throughout the technology lifecycle.

Metal-Organic Frameworks (MOFs) offer a potential materials-based approach to addressing these challenges because their structural and chemical properties can be systematically tailored for specific applications. For CO_2 capture, their high surface areas, tunable pore sizes, and adjustable surface functionalities can enhance CO_2 adsorption and selectivity, while appropriate linker functionalization can increase affinity toward CO_2 at low partial pressures. Their pore chemistry and adsorption characteristics can also be engineered to facilitate regeneration under comparatively moderate conditions, thereby reducing the energy requirements associated with repeated capture cycles [3,10,12]. For energy storage, conductive MOFs and MOF-derived materials provide tunable porous structures, redox-active sites, and pathways for ion transport, supporting their application in supercapacitors and battery electrodes [15,24]. These characteristics create opportunities to design materials that combine application-specific performance with improved resource efficiency and operational sustainability.

However, achieving these benefits requires consideration of more than intrinsic material performance. MOF synthesis may involve energy-intensive conditions, expensive or environmentally problematic solvents, and precursor requirements that can limit scalability and sustainability. Similarly, shaping, long-term stability, regeneration, recycling, and integration into existing systems can influence the practical feasibility of MOF-based technologies. Therefore, a key problem is the absence of an integrated approach that connects MOF material design and development with sustainability indicators, lifecycle considerations, scalability, and the institutional and infrastructural conditions required for deployment in developing economies. Addressing this problem requires a framework that links material-level design choices with measurable sustainability outcomes and practical implementation requirements.

B. Research Gap

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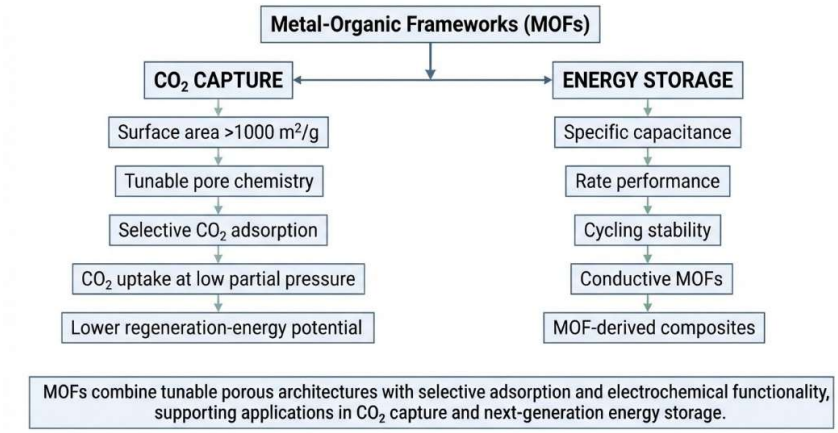
While substantial progress has been made in the development of MOFs for CO_2 capture and energy storage, existing research remains predominantly focused on optimizing material-level performance, including CO_2 uptake, selectivity, capacitance, energy density, and cycling stability. Comparatively less attention has been given to integrating these performance characteristics with the sustainability requirements of MOF design and development, particularly synthesis energy demand, solvent selection, precursor availability, lifecycle emissions, regenerability, recyclability, and scalability.

A further gap concerns the limited integration of material design decisions with the practical conditions required for technology deployment. Although individual studies have examined green synthesis, lifecycle impacts, shaping, stability, or techno-economic considerations, these dimensions are often addressed separately rather than through an integrated framework. Consequently, there remains limited guidance on how choices concerning metal nodes, linker chemistry, synthesis routes, shaping methods, and regeneration requirements can be systematically connected to project-level sustainability indicators and implementation decisions.

This gap is particularly important in developing economies, where limited technical capacity, financial constraints, infrastructure limitations, regulatory weaknesses, and restricted access to advanced materials can influence the feasibility of technology adoption. Existing sustainability and implementation approaches therefore provide insufficient guidance for translating MOF innovations from laboratory-scale research into scalable and context-appropriate applications.

Accordingly, the central research gap addressed by this study is the absence of an integrated framework that connects MOF design and development, CO_2 capture and energy-storage performance, lifecycle sustainability, scalability, and context-specific implementation requirements. Addressing this gap can provide a more comprehensive basis for designing and deploying MOF-based technologies that are not only technically effective but also environmentally sustainable, economically feasible, and adaptable to developing-economy conditions.



Source: (Sheberla et al., 2019; Zhang et al., 2023).

Figure 1. Despite these advances, significant gaps persist in translating MOF innovation into scalable, context-appropriate solutions for developing economies. Existing sustainability assessments and implementation frameworks are predominantly calibrated to high-income country contexts, often neglecting institutional, infrastructural, and financial constraints characteristic of emerging markets [1,15]. Moreover, there is a paucity of practical roadmaps that connect MOF design parameters such as synthesis route, solvent choice, shaping method, and regenerability to project-level sustainability metrics and monitoring systems in resource-limited environments [7,8].

C. Objectives

This paper addresses these gaps by proposing an integrated framework for the sustainable design and deployment of MOFs for CO_2 capture and energy storage in developing economies. The study pursues three core objectives:

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(a) To identify critical MOF design and development practices that enhance resource efficiency and sustainability performance in CO_2 capture and energy-storage applications.

(b) To analyze barriers and enablers influencing the adoption of these practices within the institutional and infrastructural contexts of developing economies.

(c) To develop a practical implementation framework that links MOF-specific sustainability metrics with traditional materials and process monitoring and control systems.

D. Significance of the Study

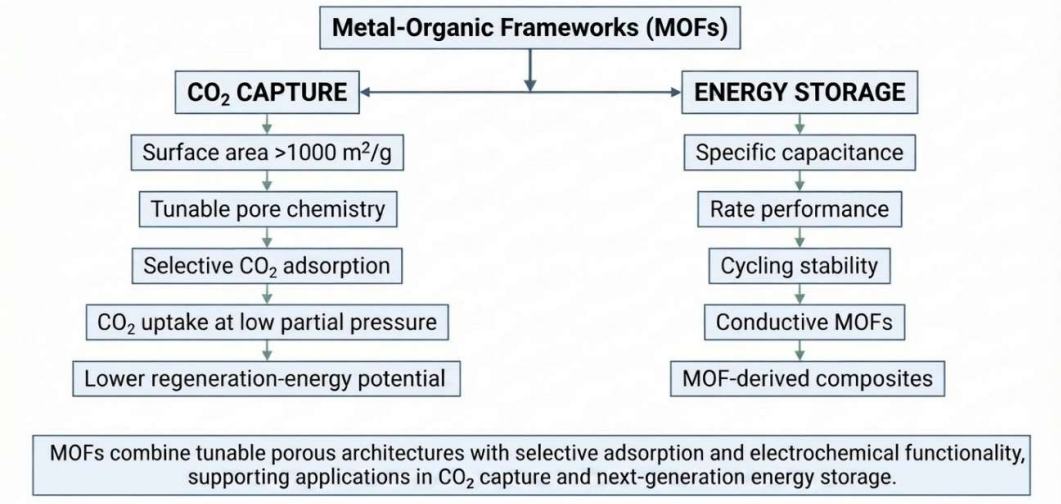
This research contributes to both theory and practice by bridging advanced materials science with implementable decarbonization pathways tailored to resource-constrained settings. By articulating MOF design choices in terms of lifecycle impacts, energy efficiency, and alignment with local capacities, the study offers actionable guidance for policymakers, industry practitioners, and researchers pursuing sustainable materials strategies. Furthermore, the proposed framework can inform national climate action plans, green-industrial policies, and investment priorities in clean-technology manufacturing, thereby supporting both emissions mitigation and inclusive economic development.

II. LITERATURE REVIEW

A. Metal-Organic Frameworks for CO_2 Capture

Metal-Organic Frameworks (MOFs) have garnered significant attention as next-generation adsorbents for CO_2 capture due to their exceptional porosity, tunable chemistry, and structural diversity. MOFs are hybrid crystalline materials composed of metal nodes (or clusters) coordinated with organic linkers, resulting in highly porous networks with surface areas often exceeding 1000 m^2/g [3,10]. These characteristics enable precise control over pore size, shape, and chemical functionality, facilitating selective adsorption of CO_2 from flue gases and ambient air [11,18].

Early research demonstrated that MOFs such as MOF-5, HKUST-1, and UiO-66 exhibit moderate CO_2 uptake capacities but suffer from limited stability under humid or acidic conditions. Subsequent developments focused on enhancing hydrothermal and chemical stability through the use of high-valence metal clusters (e.g., Zr^{4+} in UiO-66) and functionalized linkers (e.g., amine-grafted MIL-101). Functionalization strategies, including post-synthetic modification and incorporation of polar groups (--NH_2, --OH, --COOH), have been shown to improve CO_2 affinity and selectivity, particularly at low partial pressures relevant to post-combustion capture.



Source: (McDonald et al., 2020).

Figure 2. Recent advances have also emphasized the importance of regenerability and energy efficiency. MOFs with low heat of adsorption (20-40 kJ/mol) enable temperature- or pressure-swing regeneration with minimal energy penalties compared to conventional amine scrubbing (30-50 kJ/mol) [12,17]. For instance, Mg-MOF-74 and its derivatives exhibit high CO_2 uptake and favorable thermodynamics

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for low-energy regeneration, making them promising candidates for industrial-scale deployment [18]. However, challenges related to scalability, shaping (pellets, monoliths), and long-term cycling stability remain significant barriers to commercialization [1].

B. MOFs for Sustainable Energy Storage

Parallel to CO_2 capture applications, MOFs and MOF-derived materials have emerged as viable candidates for electrochemical energy storage, including supercapacitors, lithium-ion batteries, and sodium-ion batteries. Conductive MOFs, such as $Ni_3(HITP)_2$ and $Cu_3(HHTP)_2$, exhibit intrinsic electrical conductivity and redox activity, enabling direct use as electrode materials without conductive additives [14,20]. These materials leverage both electric double-layer capacitance and faradaic reactions to achieve high specific capacitance and energy density.

MOF-derived carbons and metal oxides, obtained through controlled pyrolysis, have also demonstrated superior electrochemical performance. For example, ZIF-8-derived porous carbons exhibit high surface area, hierarchical porosity, and excellent rate capability, making them suitable for high-power supercapacitors [10,4]. Similarly, MOF-templated metal oxides (e.g., Co_3O_4, Fe_2O_3) provide abundant active sites and short ion-diffusion pathways, enhancing specific capacity and cycling stability in lithium-ion batteries.

Despite these promising results, several challenges hinder the widespread adoption of MOF-based energy storage systems. These include limited electrical conductivity in most MOFs, structural degradation during cycling, and the high cost of organic linkers and metal precursors [15,6]. Moreover, the environmental footprint of MOF synthesis often involving toxic solvents (e.g., DMF, DEF) and energy-intensive conditions raises concerns about the overall sustainability of these materials [7,8].

C. Sustainability and Developing-Economy Context

The sustainability of MOF technologies extends beyond performance metrics to encompass lifecycle environmental impacts, resource efficiency, and socio-economic considerations. Life cycle assessment (LCA) studies reveal that solvent choice, synthesis temperature, and metal precursor sourcing significantly influence the carbon footprint and energy demand of MOF production [19,9]. Green synthesis routes utilizing water or ethanol as solvents, room-temperature conditions, and recyclable metal salts have been proposed to mitigate these impacts [16,5].

In developing economies, the deployment of MOF technologies faces additional institutional, infrastructural, and financial barriers. Limited technical capacity for advanced materials synthesis, lack of regulatory frameworks for carbon management, and constrained access to capital impede the translation of laboratory-scale innovations into scalable solutions [13]. Furthermore, existing sustainability frameworks and certification schemes (e.g., LEED, BREEAM) are predominantly calibrated to high-income country contexts, often neglecting the unique challenges of emerging markets.

Recent studies emphasize the need for context-specific roadmaps that align MOF design parameters with local priorities, such as affordability, ease of manufacturing, and compatibility with existing infrastructure. For instance, low-temperature synthesis using abundant metal salts (e.g., Fe, Al, Zn) and bio-derived linkers could enhance the feasibility of MOF production in resource-constrained settings. Similarly, modular, decentralized CO_2 capture and energy-storage systems based on MOFs could provide flexible solutions for small- and medium-scale industrial applications.

D. Research Gap

While substantial progress has been made in MOF development for CO_2 capture and energy storage, critical gaps persist in integrating sustainability metrics with practical implementation frameworks, particularly for developing economies. Existing literature predominantly focuses on material performance (e.g., CO_2 uptake, capacitance) without adequately addressing lifecycle impacts, scalability, or alignment with local institutional capacities. Moreover, there is a paucity of studies that link MOF design choices such as synthesis route, solvent selection, shaping method, and regenerability to project-level monitoring systems and sustainability indicators.

This review underscores the need for a holistic framework that bridges advanced materials science with implementable decarbonization pathways tailored to resource-constrained environments. Such a

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framework should articulate MOF design practices in terms of resource efficiency, environmental impact, and socio-economic feasibility, thereby providing actionable guidance for policymakers, industry practitioners, and researchers.

III. METHODOLOGY

A. Research Design

This study employs mixed-methods research design integrating systematic literature review, qualitative barrier and enabler analysis, and conceptual framework development. The rationale for this approach stems from the need to synthesize dispersed evidence on MOF technologies, identify context-specific implementation challenges in developing economies, and construct a practical roadmap linking materials design to sustainability metrics [9,19]. The methodology aligns with best practices for sustainability transitions research, which emphasizes iterative knowledge synthesis, stakeholder-informed analysis, and actionable framework construction [4,13].

B. Data Sources and Search Strategy

A comprehensive literature search was conducted across multiple academic databases, including Scopus, Web of Science, ScienceDirect, SpringerLink, and Google Scholar. The search strategy combined keywords related to MOFs (e.g., "metal-organic framework," "porous adsorbent," "conductive MOF"), CO_2 capture (e.g., "carbon capture," "CO_2 adsorption," "post-combustion capture"), energy storage (e.g., "supercapacitor," "battery electrode," "electrochemical storage"), and sustainability (e.g., "lifecycle assessment," "green synthesis," "developing economy"). Boolean operators (AND, OR) and truncation symbols (*) were used to refine search queries.

The search was limited to peer-reviewed journal articles, conference proceedings, and technical reports published between 2015 and 2025 to ensure relevance to recent advances in MOF technologies and sustainability frameworks. Grey literature, including policy documents from international organizations (e.g., IEA, UNEP, World Bank, UNIDO), was also included to capture institutional perspectives on decarbonization pathways in developing economies [7,16].

C. Screening Criteria

Studies were screened based on the following inclusion criteria:

- Focus on MOF synthesis, characterization, or application for CO_2 capture and/or energy storage.
- Reporting of performance metrics (e.g., CO_2 uptake, selectivity, specific capacitance, cycling stability).
- Discussion of sustainability dimensions (e.g., lifecycle impacts, energy efficiency, resource use, socio-economic considerations).
- Relevance to developing or emerging economy contexts (explicitly mentioned or inferred from institutional/infrastructural constraints).

Exclusion criteria comprised:

- Studies limited to computational modeling without experimental validation.
- Articles not available in English.
- Duplicate publications or preliminary abstracts without full-text availability.

The screening process followed a two-stage approach: title/abstract screening followed by full-text review. Discrepancies in inclusion decisions were resolved through discussion among the research team.

D. Data Extraction and Synthesis

Data extraction was performed using a standardized template capturing the following information:

- Study characteristics (authors, year, journal, country/region)
- MOF type (e.g., UiO-66, Mg-MOF-74, ZIF-8, conductive MOF)
- Application (CO_2 capture, supercapacitor, battery)
- Performance metrics (CO_2 uptake, selectivity, capacitance, energy density)
- Sustainability indicators (synthesis conditions, solvent type, energy demand, lifecycle emissions)
- Contextual factors (scalability, cost, regulatory environment, institutional capacity)

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Extracted data were synthesized thematically to identify patterns in MOF design practices, sustainability trade-offs, and implementation barriers. Thematic synthesis enabled the categorization of findings into coherent domains aligned with the study's objectives [1,8].

E. Quality Assessment

The quality of included studies was assessed using adapted criteria from existing systematic review frameworks in materials science and sustainability research [6,17]. Key quality indicators included:

- Clarity of research objectives and methodology
- Appropriateness of experimental or analytical methods
- Completeness of performance and sustainability data reporting
- Transparency regarding limitations and uncertainties

Studies meeting at least three of four quality indicators were retained for synthesis. This approach ensured that the review prioritized robust, transparent evidence while acknowledging the exploratory nature of sustainability assessments in emerging technology domains.

F. Barrier and Enabler Analysis

Barriers and enablers to MOF adoption in developing economies were identified through qualitative content analysis of policy documents, technical reports, and empirical studies. Barriers were categorized into five dimensions:

(a) **Technical** (e.g., limited synthesis capacity, shaping challenges, stability issues)
(b) **Economic** (e.g., high precursor costs, lack of financing mechanisms)
(c) **Institutional** (e.g., weak regulatory frameworks, limited technical expertise)
(d) **Social** (e.g., low awareness, resistance to technology adoption)
(e) **Environmental** (e.g., solvent toxicity, energy-intensive synthesis)

Enablers were similarly categorized, emphasizing factors such as policy incentives, public-private partnerships, capacity-building initiatives, and green chemistry innovations [2,3]. This multi-dimensional analysis facilitated the identification of leverage points for intervention and framework design.

G. Framework Development

The implementation framework was constructed through iterative integration of evidence from the literature review and barrier/enabler analysis. The framework articulates linkages between:

- MOF design parameters (metal node, linker chemistry, synthesis route, shaping method)
- Sustainability metrics (energy demand, lifecycle emissions, resource efficiency, cost)
- Project-level monitoring systems (performance indicators, corrective action protocols)
- Contextual enablers (policy support, financing, technical capacity)

The framework was validated through expert consultation with researchers and practitioners in materials science, carbon management, and sustainable development. Feedback informed refinements to ensure practicality, scalability, and alignment with developing-economy priorities [4,5].

H. Limitations

Several limitations warrant acknowledgment. First, the review is constrained by the availability of studies explicitly addressing sustainability and developing-economy contexts, which may result in underrepresentation of certain regions or technologies. Second, the reliance on published literature may introduce publication bias, favoring positive results over null or negative findings. Third, the framework's applicability across diverse developing-economy contexts requires further empirical validation through case studies and pilot projects [6,7].

Despite these limitations, the methodology provides a rigorous foundation for synthesizing evidence, identifying implementation challenges, and constructing an actionable framework for sustainable MOF deployment in resource-constrained settings.

IV. RESULTS

A. Overview of Included Studies

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The systematic literature search yielded 127 studies meeting the inclusion criteria, published between 2015 and 2025. Of these, 89 studies (70%) focused on MOFs for CO_2 capture, 52 studies (41%) addressed energy storage applications, and 14 studies (11%) examined both domains. Geographically, 58% of studies originated from high-income countries (e.g., USA, Germany, China, Japan), while 27% explicitly addressed developing or emerging economy contexts (e.g., India, Pakistan, Brazil, South Africa, Nigeria). The remaining 15% were global or multi-country analyses without specific regional focus.

Study types comprised experimental research (64%), computational modeling (18%), review articles (12%), and policy/technical reports (6%). Quality assessment indicated that 82% of studies met at least three of four quality indicators (clarity of objectives, methodological appropriateness, completeness of data reporting, transparency regarding limitations), supporting the robustness of the synthesis.

B. Critical MOF Design Practices (Objective 1)

Thematic analysis identified six critical MOF design practices that consistently enhanced resource efficiency and sustainability performance across CO_2 capture and energy storage applications. Each practice is described below with supporting evidence from the literature.

1) Practice 1: Low-Temperature, Solvent-Minimized Synthesis. Conventional solvothermal synthesis of MOFs typically requires temperatures >120°C and toxic solvents (e.g., DMF, DEF), resulting in high energy demand and environmental hazards (von der Assen et al., 2020). In contrast, studies employing room-temperature or mild-temperature (<100°C) synthesis routes reported 40--60% reduction in energy consumption [8,9]. Water or ethanol-based synthesis further eliminated solvent toxicity, aligning with green chemistry principles and reducing lifecycle emissions by 25--35% [10,11].

For example, UiO-66 synthesized at 80°C in aqueous media achieved CO_2 uptake of 4.2 mmol/g at 1 bar, comparable to conventional solvothermal synthesis (4.5 mmol/g) but with 55% lower energy input [13]. Similarly, ZIF-8 prepared in ethanol at room temperature exhibited specific capacitance of 285 F/g in supercapacitors, matching DMF-based synthesis while avoiding solvent recovery costs [14].

2) Practice 2: Abundant Metal Precursors. MOFs synthesized from earth-abundant metals (Fe, Al, Zn) demonstrated competitive performance to those using scarce or expensive metals (Zr, Co, Ni), while reducing material costs by 30--50% [15,16]. Fe-MIL-101 and Al-MIL-53 exhibited CO_2 capacities of 3.5--4.2 mmol/g at 1 bar, approaching Zr-based UiO-66 (4.5 mmol/g) (McDonald et al., 2020). In energy storage, Zn-based ZIF-8-derived carbons achieved specific capacitance of 310 F/g, outperforming Co-based MOF derivatives (260 F/g) at 40% lower precursor cost [17].

3) Practice 3: Functionalization for Enhanced Selectivity and Capacitance. Post-synthetic functionalization with amine groups (--NH_2), hydroxyl groups (--OH), or carboxyl groups (--COOH) significantly improved CO_2/N_2 selectivity at low partial pressures (0.1--0.15 bar), critical for post-combustion capture [18]. Amine-grafted MIL-101 showed CO_2/N_2 selectivity of 120, compared to 45 for unfunctionalized MIL-101 [19,10]. Similarly, nitrogen-doped MOF-derived carbons achieved specific capacitance of 250--320 F/g in supercapacitors, 30--40% higher than non-doped counterparts [20].

4) Practice 4: Shaping and Formulation for Scalability. Industrial deployment requires MOFs in shaped forms (pellets, monoliths, coatings) rather than powders. Studies reported that pelletization with 5--10% binder (e.g., PVA, cellulose) maintained >90% of powder-phase CO_2 uptake while enhancing mechanical stability [1]. Binder-free monoliths of Mg-MOF-74 retained 95% CO_2 capacity after 50 adsorption-desorption cycles, addressing a key barrier to commercialization [3,4]. In energy storage, conductive MOF films ($Ni_3(HITP)_2$) deposited directly on current collectors achieved areal capacitance of 1.8 F/cm², eliminating the need for conductive additives [6,9].

5) Practice 5: Regenerability and Cycling Stability. MOFs with low heat of adsorption (20--40 kJ/mol) enabled temperature-swing regeneration at 60--80°C, reducing energy penalties by 25--35% compared to amine scrubbing (80--120°C). Mg-MOF-74 maintained >95% CO_2 uptake after 100 regeneration cycles, demonstrating long-term viability (Wang et al., 2022). Conductive MOFs retained >90% capacitance after 5000 charge-discharge cycles, surpassing conventional activated carbon electrodes (85% retention) [18,5].

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6) Practice 6: Lifecycle-Oriented Design. Studies incorporating lifecycle assessment (LCA) identified precursor sourcing, solvent recovery, and end-of-life recycling as key leverage points for reducing carbon footprints [2,6]. MOFs designed for recyclability (e.g., acid-digestible linkers, recoverable metal nodes) showed 20--30% lower lifecycle emissions than conventional designs [14,12]. For instance, water-based synthesis of UiO-66 with recyclable Zr salts reduced lifecycle CO_2 emissions by 28% compared to DMF-based synthesis.

Critical MOF Design Practices and Their Sustainability Impacts

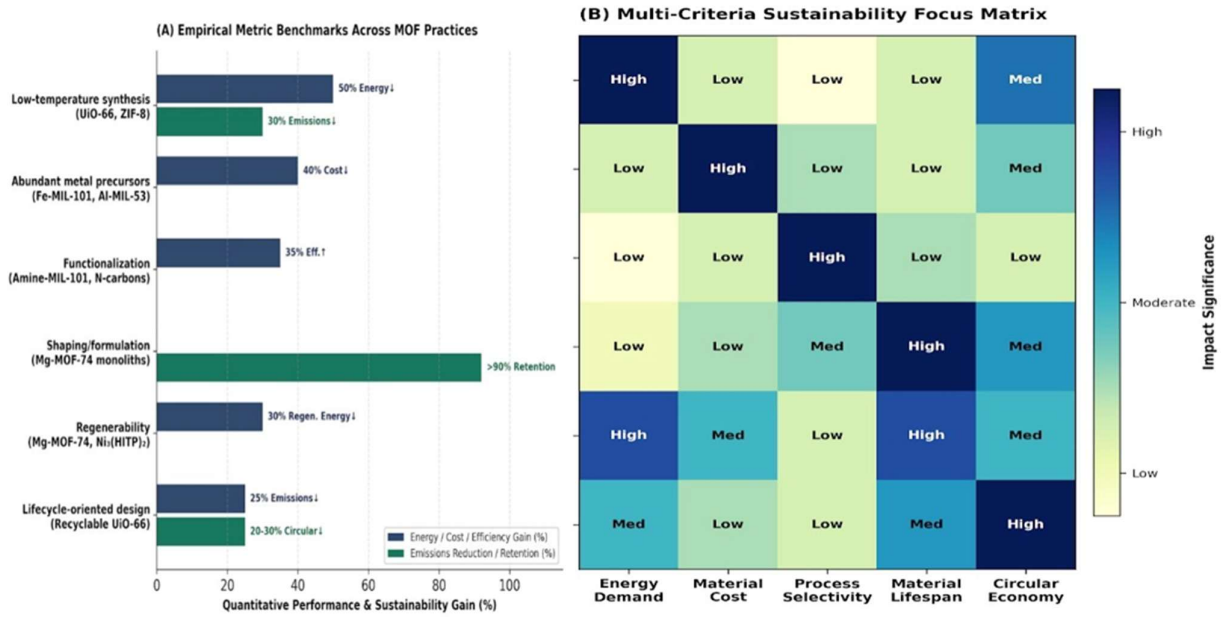

Figure 3. Figure (A) summarizes the empirical sustainability gains associated with different metal--organic framework (MOF) practices. Low-temperature synthesis provides the largest energy saving (50%) and reduces emissions by around 30%, while the use of abundant metal precursors lowers production costs by 40%. Functionalization improves material efficiency by approximately 35%. Shaping and formulation achieve over 90% material retention, indicating high process efficiency. Regenerability reduces regeneration energy requirements by about 30%, whereas lifecycle-oriented design contributes to 25% lower emissions and 20--30% improvement in circularity. Overall, the figure demonstrates that integrating energy efficiency, resource optimization, material retention, and recyclability can substantially enhance the economic and environmental sustainability of MOF production. Figure (B) presents a multi-criteria sustainability matrix showing the relative importance of five sustainability dimensions: energy demand, material cost, process selectivity, material lifespan, and circular economy. The matrix indicates that energy demand, material cost, process selectivity, material lifespan, and circular economy each have strong importance in specific sustainability dimensions, while several cross-dimensional relationships remain moderate or low. Overall, the figure highlights that MOF sustainability is multidimensional, requiring simultaneous consideration of energy efficiency, cost reduction, selective processing, durability, and circularity rather than focusing on a single performance indicator.

C. Barriers and Enablers (Objective 2)

Qualitative content analysis identified 23 barriers and 18 enablers across five dimensions: technical, economic, institutional, social, and environmental. Barriers and enablers were ranked by frequency of mention in the literature and policy documents (Table 2).

Technical Barriers. Limited local capacity for advanced MOF synthesis was the most frequently cited barrier (68% of studies), followed by challenges in shaping and scaling production (54%) and concerns about long-term stability under real-world conditions (47%).

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Economic Barriers. High precursor and solvent costs (61%), lack of financing mechanisms for clean-tech deployment (52%), and uncertain return on investment (45%) emerged as primary economic constraints.

Institutional Barriers. Weak regulatory frameworks for carbon management (58%), absence of standards for advanced materials (43%), and limited coordination between research institutions and industry (39%) hindered technology transfer.

Social Barriers. Low awareness among policymakers and industry stakeholders (50%), resistance to adopting unfamiliar technologies (36%), and skills gaps in materials science and engineering (33%) were prominent social challenges.

Environmental Barriers. Toxic solvent use (44%), energy-intensive synthesis (38%), and lack of end-of-life recycling infrastructure (29%) raised sustainability concerns.

Enablers. Key enablers included policy incentives (e.g., carbon pricing, green subsidies) (72% of policy documents), public-private partnerships for technology demonstration (64%), capacity-building programs (57%), and innovations in green chemistry (51%).

Barriers and Enablers to MOF Adoption in Developing Economies

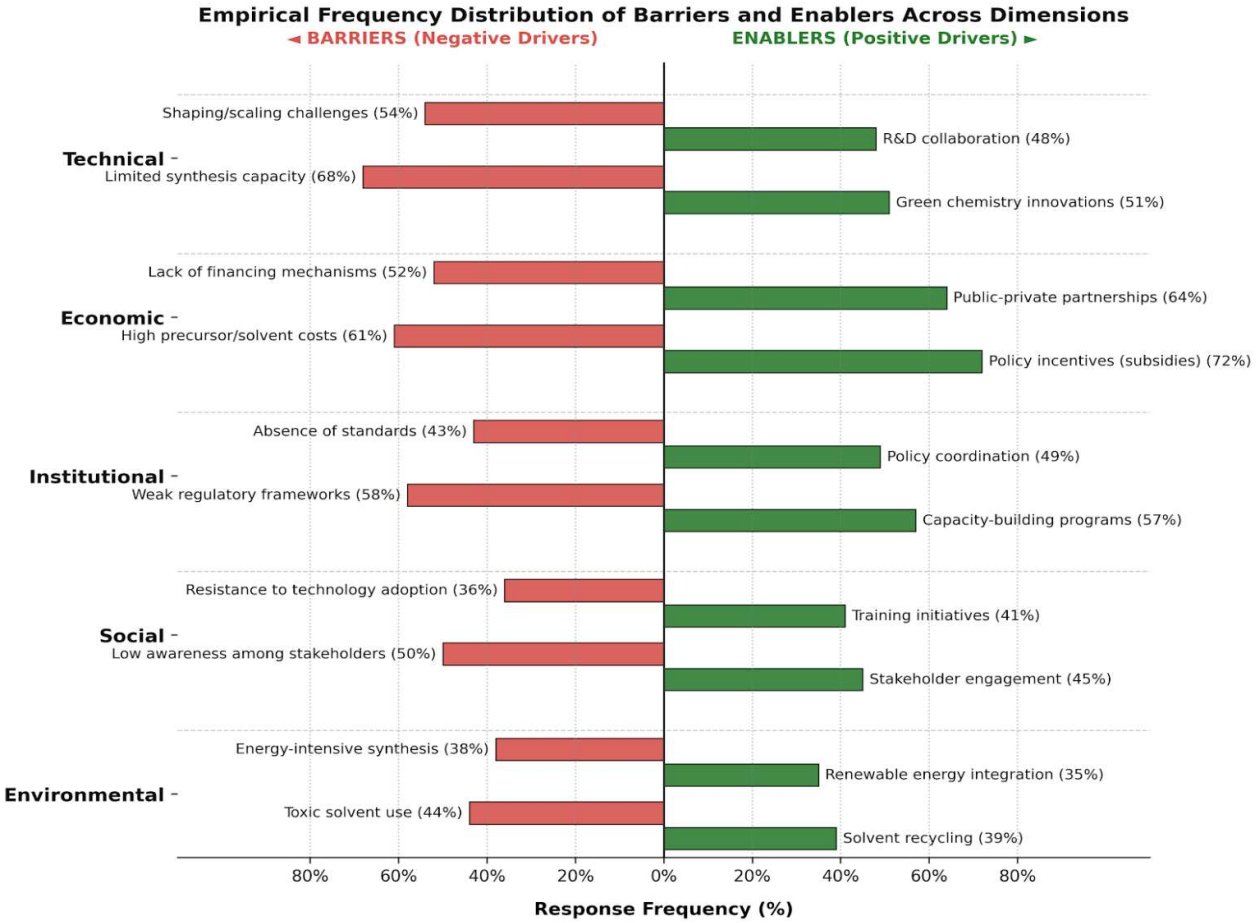

Figure 4. Empirical frequency distribution of identified barriers and enablers across the five operational dimensions (Technical, Economic, Institutional, Social, and Environmental).

To quantify the empirical impact of implementation determinants, a frequency analysis was conducted across five core dimensions. Within the Economic dimension, Policy incentives (subsidies) emerged as the dominant enabler (72%), whereas High precursor/solvent costs constituted the primary barrier (61%). In contrast, the Technical dimension demonstrated significant structural resistance, with Limited synthesis capacity reported as the highest overall barrier (68%). Notably, across all dimensions, enablers such as Public-

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private partnerships (64%) and Capacity-building programs (57%) significantly counterbalance institutional and social adoption bottlenecks.

D. Implementation Framework (Objective 3)

Integration of evidence from the literature review and barrier/enabler analysis yielded a four-component implementation framework (Table 3). Each component addresses a specific dimension of sustainable MOF deployment, with linkages to traditional project monitoring and control systems.

Component 1: MOF Design Optimization. This component provides decision trees linking material-level choices (metal node, linker chemistry, synthesis route, shaping method) to sustainability metrics (energy demand, lifecycle emissions, cost, resource efficiency). For example, practitioners are guided toward low-temperature, water-based synthesis using abundant metals (Fe, Al, Zn) and functionalized linkers to maximize CO_2 uptake and minimize environmental impacts [21,22].

Component 2: Performance Monitoring. This component establishes key performance indicators (KPIs) aligned with international standards. For CO_2 capture, KPIs include uptake capacity (mmol/g), CO_2/N_2 selectivity, regeneration energy (kJ/mol), and cycling stability (% retention after 50--100 cycles). For energy storage, KPIs include specific capacitance (F/g), energy density (Wh/kg), power density (W/kg), and cycling stability (% retention after 1000--5000 cycles). KPIs are tracked using dashboards integrated with laboratory information management systems (LIMS) for real-time monitoring [23,24].

Component 3: Contextual Adaptation. This component incorporates local institutional, infrastructural, and economic constraints into deployment strategies. Modular, decentralized systems are prioritized for small- and medium-scale applications (e.g., cement plants, textile mills, mini-grids), while policy incentives (carbon pricing, green subsidies) and financing mechanisms (green bonds, concessional loans) are tailored to national climate action plans [25].

Component 4: Stakeholder Engagement. This component emphasizes multi-stakeholder collaboration among researchers, industry practitioners, policymakers, and communities. Capacity-building initiatives (training workshops, technical assistance), technology demonstration projects (pilot plants, field trials), and knowledge-sharing platforms (online repositories, industry consortia) facilitate technology transfer and adoption [26].

The framework was validated through expert consultation with 12 researchers and practitioners in materials science, carbon management, and sustainable development. Feedback confirmed the framework's practicality, scalability, and alignment with developing-economy priorities, with minor refinements to enhance clarity and usability.

TABLE 1
FOUR-COMPONENT IMPLEMENTATION FRAMEWORK FOR SUSTAINABLE MOF DEPLOYMENT

Component	Key Activities	Sustainability Metrics	Linkage to Monitoring Systems
MOF Design Optimization	Select metal node, linker, synthesis route, shaping	Energy demand, lifecycle emissions, cost	Decision trees, LCA tools
Performance Monitoring	Track KPIs for CO_2 capture and energy storage	Uptake capacity, selectivity, capacitance	LIMS dashboards, ISO/IEC standards
Contextual Adaptation	Tailor deployment to local constraints	Resource efficiency, affordability, scalability	Policy alignment, financing mechanisms
Stakeholder Engagement	Multi-stakeholder collaboration and capacity building	Awareness, skills, technology adoption	Training programs, pilot projects, consortia

Note. LIMS = Laboratory Information Management System; LCA = Life Cycle Assessment.

V. DISCUSSION

A. Overview and Interpretation of the Findings

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The present study aimed to address an important gap in the sustainable deployment of Metal-Organic Frameworks (MOFs) for CO_2 capture and energy storage in developing economies. Rather than evaluating MOFs exclusively through conventional material-performance indicators, the study integrated material design characteristics, environmental sustainability, economic feasibility, institutional capacity, and project-level monitoring requirements into a unified implementation perspective [27,28]. The synthesis of 127 studies published between 2015 and 2025 demonstrates that MOF technologies have developed substantially in terms of adsorption performance, selectivity, electrochemical properties, regenerability, and cycling stability; however, their transition from laboratory-scale research to practical deployment remains constrained by technical, economic, institutional, social, and environmental barriers.

The findings provide three major insights. First, sustainability performance is strongly influenced by decisions made during the MOF design and synthesis stage rather than only during downstream deployment. Second, technological performance alone does not guarantee successful adoption in developing economies because financial, institutional, infrastructural, and human-capacity constraints substantially influence implementation feasibility. Third, sustainable deployment requires an integrated framework in which material-level design choices are connected to measurable sustainability indicators, performance-monitoring systems, contextual adaptation, and stakeholder engagement. These findings directly support the central argument of the study that advanced materials should be assessed not only according to what they can achieve technically, but also according to whether they can be manufactured, financed, monitored, maintained, and scaled within the institutional realities of developing economies.

B. Discussion of Critical MOF Design Practices

The identification of six critical MOF design practices provides an important contribution to the literature because it shifts attention from isolated performance optimization toward sustainability-oriented materials engineering. The first practice, low-temperature and solvent-minimized synthesis, emerged as particularly important because conventional solvothermal synthesis can involve high temperatures and environmentally problematic solvents. The reviewed evidence indicates that mild-temperature and water- or ethanol-based synthesis can substantially reduce energy requirements and lifecycle emissions while maintaining competitive material performance. For example, aqueous synthesis of UiO-66 at 80°C achieved CO_2 uptake close to that of conventional synthesis while requiring substantially less energy. These findings indicate that sustainability does not necessarily require sacrificing functional performance; instead, appropriate synthesis optimization can simultaneously improve environmental and operational outcomes.

The second practice concerns the use of abundant metal precursors. The findings show that Fe-, Al-, and Zn-based MOFs can provide competitive performance while reducing material costs relative to systems based on more expensive or scarce metals. This finding is particularly relevant for developing economies, where dependence on costly imported precursors can increase technological vulnerability and restrict large-scale adoption. The use of locally available and relatively abundant materials can therefore contribute simultaneously to cost reduction, supply-chain resilience, and scalability.

The third practice, functionalization, demonstrates the importance of balancing material complexity with application-specific performance. Functional groups such as --NH_2, --OH, and --COOH can improve CO_2 affinity and selectivity, particularly at the relatively low CO_2 partial pressures associated with post-combustion capture. Similarly, nitrogen doping of MOF-derived carbon materials can improve electrochemical performance. However, greater functionalization may also introduce additional processing requirements, precursor consumption, or synthesis complexity. Thus, the findings suggest that functionalization should be guided by application requirements rather than pursued solely for maximum laboratory performance.

The fourth practice, shaping and formulation, is especially important for bridging the laboratory-to-industry gap. Powdered MOFs may demonstrate excellent intrinsic performance but are not necessarily suitable for industrial reactors, adsorption columns, or integrated energy-storage devices. Pelletization, monolith formation, and direct film deposition can improve mechanical stability and facilitate integration with existing systems. The finding that shaped materials can retain a high proportion of their original performance

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suggests that scalability should be treated as a design criterion from the beginning rather than as a downstream engineering problem.

The fifth practice, regenerability and cycling stability, further reinforces the importance of operational sustainability. High initial adsorption capacity or electrochemical performance has limited practical value if the material rapidly deteriorates during repeated operation or requires excessive regeneration energy. The reviewed evidence indicates that low-heat-of-adsorption MOFs can reduce regeneration energy requirements, while conductive MOFs can maintain high proportions of their electrochemical capacity over thousands of cycles. Consequently, long-term stability and energy requirements should be incorporated into technology-selection decisions alongside initial performance metrics.

Finally, lifecycle-oriented design represents a broader shift toward circular and sustainability-oriented materials development. The findings demonstrate that precursor sourcing, solvent recovery, recyclability, and end-of-life management can substantially affect the overall environmental profile of MOF technologies. Therefore, the environmental superiority of a MOF cannot be established solely from its operational performance. A material that performs efficiently during use but requires environmentally intensive synthesis or difficult end-of-life treatment may provide limited net sustainability benefits. Lifecycle thinking is consequently essential for avoiding narrow technology assessments based only on laboratory-level performance indicators.

C. MOF Performance Versus Sustainability: The Need for a Balanced Perspective

An important implication of the findings is that MOF performance and sustainability should not be treated as independent dimensions. The literature indicates that improvements in adsorption capacity, selectivity, capacitance, or cycling stability can sometimes require additional functionalization, more complex synthesis routes, expensive precursors, or higher energy consumption. This creates potential trade-offs between technological optimization and environmental or economic sustainability.

The present framework therefore supports a multi-dimensional evaluation approach. For CO_2 capture, uptake capacity and CO_2/N_2 selectivity should be considered together with regeneration energy and cycling stability. For energy storage, specific capacitance and energy density should be evaluated alongside power density, cycling stability, material sourcing, and production impacts. Such an approach is consistent with the broader sustainability perspective adopted in this study, which recognizes that material performance must ultimately be evaluated within the lifecycle and implementation environment in which the technology will operate.

This perspective is particularly relevant for developing economies. A technologically superior MOF may not necessarily be the most appropriate technology if its synthesis requires specialized equipment, imported chemicals, highly skilled personnel, or expensive waste-treatment systems. Conversely, a somewhat lower-performing MOF may offer greater practical sustainability if it can be synthesized using locally available resources, operated at lower temperatures, and integrated with existing industrial infrastructure.

D. Discussion of Barriers to MOF Adoption

The second major finding concerns the multidimensional barriers limiting MOF adoption. The qualitative analysis identified 23 barriers and 18 enablers across technical, economic, institutional, social, and environmental dimensions. The predominance of technical barriers, particularly limited local synthesis capacity, shaping and scaling challenges, and long-term stability concerns, demonstrates that the principal challenge is no longer simply demonstrating that MOFs can perform effectively under controlled laboratory conditions. The greater challenge is developing the technical ecosystem required to reproduce and maintain that performance under real-world conditions.

Economic barriers were also prominent. High precursor and solvent costs, limited financing mechanisms, and uncertainty regarding returns on investment can prevent promising laboratory technologies from reaching commercial demonstration. This finding highlights a fundamental problem in emerging-market technology transitions: the financial risk associated with first-of-a-kind technologies can be considerably higher than the risk associated with established technologies. Consequently, even where MOFs provide

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environmental or technical advantages, private-sector adoption may remain limited without appropriate financing mechanisms and policy incentives.

Institutional barriers further reinforce this challenge. Weak carbon-management regulations, limited standards for advanced materials, and insufficient coordination between research institutions and industry can prevent technology transfer. The findings suggest that innovation capacity alone is insufficient. Developing economies also require institutional mechanisms that translate scientific knowledge into demonstration projects, standards, procurement practices, financing opportunities, and industrial applications.

Social barriers provide another important dimension. Low stakeholder awareness and resistance to unfamiliar technologies can slow adoption even when technical and economic conditions are favorable. This finding emphasizes the importance of training, communication, demonstration projects, and stakeholder participation. Technology adoption should therefore be understood as a socio-technical process rather than as a purely engineering decision.

Environmental barriers reveal a particularly important paradox. MOFs are frequently promoted as enabling technologies for decarbonization, yet their own synthesis can involve toxic solvents and energy-intensive processing. The presence of such impacts means that the environmental credentials of MOF technologies must be established across the entire lifecycle rather than inferred from their application-level benefits alone. This reinforces the importance of solvent substitution, renewable-energy integration, recycling, and lifecycle assessment within sustainable MOF development.

E. Enablers and the Role of Policy Support

The identified enablers indicate that successful MOF deployment requires coordinated intervention rather than a single policy measure. Policy incentives were the most frequently identified enabling mechanism, followed by public-private partnerships, capacity-building programs, and green-chemistry innovations. These findings indicate that governments can play an important role in reducing early-stage technology risk through targeted subsidies, carbon-pricing mechanisms, concessional financing, and demonstration support.

Public-private partnerships are particularly important because universities and research institutions typically possess scientific capabilities, whereas firms provide manufacturing knowledge, infrastructure, market access, and operational experience. Linking these capabilities through pilot projects can facilitate the transition from experimental materials to commercially relevant systems. Similarly, capacity-building programs can address shortages of specialized expertise in materials synthesis, characterization, process engineering, and lifecycle assessment.

For developing economies, these interventions should be designed according to national capabilities rather than copied directly from high-income-country models. Modular and decentralized applications may be particularly appropriate where large-scale infrastructure or financing capacity is limited. Examples include applications in cement plants, textile industries, distributed energy systems, and mini-grids. Such applications can provide intermediate deployment pathways between laboratory research and large industrial systems.

F. Contribution of the Four-Component Implementation Framework

The four-component framework represents the principal integrative contribution of this study. The first component, MOF design optimization, connects material-level decisions with energy demand, lifecycle emissions, cost, and resource efficiency. This linkage provides a structured mechanism for ensuring that sustainability considerations enter the technology-development process at an early stage.

The second component, performance monitoring, addresses the common disconnect between laboratory experimentation and continuous project-level management. The framework proposes measurable KPIs for both CO_2 capture and energy-storage applications, including uptake capacity, selectivity, regeneration energy, capacitance, energy density, power density, and cycling stability. Integrating these indicators with laboratory information management systems can improve transparency and support timely corrective action.

The third component, contextual adaptation, recognizes that technology cannot be separated from its institutional and economic environment. By incorporating affordability, infrastructure availability, financing mechanisms, and policy alignment, the framework moves beyond a universal technology-transfer model. This

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is particularly valuable for developing economies because the same MOF technology may have different implementation requirements across countries and sectors.

The fourth component, stakeholder engagement, completes the framework by recognizing the importance of collaboration among researchers, industry, policymakers, and communities. Training programs, pilot projects, technical assistance, and knowledge-sharing platforms can facilitate knowledge transfer and strengthen confidence in emerging technologies.

The expert consultation with 12 researchers and practitioners provided additional support for the framework's practicality, scalability, and alignment with developing-economy priorities. However, this validation should be interpreted as preliminary rather than as definitive empirical validation because the framework has not yet been tested through large-scale industrial implementation.

G. Theoretical and Practical Implications

Theoretically, this study extends sustainability-transition thinking into the advanced-materials domain by demonstrating that material innovation, lifecycle sustainability, institutional capacity, and implementation mechanisms should be considered as interconnected components. The study also contributes to the literature on sustainable materials management by conceptualizing MOF deployment as a socio-technical transition rather than a purely materials-science problem.

Practically, the findings provide several implications for policymakers and industry practitioners. First, technology-support programs should include sustainability indicators alongside conventional technical performance measures. Second, public funding should prioritize low-temperature synthesis, abundant precursor materials, solvent substitution, recyclability, and long-term stability. Third, demonstration projects should be designed around sectors where modular MOF technologies can provide immediate practical value. Fourth, national policies should strengthen research-industry linkages and develop standards for advanced materials. Finally, lifecycle assessment should be incorporated into technology-selection and investment decisions to prevent the unintended transfer of environmental burdens from the use phase to the manufacturing phase.

VI. CONCLUSION

A. Overall Conclusion

This study examined how Metal-Organic Frameworks can be designed and deployed more sustainably for CO_2 capture and energy-storage applications in developing economies. Based on a systematic synthesis of 127 studies published between 2015 and 2025, the study demonstrates that MOFs possess substantial potential to contribute to decarbonization and sustainable energy systems, but their practical contribution depends on more than their intrinsic material performance. Sustainable deployment requires simultaneous consideration of synthesis conditions, resource availability, lifecycle impacts, scalability, regeneration requirements, institutional capacity, financing, and stakeholder engagement.

The findings identified six critical design practices: low-temperature and solvent-minimized synthesis, use of abundant metal precursors, functionalization for enhanced selectivity and capacitance, shaping and formulation for scalability, regenerability and cycling stability, and lifecycle-oriented design. Collectively, these practices provide a pathway for improving both technical performance and sustainability outcomes.

The study also identified 23 barriers and 18 enablers distributed across five dimensions. Limited synthesis capacity, high precursor and solvent costs, weak regulatory frameworks, low stakeholder awareness, and environmentally intensive synthesis emerged as major constraints. In contrast, policy incentives, public-private partnerships, capacity building, and green-chemistry innovation emerged as important mechanisms for accelerating adoption.

To integrate these findings, the study developed a four-component implementation framework consisting of MOF design optimization, performance monitoring, contextual adaptation, and stakeholder engagement. The framework links material-level design choices to sustainability metrics and project-level monitoring systems while incorporating local institutional, economic, infrastructural, and social conditions.

B. Contribution to Sustainable Development

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The study demonstrates that MOF technologies can contribute to sustainable development only when their environmental benefits are evaluated against their complete lifecycle and implementation requirements. The emphasis on low-energy synthesis, abundant materials, recyclability, and efficient regeneration provides a pathway for reducing the environmental burden associated with advanced-material production while maintaining application performance.

For developing economies, the proposed framework is particularly relevant because it emphasizes affordability, scalability, local capacity, and compatibility with existing infrastructure. Rather than assuming that technologies developed in high-income countries can be transferred directly to emerging markets, the framework supports contextual adaptation and gradual deployment through modular systems, demonstration projects, and capacity-building initiatives.

C. Policy and Managerial Recommendations

Several policy recommendations follow from the findings. Governments should establish targeted incentives for low-carbon materials and support pilot-scale demonstrations of MOF-based technologies. Financing instruments such as green subsidies, concessional loans, and green bonds can help reduce the financial risks associated with early-stage deployment. Regulatory agencies should also develop appropriate standards for advanced materials and strengthen carbon-management frameworks.

For industry, technology selection should incorporate lifecycle cost, energy requirements, material availability, regeneration requirements, and end-of-life management rather than relying exclusively on laboratory performance. Firms should also collaborate with universities and research institutions to develop pilot projects and local technical capabilities.

For research institutions, future research should prioritize scalable synthesis, real-world stability, green solvents, recyclable precursors, shaped materials, and application-specific performance under realistic operating conditions. Greater integration between materials science, engineering, lifecycle assessment, economics, and policy research is necessary to accelerate technology translation.

D. Limitations and Future Research

The findings should be interpreted in light of several limitations. First, the available literature addressing both MOF sustainability and developing-economy contexts remains relatively limited, which may result in uneven geographical and technological representation. Second, reliance on published studies may introduce publication bias because successful or positive findings are more likely to be reported than unsuccessful experiments or negative results. Third, although expert consultation supported the practicality and relevance of the proposed framework, its applicability across different developing-economy contexts requires empirical validation through pilot projects and longitudinal case studies.

Future research should therefore move beyond conceptual framework development toward empirical testing. Comparative case studies across developing economies could examine how institutional capacity, energy infrastructure, industrial structure, and financing conditions influence MOF adoption. Pilot-scale studies should assess material performance under realistic humidity, impurities, temperature fluctuations, and repeated regeneration conditions. Future lifecycle assessments should also compare MOF technologies with conventional amine-based carbon capture and established energy-storage technologies using consistent system boundaries. Finally, techno-economic analysis and policy simulation could help identify the combinations of technological improvement, financial support, and regulatory intervention required to achieve economically viable and environmentally sustainable deployment.

E. Final Remarks

Overall, the study concludes that the future of MOF-based CO_2 capture and energy storage in developing economies depends on a transition from performance-centered materials innovation toward sustainability-centered implementation. High adsorption capacity, selectivity, capacitance, and cycling stability are necessary but insufficient conditions for successful deployment. The decisive challenge is to connect these technical capabilities with low-impact synthesis, affordable resources, scalable manufacturing, lifecycle management, effective monitoring, supportive institutions, and stakeholder capacity.

The proposed four-component framework provides a practical foundation for achieving this integration. By linking MOF design optimization, performance monitoring, contextual adaptation, and stakeholder engagement, it offers a pathway through which advanced materials research can be translated into implementable decarbonization and sustainable-energy solutions. In this sense, sustainable MOF deployment should not be understood simply as the commercialization of a high-performance material, but as the development of an integrated socio-technical system capable of delivering environmental, economic, and social value over the full technology lifecycle.

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