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Research Progress on Improving Energy Density Through Structural Modification Engineering of MXenes-Based Materials

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Abstract. Since the first synthesis of MXenes in 2011,researchers believe that these materials will be excellent candidates for fabricating the next-generation energy storage divices because of their own adjustable surface chemistry, superior conductivity, and high energy density. However, influenced by surface functional groups and structural instability, their energy density in energy storage applications remains relatively lower than that of lithium capacitors. Based on theoretical and experimental studies on modifying MXenes' interlayer spacing to enhance conductivity and energy density, this review briefly discusses the charge storage mechanism of MXenes and the research progress in improving energy density through various structural modification engineering approaches. Specifically, it introduces advances in modifying traditional MXene structures via multiple methods to boost energy density. This review concludes that structural modification engineering of MXenes exhibits remarkable effects in improving their electrochemical performance. In the future, such engineering will aim to provide new insights for optimizing MXenes and further enhancing their energy density.

Keywords: Two-dimensional Material, MXenes, Intercalation, Energy Density

1. Introduction

With the rapid development of the global energy industry, solar energy and others are regarded as clean energy sources have garnered significant attention. Nonetheless, because of the unstable properties of storing energy, researchers are compelled to develop efficient conversion and energy storage devices. Two-dimensional (2D) materials have been extensively explored in the energy storage field owing to their excellent physical and chemical properties, including the ability to store a large number of ions between layers without significant structural changes and the provision of high capacitance even at high discharge rates [1]. As a newly discovered class of two-dimensional layered materials, MXenes are composed of transition metal carbides, nitrides, or carbonnitrides, which can be prepared by chemical etching and exfoliation from MAX phases. They have developed rapidly due to their unique structures [2,3]. MXenes, as a novel category of 2D materials, follow a formula of Mn+1XnTx (n = 1-4), M can be represented as transition metal element(e.g., Ti, Nb, Mo, etc.), X denotes carbon and/or nitrogen, Tx refers to surface terminals [4]. Benefiting from their

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remarkable intrinsic properties such as considerable mechanical strength, tunable interlayer spacing, high metallic conductivity, and intercalation charge storage capability, MXenes have been widely applied in energy storage [1]. Despite their excellent performance, MXenes still face challenges such as interlayer restacking and insufficient conductivity, which affect specific surface area, charge storage capacity, ion diffusion rate, and other key properties, thereby limiting their energy storage potential [5]. To address these issues and further exploit their application prospects in energy storage, structural modification methods for MXenes have been developed.

The main structural modification approaches for MXenes include intercalation engineering and heterostructure synthesis of composite materials. Intercalation engineering modifies the interlayer spacing by inserting different substances (e.g., metals, organic materials) between MXene layers, effectively improving the ion diffusion environment. Heterostructure synthesis of composites involves introducing impurity particles onto the material surface or forming hybrid structures with carbon materials, polymers, etc., which modulates charge distribution and synergistically integrates the advantages of each component to enhance electrical performance [5]. Based on the above aspects, this review briefly introduces various modification methods for MXenes, discusses their unique characteristics, summarizes the mechanisms and features of similar methods, and finally prospects new approaches for improving the electrochemical performance of MXenes.

2. Improvement of energy density by intercalation mechanism

2.1. Metal-based intercalation

Among MXene materials, Ti3C2Tx has been extensively studied due to its abundant and easily modifiable surface functional groups and unique 2D nanosheet structure. However, the interlayer restacking of Ti_3C_2Tx limits its energy density. To address this, nanoparticles (NPs) can be introduced into the Ti_3C_2Tx structure through insertion or filling: Ti3C2Tx is mechanically mixed with nickel NPs in a paste mixer to obtain 10% Ni-MXene [6]. The diffraction peak of the hybrid MXene shifts from 7.5° (pure MXene) to a lower angle of $2\theta = 6.1°$ (10% Ni-MXene), accompanied by a gradual increase in full width at half height (FWHM), indicating expanded interlayer spacing of MXene due to nickel NP intercalation [6]. The resulting 10% Ni-MXene exhibits a cyclic stability of 83.7% after 10,000 cycles, achieved a high power of 1872 W per kilogram, and an energy density of 26 Wh kg^{-1}. In hydrogen evolution reaction (HER) measurements, it achieved an overpotential (OP) of 109 mV at 10 mA cm^{-2} and a maximum current density (J) of 200 mA cm^{-2} [6]. This intercalation effectively expands the interlayer spacing and improves electrochemical performance, demonstrating the effectiveness of the intercalation mechanism.

Metal ion intercalation also shows significant modifications to MXene materials. Treatment of MXenes with Lewis basic halides can similarly expand their interlayer spacing [4]. Eutectic molten salts of $AlBr_3$/NaBr/KBr and AlI_3/NaI/KI were used to treat Ti_3C_2Tx to form Lewis basic halide-modified MXenes (LB-Ti_3C_2Tx). The interlayer spacing increased from 11.2 Å (pristine Ti_3C_2T) to 14.7 Å (LB-Ti_3C_2T). In storage performance measurements, the specific capacity of the LB-Ti_3C_2Tx electrode was 168 mAh g^{-1}, corresponding to 215 F g^{-1} ,and the scan rate is 0.5 mV s^{-1}. Under the same conditions, the specific capacity of pristine Ti3C2Tx was only 78 mAh g^{-1} (99 F g^{-1}). When the scan rate increased to 100 mV s^{-1}, the specific capacity of Ti_3C_2Tx was 14 mAh g^{-1}, while that of LB-Ti_3C_2Tx was 42 mAh g^{-1}, three times higher than that of Ti_3C_2Tx [4]. Additionally, at a specific current of 0.1 A g^{-1}, LB-Ti_3C_2Tx achieved a maximum capacity of 229 mAh g^{-1} with a high Coulombic efficiency of 96%, significantly outperforming pristine Ti_3C_2Tx [4]. Furthermore, intercalation of K into Ti_3C_2Tx reduces the concentration of surface functional groups and improves

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material conductivity, while subsequent insertion of Ag nanowires compensates for the conductivity loss caused by intercalation and annealing. Meanwhile, the unique structural characteristics of Ag nanowires can promote charge transfer processes [4,7]. This hybrid intercalated MXene material achieved a high energy density of 6.9 mWh g^{-1} at a power density of 350 mW g^{-1}, significantly higher than previous MXene-based devices, demonstrating its potential in energy storage [7].

2.2. Organic and non-metal material intercalation

Given the remarkable achievements of intercalation engineering in MXenes, research has extended beyond metal-based intercalants to other materials, particularly non-metals and organic molecules. Due to their structural features, non-metallic materials and organic molecules can be used for precise regulation of MXene properties [8-10]. For example, alkyl ammonium cations of different chain lengths are introduced into the MXene interlayer via electrochemically driven cation intercalation (ECI). Supercapacitors (SCs) using this composite MXene as the anode achieved a high energy density of 56.7 Wh L^{-1} at a power density of 0.15 kW L^{-1}, along with excellent cyclic stability of 30,000 cycles at 10 A g^{-1}. Moreover, it maintained a high energy density of 36.7 Wh L^{-1} even at a high power density of 30.1 kW L^{-1} [8]. Additionally, chlorophyll, which easily forms aggregates in solutions and offers advantages like extremely abundant reserves, inexpensive and high environmental friendliness, has been explored for modifying MXenes. Specifically, the chlorophyll derivative zinc 3-hydroxymethyl chlorin (Chl) is considered a promising candidate [2]. Researchers physically mixed Chl with Nb2C in tetrahydrofuran (THF), resulting in a Nb2C composite with significantly expanded interlayer spacing. The Li capacity of the composite exceeded 300 mAh g^{-1}, reaching 350 mAh g^{-1} at a current density of 100 mA g^{-1}. It also maintained a high specific capacity after 200 cycles, with a Coulombic efficiency of over 99% throughout the charge-discharge process, outperforming pristine MXenes [2].

Research on MXene intercalation engineering is not limited to traditional molecular insertion; emerging methods have also been developed to improve MXenes. For instance, modified silica nanospheres were inserted into Ti_3C_2Tx to reduce triboelectric charge dissipation and inhibit MXene layer restacking. This effectively increased the interlayer spacing and specific surface area of MXene, enhanced the constant of dielectric and the density of surface charge, and observably improved the output capability of triboelectric nanogenerators, with a power density increased to 691.2 $\mu W \cdot cm^{-2}$, providing an alternative effective strategy for MXene modification [5,11].

In summary, due to their unique molecular structures, organic and non-metallic materials can precisely regulate the interlayer spacing of MXenes, introduce additional surface active terminations, and inhibit self-restacking, thereby significantly enhancing the performance of MXene materials [5].

3. Improvement of electrochemical performance by heterostructures

3.1. Heteroatom doping

Heteroatomic doping of MXenes is the direct dispersion of different elements required into the crystal lattice of MXenes, creating abundant defective ion channels and increasing carrier density, leading to synergistic enhancement of overall electrochemical performance [5]. For example, a layer-by-layer N-doped mesoporous carbon (NMC)-MXene heterostructure based on Ti_3C_2Tx was constructed via electrostatic self-assembly, forming a stable layered alternating structure. This reduces MXene self-restacking and increases the specific surface area of the material [3]. The

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electrostatic self-assembly strategy forms a hierarchical structure with expanded interlayer spacing, facilitating rapid ion transport during charge-discharge processes. Meanwhile, the interaction between NMC and Ti reduces the electron density of Ti, improving material conductivity. This composite material combines the advantages of both NMC and MXene, shows the maximum specific capacitance of 439 F $g^{-1}$when the current density of 1 A g^{-1}, the maximum specific capacitance is, and the durability is excellent [3].

3.2. Composite heterostructures

Given the issues such as self-restacking of MXenes, combining MXenes with composite materials has been recognized as an effective solution. Heterostructures formed by MXenes and composites integrate the advantages of both components and have attracted considerable attention in recent years. For example, carbon nanomaterials, with their high mechanical strength and structural advantages, have been explored for MXene heterostructure engineering. Notably, Ti_2C_2 intercalated with C60 reach the maximum capacitance of 348 F g−1 is achieved at the ratio 90% MXene-10% C60 [12]. In a recent study by the same research group, carbon nanotubes (CNTs) were co-intercalated with C60 into MXene based on the C60 intercalation strategy. The composite with a composition of 60% MXene + 30% CNT + 10% C60 exhibited excellent performance, including a maximum specific capacitance of 215 F g^{-1}, a maximum specific energy of 26.87 Wh kg^{-1}, and a maximum power density of 387 W kg^{-1}. In this system, C60 expanded the MXene interlayer spacing, while CNTs provided efficient conductive pathways for charge carriers, synergistically enhancing MXene performance [9]. Additionally, based on long-term research on 2D materials, combining different types of 2D materials has also been proposed as a solution. For example, GeMXene, a 2D layered heterostructure of GeH and MXene, exhibits pseudocapacitive behavior through cation intercalation between layers. Meanwhile, the conductive MXene sheets compensate for the low electrochemical properties of GeH. In cyclic voltammetry (CV) tests with the scan rate of 50 mV s^{-1}, GeMXene maintained a capacitance retention of ~92% after 5000 cycles [1]. GeMXene showed the highest capacitive performance in electrolytes containing small-sized cations and acidic conditions. Density functional theory (DFT) calculations reveal the thermodynamic state of Li+ embedded in the GeMXene layer is more favorable than that into O-terminated MXene layers [1], providing a reference for the research of other MXene heterostructures.

Similarly, polyoxometalates (POMs), a class of metal oxide clusters with diverse internal structures, high surface area-to-volume ratios, and excellent redox properties, have been widely applied in energy, catalysis, biology, and other fields. MXenes and POMs possess complementary properties and dimensionalities, making them promising for synergistic effects. For example, expanding interlayer spacing with various quaternary ammonium cations followed by reaction with POMs can significantly enlarge the interlayer space, forming cationic nanolayered structures to anchor POM clusters [10]. Through hybridization of Ti3C2Tx with cetyltrimethylammonium bromide (CTAB) and 12-phosphotungstic acid (PW12), the resulting CTAMX-PW12 showed a peak current of 104% of the first cycle even after 100 cycles in CV measurements, and after 5000 cycles, 85% capacitance is maintained. Furthermore, CTAMX-PW12 exhibited a specific capacitance of over 35 F g^{-1} at a current density of 0.5 A g^{-1}. Although its enhancement in specific capacitance is moderate, it shows excellent performance in volumetric capacitance [10]. Therefore, intercalating and stabilizing POMs in MXenes enables the complementary integration of the two materials, leveraging the electrochemical activity of POMs to explore the full potential of MXenes.

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4. Conclusion

In conclusion, structural modification engineering exhibits remarkable effects that can improve the electrochemical performance of MXenes, including but not limited to energy density. Various approaches can precisely regulate the interlayer spacing and surface terminations of MXenes, optimizing their structure and providing effective solutions to issues such as self-restacking and oxidative instability. Additionally, different intercalation strategies introduce unique advantages to MXenes, offering new insights for further exploiting their potential.

Despite the promising progress in improving the energy density of MXenes through structural modification engineering, challenges such as insufficient precise regulation of material properties remain. Future research should focus on constructing hybrid architectures with more composite materials, further refining surface chemistry to enhance electrochemical performance, and reducing environmental sensitivity. Furthermore, leveraging the advantages of computational chemistry can provide support for the design and simulation of MXene materials. Integrating material science, electrochemistry, computational chemistry, physics, and engineering will further unlock the potential of MXenes in the energy field, enabling them to occupy a significant position in this domain.

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