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Application of MOF Materials in Electrochemical Energy Storage Devices

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Abstract. Metal-organic frameworks (MOFs), due to their highly ordered structure, ultra-high specific surface area, and adjustable porosity, have become highly promising new energy storage materials. This article reviews the applications of MOFs and their derivatives in energy storage devices such as supercapacitors and lithium/sodium-ion batteries, and discusses the design principles for enhancing their conductivity, optimizing their porous structures, and strengthening their structural stability. Although MOFs can be directly used as electrode materials due to their advantages such as adjustable structure and large specific surface area, their inherent poor conductivity and the decrease in ion transmission efficiency with increasing thickness limit their practical applications. Through carbonization treatment, the conductivity can be significantly enhanced and a stable porous carbon framework can be formed, such as the C-ZIF-67 material; while when combined with carbon materials, conductive polymers or metal oxides (such as PANI/MIL-101), multiple advantages can be integrated, significantly improving the electrochemical performance, mechanical strength and cycle life, thus becoming an effective strategy to break through the practical application bottleneck of MOFs. This article summarizes the current challenges in the industrialization process of MOF materials, such as costs, structural control, and processing difficulties. It proposes solutions including green synthesis, machine learning-assisted design, and the construction of conductive composite structures.

Keywords: Supercapacitor, Conductivity, Carbon-based materials, Composite materials, Structural Design

1. Introduction

With the development of human society, the demand for electrochemical energy storage devices has been continuously increasing due to the widespread popularity of renewable energy sources such as solar and wind power, as well as electric vehicles and portable electronic devices. Such types as lithium-ion batteries, supercapacitors, and sodium-ion batteries have gradually become key components of green energy systems. To meet the requirements of daily use for higher energy storage density and longer cycle life performance. Metal Organic Frameworks (MOFs) have gradually demonstrated unique advantages in the field of electrochemical energy storage due to their

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highly ordered crystal structure, extremely high specific surface area, multiple pore diameters, and diverse selection of metal/organic components [1]. Compared with traditional carbon materials, metal oxides, or conductive polymers, MOFs can achieve higher exposure of active sites and better ion transmission channels. Moreover, their conductivity and structural stability can be further optimized through post-treatment methods (such as carbonization, doping, and composites, etc.). Therefore, MOFs and their derivative materials are becoming an important research direction for the next generation of high-performance energy storage electrode materials.

This paper explores the application value of MOFs in various electrochemical energy storage devices, and this advancement plays a positive role in promoting the continuous development of energy storage technology.

2. Definition of MOF materials

MOFs a one-dimensional or multi-dimensional structures which is synergistically affected by the metal ions or metal clusters and organic ligands [2]. It has a highly ordered pore structure, a huge surface area, and adjustable chemistry. Therefore, it is considered the molecular sponge. The basic structure of MOFs consists of metal nodes and organic ligands. Metal nodes are composed of transition metal ions, like Fe^{2+}, Zn^{2+}, and Cu^{2+}, and metal clusters, like Zn_4O and Cr_4O. The specific capacity of Fe-MOFs is generally higher than that of Zn-MOFs. Howver, the stability is poor. organic ligands are composed of Carboxylic acids, like the phthalic acid and the trimesic acid,and Nitrogen-containing, like the imidazole and the triazole. The conductivity of nitrogen-containing ligands is greater carboxylic acid ligands. The meaning of MOFs has important application prospects in physics, including gas separation and sensing, chemistry, including catalysis and luminescence, and even the biomedical sciences.

3. Performance parameters of MOF materials

The performance parameters of MOF materials can be analyzed into three parts, including the specific surface area, the pore structure, and the conductivity.

First, the metal organic materials have extremely high specific surface area, and the specific surface area means the sum of the total external surface area of all particles per gram of substance, the international units are g/m^2. The specific surface area determines the material's reactivity and the mass transfer efficiency. Metal organic materials' specific surface area can get 4500 to 6000g/m^2 [3]. Therefore, MOFs have good catalytic properties.

Second, MOF materials have high porosity. Porosity refers to the size and distribution of pores. According to the size of the pores, we can divide them into macropores (greater than 50nm), mesopores (2-50nm), and micropores (less than 2nm). The pore size of MOFs can range from 2.28 to 3.8 [4]. This makes MOFs have great potential in chemical energy storage, gas separation, and so on.

Finally, MOFs have better conductivity. Conductivity means a material's ability to conduct electric current. The nature of the MOFs is that free electrons within a material to move in a directed manner. The SI unit is siemens per meter S/m. In the past decade, the conductivity of MOFs has reached more than 10^{-3} S/cm. Some of them can even reach 40S/m. This makes metal-organic materials suitable for energy storage and sensing fields such as electrocatalysis and chemiresistive sensors.

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4. Specific applications of MOFs in the electrochemical energy storage field

4.1. MOFs' intrinsic materials

MOFs can be directly used as electrode materials in the electrochemical energy storage field. In 2009, Takaishi et al. discovered an electrode material prepared from $Cu[Cu(2,3\text{-}pdt)_2]$. The electrical conductivity of this kind of material is 6×10^{-4} S cm^{-1} at 300 K, which is an ultra-high data [5]. This material is an ideal supercapacitor material. In 2017, Sheberla et al. developed a highly conductive MOF material that can be used as the only electrode material in double-layer capacitors [6]. This is the first time that a supercapacitor can be made entirely of neat MOFs as active materials. The electrode made in this way does not contain conductive additives or other binders. It can retain more than 90% of its capacity after 10,000 cycles, and its active electrode material can be tuned at the molecular level [6]. This research heralds a new generation of supercapacitors that will come.

MOFs' intrinsic materials have structural advantages. This is because their crystal structure is clear and can be controlled precisely. Through techniques such as single-crystal X-ray diffraction, the structure of MOFs can be characterized at the atomic level. Therefore, their structure-activity relationship can be deeply clarified and understood. Then the structure of MOFs can be further optimized. In addition, since the pore structure of MOFs can be designed directionally, it is beneficial to optimize the conductivity of electrode materials. However, in practical applications, the preparation of these materials still faces many challenges. For example, the conductivity of most MOFs' intrinsic materials is insufficient. This is because when preparing electrodes with a certain thickness, due to the presence of a large amount of highly active substances, the load on the electrode becomes larger, and the ion transmission efficiency will be reduced significantly. To overcome these limitations and improve the performance of materials, researchers need to design structures with special conductive networks and adopt highly difficult preparation processes.

4.2. MOF-derived electrode materials

Since MOFs have inherent defects when used directly as electrode materials, MOF derivatives are more widely used in the field of electrochemical energy storage. In 2022, statistics from Zhang et al. showed that MOF derivatives had accounted for 62% of the energy storage field, exceeding the proportion of intrinsic MOF materials [7]. MOF-derived materials mainly include carbonized materials and composite materials.

4.2.1. MOF-derived carbonized materials

MOF carbonized materials are mainly prepared by pyrolyzing MOF precursors. At high temperatures, organic ligands undergo carbonization reactions and form a carbon skeleton with a porous structure. Due to the existence of this structure, by reasonably controlling the reaction temperature and other conditions, the structure of the product can be accurately controlled. The materials prepared in this way will have superior properties. Compared with other materials, MOF carbonized materials have a higher specific surface area, and their pore structure can be precisely controlled. These properties make them ideal materials for high-performance supercapacitor electrodes. In 2025, Zou et al. used an organic framework material (ZIF-67) based on cobalt metal with high surface area and good crystallinity as a precursor, prepared C-ZIF-67/PANI composite materials through high-temperature calcination and in situ polymerization [8].

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The specific capacitance of this capacitor material is 450.5 F g^{-1} [8]. After 5000 charge and discharge cycle tests at a current density of 8 A g^{-1}, the specific capacitance value still maintains 71% of the initial value [8]. The research results show that C-ZIF-67/PANI has excellent cycling stability.

MOF-derived carbonized materials can also be obtained by carbonization directly, a typical example of which is Ni-BPA. In 2025, Tai et al. developed a new 3D nitrogen-rich nickel-based c-MOF material Ni-BPA, which has a carbon-carbon triple bond. Its rigid structure gives MOF strongerπelectrons. Theσof Ni-BPA is 5.64×10^{-3} S m^{-1}, showing excellent conductivity [9]. Ni-BPA produces a high specific capacitance of 532.4 F g^{-1} at 1 Ag^{-1} [9]. The Ni-BPA//AC device has a capacitance retention rate of 91.9% and a coulombic efficiency of 98.6% after 10,000 cycles, showing excellent cycle stability [9].

4.2.2. MOF-based composite materials

MOF composite materials are formed by combining MOFs with other functional materials. Common composite methods include composites with carbon materials, composites with conductive polymers, and composites with metal oxides. Examples of composites with carbon materials include HKUST-1 composite nanomaterials. In 2019, N.H et al. composited HKUST-1-derived copper sulfide polyhedrons and nitrogen-doped carbon polyhedrons to form supercapacitors interspersed in carbon nanotube films [10]. The material exhibited an excellent energy density of 38.4 Wh kg^{-1} at a power density of 750 W kg^{-1}, making it an excellent flexible composite electrode [10]. In 2024, a new type of conductive porous metal-organic framework material $Ni_3(HITP)_2$ was developed and synthesized by B.S et al. [11]. By growing $Ni_3(HITP)_2$ films on a variety of 2D substrates and 3D nanostructured substrates, the B.S. team successfully developed a micro supercapacitor with a thin film interlaced structure[11].

An example of a composite with conductive polymers is PANI/MIL-101. In 2024, Wang et al. successfully prepared a composite material named PANI/MIL101 [12]. The flexible supercapacitor prepared from this material has a specific capacity of up to 1197F/g, and the specific capacity only decays by 10% after 1000 bending cycles [12]. The specific capacity can be maintained at more than 90% after 10,000 cycles of the cycle stability test [12]. The data above shows that PANI/MIL101 has good application prospects in flexible electronic devices and energy storage.

Examples of MOFs composite with metal oxides are $MoO_3@TiO_2$and so on. In 2018, Lou, X. W. et al. used a MOF-assisted synthesis method to embed Fe_2O_3 nanotubes on Co_3O_4 particles to prepare a hierarchical composite nanostructure [13]. The structural and compositional characteristics of this hierarchical composite material are conducive to improving its lithium storage performance. The energy storage device prepared from this material will have an initial charge and discharge capacity of 709.89 and 921.9 mAh/g at 0.5 A/g [13]. After 80 cycles, the discharge capacity remains at 951 mAh/g, providing a new idea for the controllable synthesis of complex hollow nanostructures and has broad development prospects in the field of energy storage [13]. In addition, in 2022, Wang et al. coated an ultra-thin TiO_2 shell on MoO_3 nanorods to prepare $MoO_3@TiO_2$ [14]. The full battery prepared from this material can provide an energy density of up to 252.9 Wh kg^{-1} and a power density of 18.3 kW kg^{-1}, showing excellent electrochemical performance [14].

Through carbonization and composite strategies, MOF-derived electrode materials can have stronger conductivity and more stable structures. The rich porous structure of MOF-derived materials can promote the penetration of electrolytes and improve ion transfer efficiency. However, there are still some challenges in the preparation process of MOF derivative electrode materials. For

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example, carbonized materials may experience structural collapse during the pyrolysis process, and it is difficult to achieve accurate composite bonding at the interface of composite materials.

5. Challenges and solutions of MOF materials in electrochemical energy storage

5.1. Main challenges

MOF materials are often expensive, as certain variants with superior electrochemical performance rely on noble metals (e.g., Ru, Pt, Pd) as metal centers. These noble metal MOFs, although possessing excellent electrochemical activity, are severely limited in practical application in large-scale energy storage devices due to their high raw material costs and scarce resources [15]. The synthesis of MOFs' crystallinity is highly sensitive to parameters such as temperature, reaction time, and solution concentration. Even minor changes can lead to significant differences in the crystal structure, pore size distribution, and even composition, thereby affecting its specific surface area, conductivity, and cycling stability. This poses a challenge for large-scale manufacturing [16]. Most MOFs exist as microcrystalline powders, exhibiting limited processability, inadequate mechanical strength, and low electrical conductivity. These drawbacks hinder their direct application in fabricating high-performance electrodes. Limited its practical integration and application in batteries and supercapacitors [17].

5.2. The current solution approach

A green and low-cost synthetic route is needed to reduce the environmental burden and production costs. Many studies have focused on green synthesis methods, such as the hydrothermal method, solvent-free ball milling method, and room-temperature self-assembly. These methods can reduce the use of harmful organic solvents and have strong scalability [15]. The combination of machine learning and first-principles calculations has been applied to predict and screen the structural properties of MOFs, significantly accelerating the development of new energy storage materials. By constructing structural descriptors and performance models, it is possible to accurately predict key indicators such as the conductivity, stability, and capacity of MOFs [18].Constructing conductive composite structures involves combining MOFs with conductive materials (such as carbon nanotubes, graphene, MXene, or conductive polymers). This process significantly enhances the electronic transmission performance and structural stability of the composite materials. For instance, the MOF/MXene composite electrode exhibits excellent rate performance and cycle life in supercapacitors [19].

6. Conclusion

MOFs and their derivatives, with their highly ordered structure, extremely high specific surface area, and tunable porosity, demonstrate unique advantages in the field of electrochemical energy storage. By undergoing carbonization treatment or combining with carbon materials, conductive polymers, and metal oxides, the conductivity and structural stability of the material can be significantly improved, thereby enhancing the cycle life and energy density. However, problems such as high cost, complex structural control, and poor processing performance still limit its large-scale application. The main trends for future development are reflected in four aspects: Firstly, a multi-functional integrated structure is constructed to achieve the collaborative design of energy storage, electro-catalysis, and conductive network. Secondly, develop low-cost systems centered on common transition metals such as Fe, Ni, and Co, and introduce green and renewable ligands to reduce the

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production cost. Fourth, establish a standardized production system covering design, synthesis, and evaluation, to facilitate the implementation of industrialization. Overall, the development of MOFs and their derivatives has provided new ideas for the research on energy storage materials and has laid an important foundation for the future energy transition and sustainable development.

Authors contribution

All the authors contributed equally and their names were listed in alphabetical order.

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