

Application of MXene Materials in Aqueous Zinc-Ion Batteries

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Abstract: As the global requirement for renewable energy grows, zinc-ion batteries (AZIBs) are an ideal replacement for lithium-ion batteries due to their plentiful zinc resources, inexpensive, and high level of security. Nevertheless, the energy density, circulation reliability, and zinc dendrite formation issues of AZIBs limit their widespread application. MXene materials, featuring a distinctive two-dimensional structure, high-conductivity, and abundant surface functional groups, show great potential in the cathode, anode, separator, and electrolyte of AZIBs. This study systematically explores the applications of MXene materials in various AZIB components, including their roles in enhancing zinc ion transport efficiency, suppressing dendrite growth, and improving battery cycling life.

Keywords: Aqueous Zinc-Ion Batteries (AZIBs), MXene Materials, Cathode Materials, Anode Materials, Separator, Electrolyte, Zinc Dendrite Suppression, Cycling Stability.

1. Introduction

As the global requirement for energy increases, electrochemical energy storage technology has gradually attracted widespread interest. Lithium-ion batteries (LIBs), due to their expanded vitality thickness and long lifetimes have ended up the standard choice for control reserve funds in versatile electronic gear and electric automobiles. However, the restricted accessibility of lithium assets, tall costs, and security issues oblige the advance application of lithium-ion batteries in large-scale vitality capacity [1]. In differentiate, watery zinc-ion batteries (AZIBs), with their copious zinc assets, moo fetched, and tall security, are continuously developing as an elective to lithium batteries.

Despite the clear advantages of AZIBs, they still face some challenges in practical applications. Water particles in fluid electrolytes can effectively lead to the arrangement of zinc dendrites, which in turn cause battery brief circuits and failure. Furthermore, the vitality thickness and cycling solidness of AZIBs got to be progressed [2]. To address these challenges, MXene materials, due to their amazing electrical conductivity, tall particular surface region, and great mechanical properties, have pulled in impressive consideration within the field of battery materials in later a long time.

MXene materials, as a two-dimensional layered material first discovered in 2011 [3], have made significant progress in research related to energy storage applications in recent years. They can not only serve as cathode materials but also play roles in anodes, electrolyte additives, and separators, significantly enhancing the overall performance of AZIBs. Nonetheless, the specific applications of MXene in AZIBs are still in the exploratory stage, especially in studies aimed at improving cycling stability and inhibiting zinc dendrite formation [4].

Therefore, this study aims to systematically explore the utilization of MXene in aqueous zinc-ion batteries, particularly their roles in cathodes, anodes, electrolytes, and separators, to provide new insights and theoretical support for enhancing AZIB performance.

2. MXene in Aqueous Zinc-Ion Batteries

2.1. Cathode Materials

In recent years, MXene materials, owing to their distinctive two-dimensional structure, excellent electrical conductivity, large specific surface area, and modifiable surface chemistry, have increasingly attracted attention as potential cathode materials for aqueous zinc-ion batteries (AZIBs). Research has predominantly concentrated on the superior electrochemical characteristics of MXene materials and their composites, particularly those combined with metal-based oxides like vanadium and manganese oxides. [5].

2.1.1. Electrochemical Performance of MXene Materials

The layered structure of MXene materials provides rapid pathways for the intercalation and deintercalation of zinc ions, while their surface rich in functional groups facilitates the adsorption and storage of zinc ions. Optimization of interlayer spacing in MXene materials enhances zinc ion diffusion rates and transmission efficiency; larger interlayer spacing typically increases ion storage capacity and reduces ion diffusion barriers.

MXene surfaces are fond of in functional groups, and modifying these groups can significantly enhance the electrochemical performance of electrode materials. By surface oxidation modification of Ti_3C_2Tx MXene to increase oxygen functional groups ($-O$, $-OH$), these groups provide more active sites for zinc ion adsorption and intercalation, while stabilizing the zinc ion intercalation and deintercalation process. For example, Naguib et al. oxidized Ti_3C_2Tx MXene under specific conditions to produce more $-O$ and $-OH$ functional groups on its surface [6]. These oxygen groups not only enhance the hydrophilicity and zinc-ion affinity of the material but also provide more active sites for electrochemical reactions, aiding in improving electrode cycling stability and zinc ion transmission efficiency. This research shows that tuning the functional groups on the surface of MXene can optimize its property in energy storing solutions to be used in

e.g. zinc-ion water batteries.

2.1.2. MXene-Based Composite Materials

MXene materials can be integrated with other substances, including oxides, conductive polymers, or carbon-based materials, to further enhance their electrochemical properties.

Vanadium oxides (such as V_2O_5) possess a high theoretical specific capacity and layered structure, enabling reversible multivalent state changes (e.g., V^{5+}/V^{4+}) for zinc ion intercalation/deintercalation reactions, which makes them well-suited in zinc-ion water batteries. However, Vanadium oxides have poor electrical conductivity which limits their rate performance and electrochemical stability. MXene materials, with high conductivity, can provide effective electron transport channels for vanadium oxides, thereby enhancing the rate performance of cathode materials. Additionally, the layered structure of MXene can synergize with that of vanadium oxides, offering more pathways for zinc ion diffusion and increasing zinc ion storage capacity. The 2D layered structure of MXene also helps to prevent structural damage to vanadium oxides from occurring over the course of charge/discharge cycling. In the V_2O_5/V -MXene composite prepared by Narayanasamy et al., V_2O_5 nanoparticles are uniformly attached to V_2C MXene nanosheets, maintaining a capacity retention rate of over 90% at high current densities, exhibiting excellent rate performance and cycling life^[7].

2.2. Anode Materials

MXene materials show considerable potential as anode components for water based zinc ion batteries. In these kinds of zinc ion batteries, the anode usually consists of Zn, and during the charging process, the Zn ions migrate through the electrolyte towards the anode surface, where on they are subsequently returned to zinc atoms and deposited; If this deposition occurs unevenly, zinc atoms tend to accumulate in localized regions, forming irregular protrusions that progressively grow into dendrites. In order to mitigate dendrite formation in aqueous zinc-ion batteries, researchers introduce conductive materials into the zinc anode to achieve a more uniform deposition layer. Due to their unique two-dimensional layered structure, MXene materials provide a smooth, homogeneous interface during zinc atom deposition, reducing zinc atom accumulation and consequently the formation of dendrites. Local high electric fields also contribute to dendrite formation; however, the high conductivity of MXene materials enables uniform electric field distribution, reducing field concentration and thus preventing localized zinc atom accumulation to inhibit dendrite growth. Studies have shown that by coating the zinc anode surface with Ti_3C_2Tx MXene materials, zinc deposition behavior is significantly improved, and dendrite growth is suppressed. Kundu et al. found that Ti_3C_2TxM Xene@Zn paper effectively suppresses Zn dendrite growth by providing a consistent spread of electric current on the surfaces of the electrodes, it promotes the uniform deposition of zinc, thereby significantly extending the battery's cycle life^[8].

2.3. Separator Materials

The key qualities that an optimal separator should possess are: high mechanical strength with minimal thinness, adequate porosity, homogeneous microstructure, high thermal stability, and good electrochemical properties and wetting.^[9] MXene materials have a favorable two-dimensional layered structure and mechanical flexibility, enabling them to act as a

physical barrier in the separator to prevent zinc dendrite penetration. The two-dimensional layered structure of MXene can form a dense protective layer within the separator, effectively blocking zinc dendrite penetration. This layered structure makes it difficult for zinc dendrites to penetrate vertically, enhancing the separator's dendrite resistance and extending battery life.

In aqueous zinc-ion batteries, the separator needs to have good ion selectivity, allowing only zinc ions (Zn^{2+}) to pass freely while blocking other secondary reaction ions (such as H^+ , OH^-). However, current separator materials exhibit poor ion selectivity, which may increase side reactions and affect battery efficiency. MXene materials are rich in surface functional groups (e.g. $-OH$, $-O$) that allow them to interact with cations in the ionic matrix, thereby modulating selective conduction of and reducing interference from other secondary ions of zinc ions. MXene surfactant interacts with Zn^{2+} ions, enhancing Zn^{2+} ion conduction rate. At the same time, it can inhibit unnecessary side reactions by reducing the conduction of side reaction ions (such as H^+ , OH^-), preventing side reactions and thus improving battery efficiency. Su et al. found that by altering the separator, a full cell watery zinc-ion battery collected with a Janus MXene-GF separator accomplished a great capacity maintenance rate of 77.9% after 1000 cycles at 5.0 A g^[10].

Traditional separator materials (such as polypropylene PP, polyethylene PE) are non-conductive, while MXene materials have high conductivity; introducing MXene into the separator can enhance overall conductivity, making a difference to diminish inside resistance and hence make strides the charge-discharge productivity and control thickness of the battery. Researchers designed one lightweight zinc-philic MXene/nano-porous oxygen heterostructure separator used to stabilize zinc-metal anodes. The rate performance of full cells with MXene@NiO modification of the separator was significantly improved at different current densities, with capacities as high as 224.0 mA h g⁻¹ and a volume maintenance of 99.03%^[11].

2.4. Electrolyte

In fluid zinc-ion batteries, the electrolyte is one of the center components, specifically affecting particle conduction, chemical solidness, cycling execution, and security of the battery. Traditional aqueous zinc-ion battery electrolytes, such as $ZnSO_4$ (zinc sulfate), $Zn(CF_3SO_3)_2$ (zinc trifluoromethanesulfonate), and $ZnCl_2$ (zinc chloride), although offering good conductivity and low cost, still have certain drawbacks in practical applications. The main problems centered on side reactions (evolutionary hydrogen reactions) as well as the development of zinc branching dendrites. To address these issues, researchers have proposed introducing additives (MXene materials) into the electrolyte for improvement.

Due to their high electrical conductivity, MXene materials are effective as additives to improve the overall electrical conductivity of the solute, while also interacting with the aqueous elements in the solute to reduce hydrogen evolution reactions. The hydrogen evolution reaction ($2H^+ + 2e^- \rightarrow H_2$) is typically a side reaction in aqueous zinc-ion batteries. The reduction reaction of water molecules generates hydrogen gas, consuming some of the battery's charge and reducing Coulombic efficiency. The interaction between MXene surface functional groups and water molecules can passivate the water molecules, making their reduction potential more

negative, thus preventing reduction reactions within the electrode's operating voltage range.

Traditional electrolytes cannot effectively control the uniform deposition of zinc ions, especially at high current densities, where zinc ions easily accumulate locally, forming dendrites. MXene materials possess Enriched with surface functional groups (e.g. -OH, -O) that interact with Zn^{2+} ions to stabilize them, maintaining their uniform distribution in the electrolyte. This interaction effectively reduces excessive accumulation of zinc ions in local areas, preventing the rapid deposition of zinc ions in localized areas within the electrode screen, thereby minimizing the strengthening influence of the local electric field and inhibiting the growth of dendritic protrusions.

Sun et al. used Ti_3C_2Tx as an additive to the electrolyte to control the nucleation and formation of Zn, promoting uniform Zn deposition; this electrolyte achieves dendritic grain-free zinc coating/stripping with strong Coulombic efficiency (99.7%) and excellent cyclability (consistent cycling for 1,180 cycles). MXene's great potential as an electrolyte additive for zinc ion batteries was shown in this research.^[12]

3. Conclusion

With its unique two-dimensional layered structure, good conductivity, and rich surface radical, MXene materials demonstrate great promises for a variety of key components in water-based zinc-ion batteries. In the cathode, MXene materials significantly enhance the electrochemical properties of cathode materials by increasing electrical conduction and ion transport capacity; particularly in composites, MXene combined with manganese- and vanadium-based cathode materials exhibits superior rate performance and stability. In the anode, the two-dimensional layered structure of MXene effectively inhibits zinc dendrite formation, smooths the zinc ion deposition interface, and reduces side reactions, thereby extending the cycle life of the galvanic cathode and improving its charging and discharging performance. In the separator, MXene provides efficient ion conduction pathways, enhances the separator's physical resistance and electrical properties, and significantly reduces the risk of zinc dendrite infiltration, improving battery safety and stability. In the electrolyte, MXene optimizes zinc ion distribution and migration by interacting with zinc ions and water molecules, reducing Reduction of secondary effects including the hydrogen evolution, while improving Coulombic efficiency and overall battery lifespan.

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