Environmental Science and Ecotechnology 24 (2025) 100545

Contents lists available at ScienceDirect

Environmental Science and Ecotechnology

journal homepage: www.journals.elsevier.com/environmental-science-and-ecotechnology/

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Innovative MOF materials for a sustainable future: Tackling energy and environmental challenges

1. Introduction

The development of human society has caused global energy demand and consumption to grow rapidly. The extensive consumption of fossil fuels (e.g., oil and coal) has dramatically increased environmental pollution and greenhouse gas emissions, seriously threatening the ecological system and human health. Developing green and sustainable technologies should be investigated and pursued to benefit human society. In addition, designing efficient and multifunctional materials is vital in new energy and environmental development. The metal-organic framework (MOF) is a kind of functional and highly porous nanomaterial composed of metal-based nodes and organic ligands, providing reactive sites for energy and environmental fields. In recent years, a series of derived MOFs has ushered in the extensive development of covalent organic frameworks, hybrid porous materials, hydrogen-bonded organic frameworks, dynamic and intelligent MOFs, flexible MOFs, and the like. MOFs have large specific surface areas, rich active sites, controllable chemical structures, and different growth morphologies, including three-dimensional networks, two-dimensional (2D) sheets, and one-dimensional nanorods. MOFs have attracted extensive attention for their unique properties and structures in several fields, including carbon dioxide separation, carbon dioxide capture, carbon dioxide catalysis, hydrogen storage, and batteries and supercapacitors. While most MOFs have poor stability and conductivity, conductive MOFs have been extensively investigated. When MOFs are applied as electrode materials, they are mainly utilized to obtain MOF composites, MOF-derived materials, and modified MOF-derived materials. This commentary primarily focuses on the applications of MOFs in electrocatalysis, electrochemical energy storage, and electrosorption.

2. Engineering MOFs for diversified energy storage and conversion systems

The emergence of efficient energy storage and conversion systems is significant in developing renewable energy. The most widely studied energy storage devices thus far are batteries, supercapacitors, hydrogen storage, methane storage, photovoltaic cells, and fuel cells. Device performance when charging or discharging mainly depends on the development of advanced materials. Lithium batteries are the most commonly used energy storage devices and function as various secondary batteries; however, their poor energy density and cycle life have limited their long-term development. MOF-based batteries suffer from power loss, performance deterioration, and dendrite formation. Furthermore, electrodes, electrolytes, and cell resistance induce power dissipation, causing by the resistance of the electrodes, electrolytes, and internal cell components. While this inefficiency might reduce energy storage capacity and performance, refining electrode materials and cell design can help solve this problem. MOF-based batteries lose performance due to electrode degeneration and electrolyte breakdown; thus, they require better materials and innovative battery management. Moreover, common dendrite formation causes short circuits and battery life. Protective coatings and electrolyte additives are necessary for battery safety and dendrite prevention. These difficulties demonstrate the need for ongoing research to improve MOF-based battery performance for various applications.

$Al(OH)[O_2C\text{-}C_6H_4\text{-}CO_2]$@graphene composite created by inducing structural disorder in MOF crystals through the extraction and insertion of lithium were prepared and applied to lithium-ion batteries [1]. Specific capacity increased rapidly (from 60 to 400 mAh g^{-1}) at a current density of 100 mA g^{-1}. This strategy of inducing structural change enhanced the diffusion and storage of Li^+, and the conductivity of Al-MOF was enhanced due to conductive graphene. This method indicated that MOFs could be used in energy storage devices and could be extended to next-generation energy storage devices, such as lithium sulfur batteries and lithium air batteries. Hanna Breunig et al. reported using economic analysis on MOFs for hydrogen storage and found them to be economically comparable to modern energy storage technologies when designed appropriately by optimized equipment. Furthermore, future research in this area could focus on MOFs capable of adsorbing 15 g of hydrogen per kg at production costs under USD 10 per kg, making them important alternative materials for energy storage [2]. Donald J. Siegel et al. filtrated nearly half a million metal—organic frameworks and found that SNU-70, UMCM-9, and PCN-610/NU-100 had higher excellent capacities than IRMOF-20 [3]. Wu et al. achieved high power conversion, long-term stability, and low lead leakage in solar cells by preparing thiol-functionalized 2D conjugated metal—organic frameworks as solar cell materials [4]. Oxygen reduction reaction (ORR), oxygen evolution reaction (OER), and hydrogen evolution reaction (HER) are the dominant reactions in the development of sustainable energy technology. They are also essential in conversion reactions between chemical energy and electric energy. The properties of electrocatalysts affect these electrochemical reactions, including surface area, conductivity, stability, active site density, etc. Mukhopadhyay et al. reported on a nitrile-modified MOF film that had a significant CO_2 solvation layer, which was locally 27-fold higher than the intrinsic electrolyte and was able to reach a concentration of 0.82 M. This significantly improved the conversion of CO_2 to formic acid, with a selectivity

https://doi.org/10.1016/j.ese.2025.100545

of more than 90 % [5]. A Co-N co-doped porous carbon catalyst converted via the pyrolysis of ZIF-67 attracted the limelight. Due to its large surface area and pore volume as well as the synergistic effect of Co-N, the catalyst improved mass transfer and electron transfer and indicated excellent ORR activity and stability. In 2019, ZIF-67-derived nickel cobalt oxide sulfide nanocomposites were proven to have high activity. The synergistic effect of ZIF-67 and metal sulfides enhanced the catalytic activities of these three reactions. ZIF-67 also had excellent durability and stability. It could be directly applied to electrochemical water decomposition to facilitate hydrogen production in zinc-air batteries. Like MOF-74 series of NiCoFe-MOF-74, the reports have confirmed their stable OER currents and excellent OER performance. Through the density functional theory calculations, the synergistic effect of Ni, Co, and Fe_3O_4 could enhance the catalyst's activity. Fe-Zn MOF also served as the precursor to creating Fe with a hierarchical structure through pyrolysis. This resulted in an Fe_3C@N-C double-function electrocatalyst, demonstrating outstanding electrocatalytic performance in HER and ORR. In recent years, the development of tri-functional electrocatalysts has gained much scholarly interest, facilitating the progress of large-scale commercialization. Cobalt porphyrin has been linked into covalent organic frameworks (COF-366 and COF-367) by imine bonds and could be investigated to reduce CO_2 to CO. COF-367-Co had a higher Faradaic efficiency of 91 % for the reduction reaction. In 2022, the MOFs/COFs (UiO-66-NH_2/COF-366-OH-Cu) attracted attention due to the high adsorption capacity of CO_2 and the conversion of CO_2 to CH_4. It reached a high current density of -398.1 mA cm^{-2} and a Faradaic efficiency of 76.7 %. These conversions could potentially contribute to carbon neutrality and clean energy production.

Improving the stability, conductivity, and creation of MOF-derived carbon materials with precisely tuned pore diameters is essential for collectively enhancing the effectiveness of MOF-based energy storage devices. Cost-effective MOFs for hydrogen storage can compete with existing storage technologies. Advancements in MOF-based electrocatalysts can significantly augment mass and electron transport, thereby enhancing catalytic activity.

3. Superior purification role of MOFs in aquatic environments

The lack of fresh water is a key environmental problem in the 21st century. Population growth has increased the demand for fresh water; thus, various water desalination technologies such as electrocoagulation, electrodialysis, and capacitive deionization, have been investigated. Capacitive deionization (CDI) technology is a new type of water treatment technology based on electric double layer theory, which has the advantages of being environmentally friendly, large-scale, energy efficient, and easily operable. CDI has become an alternative desalination method for water purification due to lower energy consumption, faster regeneration cycles, etc. Electrode materials are important to CDI batteries, as they largely determine CDI performance. At the time of this writing, the electrode materials used in CDI include various porous carbons, such as activated carbon, carbon nanotubes, and graphene oxide. However, carbon electrodes have low stability and are ineffective at the desalination and removal of ions. MOF-derived carbon materials have become one of the most promising electrode materials in the field of capacitive deionization technology due to their varied structures, well-developed pores, and excellent electric double-layer properties. It was also conducive to ion transport and charge transfer. Through element doping in MOF materials, multiple synergistic effects are helpful in enhancing MOF's ability to mitigate pollution. ZIF-8 was combined with N, P, and S co-doped hollow carbon polyhedron materials, indicating excellent stability and high specific capacitance. When combined with other carbon materials, MOFs can form compounds that result in new, high-efficiency electrode materials. Similarly, a series of multi-metal source-derived ZIFs were used to form nitrogen-rich, hierarchical hollow carbon materials for capacitive deionization desalination. Performance was significantly enhanced by trace doping with Ni, achieving a capacity of 37.8 mg g^{-1} [6]. In addition to its use in the desalination field, CDI technology has also been applied to remove pollutants in water. Some research innovatively combined CDI and photocatalysis technology to extract heavy metal chromium from water. Jiang et al. prepared three-dimensional layered conductive MOF/layered double hydroxide/carbon fiber materials that were then employed in applied hybrid capacitive deionization batteries, which exhibited excellent salt adsorption capacities of up to 147.8 mg g^{-1}. Furthermore, the performance remained constant at 91.4 % after 50 cycles [7]. By electro-depositing Ce/Zn-BDC-NH_2/polypyrrole/graphite substrate as the anode and flower-like manganese dioxide as the cathode, one study found that the electro-adsorption capacity for removing fluoride reached 55.12 mg g^{-1} when the electro-adsorption voltage was 1.2 V with an initial fluoride concentration was of 100 mg L^{-1} F^- [8]. In sum, this represents a new mechanism in using MOFs for capacitive deionization.

4. Conclusion

This article primarily discusses the development status of MOF materials in the fields of electrochemistry, energy storage, electrocatalysis, and electrosorption-multifaceted and diverse fields. We hope to provide guided themes to researchers in related fields. We also look to inspire scientists to achieve even more exciting results in these research areas, and promote further innovation in this field. Artificial intelligence technology is also expected to improve the development of energy and environmental areas through the use of metal-organic frameworks.

CRediT authorship contribution statement

Junye Cheng: Writing – original draft, Supervision, Resources, Methodology, Formal analysis, Conceptualization. **Lei Huang:** Writing – review & editing, Resources, Formal analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

This project is financially supported by the National Natural Science Foundation of China (52372289, 52102368, 5251101192), Guangdong Special Fund for key Areas (20237DZX3042), State Key Laboratory of New Ceramic Materials Tsinghua University (No. KF202415), and Shenzhen Stable Support Project.

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8 November 2024