

Dye-Sensitized Metal-Organic Frameworks (MOFs): Design, Mechanisms, and Application Advances

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Abstract

Metal-organic frameworks (MOFs) have emerged as ideal carriers in photocatalysis owing to their high specific surface area, precisely tunable pore channels, and adjustable electronic structures. However, most MOFs suffer from weak visible-light response and facile recombination of photogenerated charge carriers. The dye-sensitization strategy, which constructs dye-MOF heterojunctions, can effectively broaden the light absorption range of materials and enhance interfacial charge separation and transport, representing an important pathway to overcome the limitations of traditional MOF and inorganic semiconductor-sensitized systems. This review summarizes the characteristics of dye-sensitized MOFs; elaborates on the mechanisms of electron injection, energy transfer, interfacial interactions, and multi-component synergistic catalysis in heterojunction construction; and surveys the research progress of these materials in photocatalysis

Keywords

Dye Sensitization; metal-organic framework (MOF); photocatalysis; heterojunction; charge carrier separation

1. Introduction

Metal-organic frameworks (MOFs) are crystalline porous materials formed through coordination self-assembly of metal ions or metal clusters with organic ligands. Leveraging their high specific surface area, tunable pore structures, and coordination environments, MOFs have become ideal platforms for optical property modulation and efficient photogenerated charge separation. Through ligand design and metal center regulation, the band structures and charge transfer mechanisms of MOFs can be precisely optimized, demonstrating tremendous application potential in photoelectric conversion, photocatalysis, and related fields.

As illustrated in Figure 1, dye sensitization refers to the process where dye molecules are excited to their excited states upon visible-light irradiation, subsequently injecting photogenerated electrons into the host material, thereby achieving light absorption-charge injection-charge separation. In dye-MOF composite systems, MOFs replace traditional inorganic porous hosts, utilizing their well-defined pore channels and coordination interactions to achieve high dispersion of dye molecules, strengthen interfacial electron transfer, and significantly improve photogenerated charge separation efficiency and material stability—representing a significant material upgrade from conventional sensitization systems.

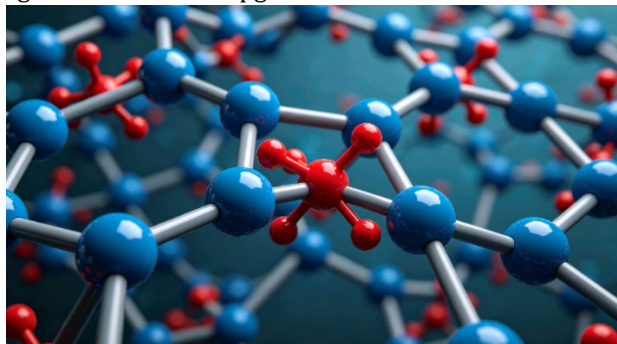


Figure 1. Binding modes between MOF frameworks and dye molecules

2. Characteristics of Dye-Sensitized MOF Materials

Dye-sensitized metal-organic framework (MOF) materials exhibit unique and remarkable characteristics that render them promising candidates for photocatalytic applications.

(1) Light Absorption Range

A core advantage of dye-sensitized MOF materials lies in the highly tunable nature of their light absorption range. By selecting dye molecules with distinct absorption spectral characteristics, the photoresponsive region of MOF materials can be effectively extended from ultraviolet (UV) to visible (Vis) and even near-infrared (NIR) regions. This capability is crucial for maximizing solar energy utilization, as the majority of solar energy resides in the visible and near-infrared regions. For instance, while certain organic ligands are limited to UV absorption, the incorporation of visible-light-sensitive dyes significantly enhances the overall light-harvesting efficiency of MOF-dye composites, enabling more effective driving of photocatalytic reactions.

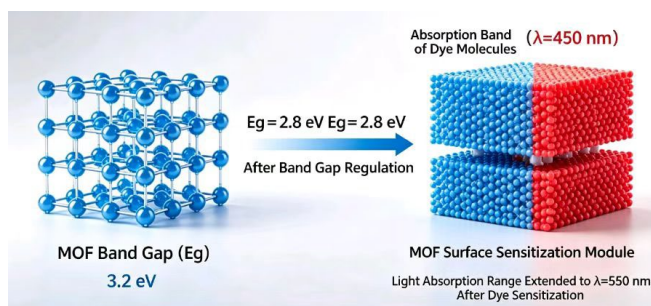


Figure 2. Schematic illustration of bandgap engineering and dye sensitization for extended light absorption

(2) Photogenerated Charge Carrier Separation Efficiency

The heterojunction interface formed between dyes and MOFs plays a pivotal role in enhancing the separation efficiency of photogenerated charge carriers (electron-hole pairs). Upon photoexcitation of dye molecules, their excited-state electrons can be efficiently injected into the conduction band or metal clusters of MOFs, thereby achieving rapid charge separation. This interfacial charge transfer mechanism effectively suppresses the recombination of photogenerated charge carriers, prolongs their lifetime, and consequently improves photocatalytic activity. Through rational interfacial design, Type II or Z-scheme heterojunctions can be constructed to further optimize charge transport pathways and minimize energy losses.

(3) Active Sites

MOF materials inherently possess abundant metal sites and organic ligand functional groups that can serve as catalytically active centers for reactions. The introduction of dye molecules not only augments light-harvesting capability but may also introduce new active sites or alter the electronic environment of existing sites, thereby diversifying reaction pathways and enhancing catalytic activity. For example, dye molecules can directly participate in redox reactions or form intermediates with reactants through their structural features, synergizing with the intrinsic catalytic functions of MOFs.

(4) Structural Stability and Designability

The high crystallinity and structural tunability of MOF materials provide stable scaffolds and flexible modulation space for dye sensitization. This structural stability and designability enable precise optimization of material structure, pore size, and channel functionality through controlled selection of metal nodes, organic ligands, and dye incorporation methods to accommodate specific photocatalytic applications.

3. Mechanisms of Dye Sensitization in MOF-Based Heterojunction

Construction

Dye-sensitized metal-organic frameworks (MOFs) enhance photocatalytic performance through heterojunction construction primarily via the following mechanisms.

3.1. Electron Transfer Mechanism

Upon light absorption, dye molecules are excited, and their energy levels in the excited state undergo significant changes. In this excited state, dyes inject electrons into the conduction band or metal clusters of intimately contacted MOF materials. This process achieves effective separation of photogenerated charge carriers, with electrons transferring from dyes to MOFs, thereby suppressing rapid electron-hole recombination, extending the lifetime of photogenerated charges, and consequently improving photocatalytic efficiency. This interfacial charge transfer constitutes one of the core mechanisms by which dye-sensitized MOF heterojunctions function.

3.2. Energy Transfer Mechanism

Beyond direct electron injection, dyes can also activate MOF catalytic activity through energy transfer upon light absorption. The most common energy transfer mechanism involves Förster resonance energy transfer (FRET). In this mechanism, excited dye molecules transfer their excitation energy non-radiatively to acceptors within the MOF, activating the MOF for catalytic participation. This energy transfer broadens the photoresponsive range of MOF materials, enabling catalytic activity under more extensive spectral illumination.

3.3. Interfacial Interactions

The intimate interface between dyes and MOFs is crucial for efficient photocatalysis. Dye molecules can form heterojunctions with MOFs through various modes, including non-covalent interactions (such as π - π stacking, hydrogen bonding), coordination bonds, or covalent bonds. These interactions ensure good contact between dyes and MOFs, providing favorable pathways for efficient electron or energy transfer. Optimized interfaces can significantly enhance electron or energy transport efficiency, reduce interfacial losses, and maximize catalytic performance. Fine-tuning of interfacial structures represents a key design strategy for improving dye-sensitized MOF material performance.

4. Application Advances

4.1. Pollutant Degradation

Toxic organic pollutants in water bodies, including dyes, antibiotics, and phenolic compounds, pose severe threats to ecosystems and human health. Many pristine MOFs exhibit insufficient visible-light response due to their wide bandgaps. As

shown in Figure 3, dye-sensitized MOF heterojunctions enhance visible-light response and photocatalytic efficiency by introducing dye molecules as light-harvesting units that absorb visible light and transfer energy or electrons to MOFs. This strategy has been successfully applied to the efficient degradation of various organic pollutants, including emerging organic contaminants (EOCs). Meanwhile, MOF-derived catalysts demonstrate exceptional performance in persulfate-based advanced oxidation processes, efficiently generating reactive radicals for rapid mineralization and removal of organic pollutants. Dye-sensitized MOF heterojunctions not only possess excellent photocatalytic activity but also provide abundant adsorption sites for pollutants through their porous structures, achieving an "adsorption-degradation" synergistic effect that enhances pollutant treatment efficiency.

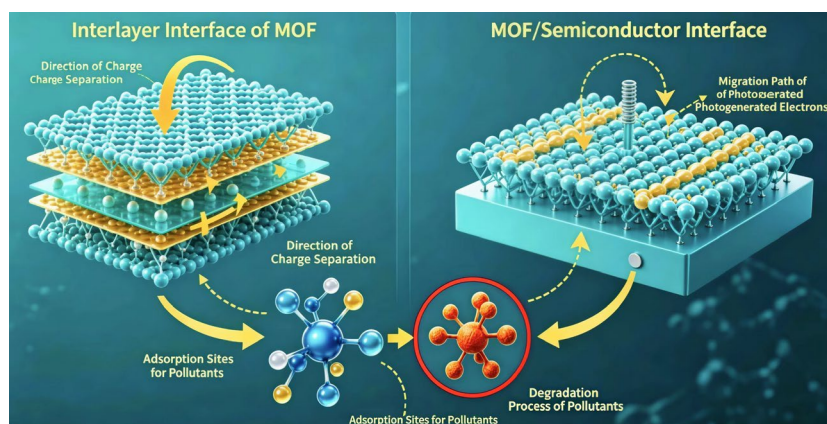


Figure 3. Charge separation and pollutant degradation pathways in MOF/semiconductor heterojunctions

4.2. Application of Dye-Sensitized MOFs in Photocatalytic CO₂ Reduction

Dye-sensitized metal-organic frameworks (MOFs) demonstrate significant application potential in photocatalytic carbon dioxide (CO₂) reduction. The primary mechanism involves effective light energy capture by dye-sensitized MOFs, followed by transfer of photogenerated charge carriers to adsorbed CO₂ molecules, thereby reducing them to high-value-added products such as carbon monoxide (CO), methane (CH₄), or methanol.

The introduction of dyes further enhances the light-harvesting capability of MOFs. Strategies including ion-exchange encapsulation of cyanine dyes [14], post-synthetic modification with acetylacetone [16] (AA), and construction of porphyrin-based MOFs [18] (PMOFs) have broadened their absorption range to visible and even near-infrared light, which is essential for maximizing solar energy utilization [17]. As illustrated in Figure 4, upon light absorption, dyes activate MOF catalytic activity and promote charge separation through electron transfer or energy transfer

mechanisms. This efficient charge separation suppresses recombination of photogenerated electron-hole pairs, prolongs carrier lifetime, and ultimately achieves substantial enhancement in CO₂ reduction efficiency while effectively regulating product selectivity, significantly improving both the photocatalytic efficiency and product selectivity of CO₂ reduction[19].

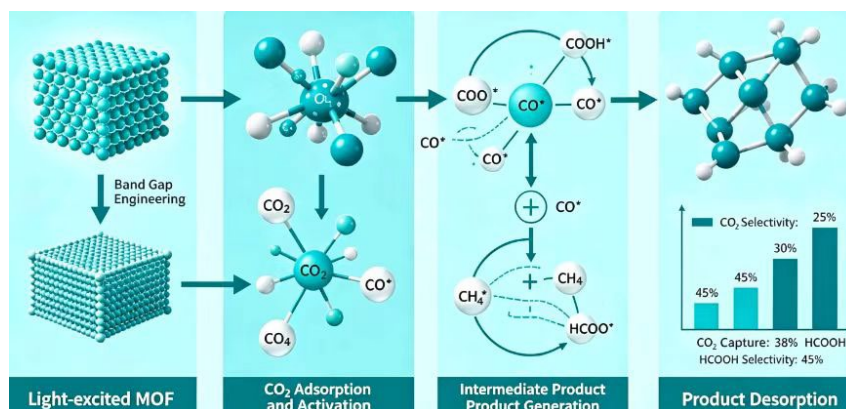


Figure 4. Overall reaction pathways and product distribution in MOF-based photocatalytic CO₂ reduction

4.3. Catalysis

Beyond photocatalysis, MOFs exhibit tremendous application potential in conventional non-photocatalytic reactions. Metal nodes or organic ligands of MOFs (such as those containing -NH₂, -COOH, -SO₃H functional groups) can serve as catalytically active centers for various organic reactions, redox reactions, and enzyme-mimetic reactions. Their inherent porous structures provide nanoscale reaction vessels that enhance reaction selectivity and allow efficient reactant access to active sites. Furthermore, the structural diversity of MOFs enables precise regulation of catalyst activity and selectivity through modification of metal centers, organic ligands, or post-synthetic modification. For instance, in organic reactions, Zr-UiO-66 series MOFs can catalyze esterification[21] For instance, in organic reactions, Zr-UiO-66 series MOFs can catalyze esterification [21] ; as shown in Figure 5, in nitrogen reduction reactions, Fe- and Mo-containing MOFs can activate N₂ molecules for ammonia synthesis, , while post-synthetic modification can further endow MOFs with specific properties and expand their applications.

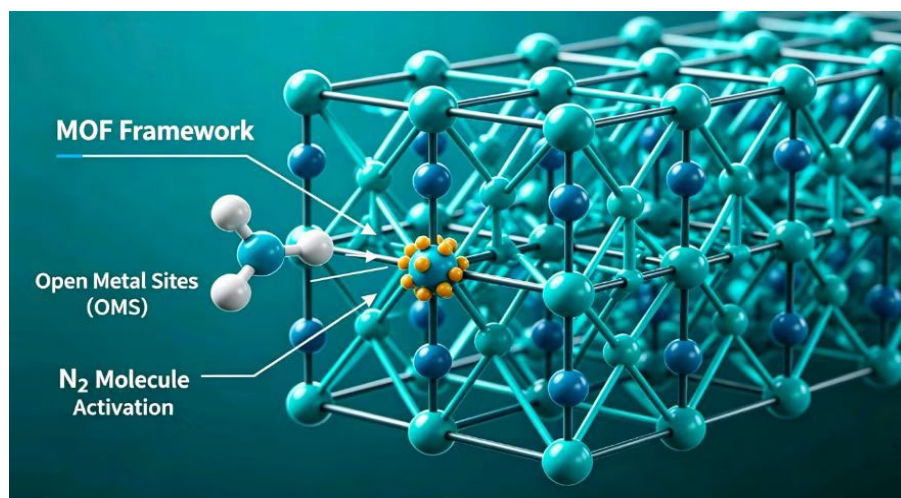


Figure 5. Activation of N_2 molecules by open metal sites (OMS) in MOFs

5. Conclusion

Significant progress has been achieved in the research of dye-sensitized metal-organic frameworks (MOFs) for constructing heterojunctions in photocatalytic pollutant degradation and catalytic reduction reactions. Research in this field has not only advanced the application of MOF materials in environmental remediation and energy conversion but also laid foundations for developing next-generation high-efficiency photocatalytic materials.

Looking forward, dye-sensitized MOFs demonstrate broad prospects as new-generation high-efficiency photocatalytic materials. Research will continue focusing on enhancing material stability and durability, particularly long-term operational performance under complex aqueous environments, acidic/alkaline conditions, and intense illumination. The development of novel efficient, environmentally friendly dyes with broad-spectrum absorption capabilities, alongside MOF materials with superior photoelectric properties, will be critical directions. Fine-tuning of heterojunctions through interfacial engineering, morphology control, and post-synthetic modification to optimize dye-MOF interactions and electron transport pathways will further enhance catalytic efficiency. Moreover, integrating dye-sensitized MOFs with other functional materials such as semiconductors, noble metal nanoparticles, and carbon materials may achieve multi-functional synergistic effects, thereby comprehensively improving their photocatalytic performance.

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