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Towards Next-Generation Lithium-Ion Batteries: The Promise of MXENE Materials

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ABSTRACT

2D nanomaterials have great potential in energy storage because of their high surface area, electrical conductivity and mechanical strength. MXene has got quick attention compared to other 2D materials for its physiochemical and tailoring properties. Recently, its use in Li-ion batteries showed great potential for their layered structure and excellent electrical conductivity. Thus, MXene can be used as anode and cathode materials in Li-ion batteries. Though, it faces some complexities like structural degradation, limited voltage window, restacking and aggregating issues and production cost. Through the article a study has shown that increasing the interlayer spacing, changing the functional groups of MXenes, and structural design MXenes are the most important ways for developing highly efficient Li-ion batteries. Besides these, structural design and properties of MXene, and Li-ion batteries applications are also discussed. In this review, the most essential part for MXene based Li-ion batteris is anode material is summarized. Overall, a comprehensive review of MXene-based Li-ion batteries and their future outlooks is presented in the article.

Keywords: MXene, Li-ion Batteries, 2D Materials, Nanostructures, Energy Storage.

1. Introduction

The use of lithium-ion batteries (LIBs) as the basis of portable electronics, electric mobility, and grid storage is due to their offering a combination of high specific energy and long cycle life[1]. The next application, however, is limited due to the following intertwined factors: safety and thermal runaway risks in flammable electrolytes, capacity decay caused by parasitic interfacial reactions, and rate limitations during fast charging, where Li plating, electrolyte decomposition, and electrode cracking may occur[2]. Recent reviews underline that to attain minutes-scale charging and maintain energy density, it is necessary to have a better electron/ion transport, engineered solid electrolyte interphase (SEI), and stable interfaces on both electrodes[3].

Traditional graphite anodes and composite cathodes experience bottlenecks in transport and interfacial instability at high current densities. Strategies of materials are aimed at (i) high-conductivity scaffolds to minimize electronic/ionic resistances, (ii) surface chemistries to develop strong, inorganic-based SEIs to prevent continuous usage of electrolytes, and (iii) architecture to preserve accessible pathways to practical areal loadings. The literature review of fast-charging LIBs and interface-driven design recurrently identifies the necessity to design electrode frameworks capable of homogenizing current, buffering mechanical load, and controlling interphase composition, all at scale[2], [3].

MXenes are a vast group of 2D transition-metal carbides/nitrides, the general formula of which can be represented as $M_{n+1}X_nT_x$ (M is an early transition metal, X is C/N, T is a surface trapping: -O/-OH/ -F/-Cl). They are fabricated by selectively etching the A-layer of layered MAX phases to produce few-layer or delaminated sheets, which can integrate metallic-level electrical conductivity and hydrophilicity with tunable surface chemistry, which is not commonly found on battery electrodes and interlayers[4]. Such properties permit several Li-storage modes (intercalation, surface redox, pseudo capacitance), rapid charge transfer, and abundant possibilities to engineer interphase through controlled terminations. The crystallographic origin of MXenes, as well as the key importance of surface terminations in determining electrochemical behavior, is established by scientific research[5].

Synthesis The traditional fluoride-based pathways (HF or in-situ HF) are consistent and efficient at synthesizing $Ti_3C_2T_x$ and other preparations but are associated with safety and ecological issues and leave behind F-functionalized surfaces[6]. The fluorine-free methods of a new generation, including Lewis-acid molten-salt etching, electrochemical/alkaline approaches, and emerging bottom-up approaches, have provided greater control of terminations (including mostly predominant -Cl/ -O/ -OH), expanded MXene chemistries, and enhanced scalability processability. The direct consequences of these greener routes on LIB performance are changes in the interlayer spacing, surface acidity, basicity, and SEI chemistry[7], [8].

Altogether, MXenes are in line with the key requirements of next-generation LIBs: fast charge/discharge through high electronic conductivity and accessibility of interfaces and interlayers, designable interfaces through termination and interlayers control, and more green synthesis pathways with scale-up compatibility. The rest of this paper summarizes the

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progress in (i) termination and interlayer engineering to Li-storage engineering and SEI control, (ii) MXene-based hybrids to high-loading anodes (particularly, Si-MXene),(iii)MXene-enabled separators/electrolytes to control cell-level stability and fast-charge tolerance, and (iv) HF-free synthesis and anti-oxidation initiatives that bridge the gap between laboratory performance and high-performance, durable, manufacturable devices[9], [10].

2. Structure and Properties of Mxenes

A general structure of MXene (M_3X_2) is shown in Figure 1. Generally, M3X2 is derived from M_3AX_2 where the atoms from A layer are chemically removed by etching, leaving highly active M layer atoms outside keeping inside X layer atoms. For example, consider a layer of A atoms along (111) place in FCC structured titanium carbide layer is extracted. The fabricated MXene has a hexagonal closed pack (HCP) structure. The ordering of MXene depends on "n". For n=1, the stacking sequence is in ABABAB form while for n>1 has ABCABC sequence.

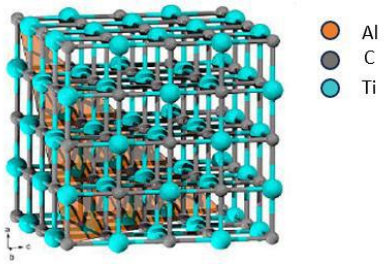

Fig. 1 Typical lattice of transition metal carbide MXene

MXene achieved more attention in short time than MXene and MoS2 because of their tailoring properties. Where graphene only allows functionalization, MXene properties can be tuned by functionalization, processing and doping [11]. It is possible to control the final properties by adjusting MXene phase composition. By doping the MAX phases, unique properties can be obtained. For instance, Sn doping in A layer of Ti3AlC2, the resistance to oxidation increases by 33% at 900˚C [12]. It is also possible to modify the properties by changing inter-flake spacing. MXene showed metallic conductivity by nature, however, semiconductive nature is observed by increasing c- lattice spacing [13]. Furthermore, surface functionalization, usually by terminating -O, -F and -OH, plays an important role in enhancing the performance of MXene. By this, electron mobility, 2D ferromagnetism, biocompatibility, conductivity etc. can be modified [14].

3. MXENEs as Anode Materials in Lithium-Ion Batteries

3.1 Elucidation of Multi-Modal Lithium Storage Kinetics

The MXene architecture, defined by its two-dimensional (2D) structure and diverse surface functional groups ($-T_x$), facilitates a highly versatile lithium storage mechanism that significantly surpasses conventional anode materials [15]. Fundamentally, the intercalation of Li^+ ions into the interlayer spacing is the dominant capacity pathway, where the robust structural framework effectively mitigates the typical volumetric changes associated with charge/discharge cycles. Furthermore, surface-mediated adsorption on the accessible terminal groups (-O, -OH, -F) provides substantial supplementary capacity by introducing additional active sites. For specific transition-metal chemistries within the MXene matrix (e.g., V- or Nb-based systems), a conversion-type reaction mechanism is also implicated, contributing to the overall reversible capacity. This synergistic, multi-modal storage mechanism is crucial, enabling reported specific capacities for $Ti_3C_2T_x$ to exceed 400 mAh g-1, a figure notably higher than the theoretical limit of graphite (372 mAh g-1) [16], [17], [18].

3.2 Rate Performance and Structural Integrity Analysis

The exceptional electrochemical performance metrics of MXene anodes are directly attributed to their intrinsic metallic-level electronic conductivity. This high conductivity is paramount, guaranteeing rapid charge transfer kinetics and a minimal internal resistance, which subsequently manifests as outstanding rate capability, a prerequisite for high-power battery applications [16], [17]. The 2D structural integrity is equally vital, serving as a highly stable mechanical scaffold and particle pulverization commonly observed in high-capacity alloy-type materials. This structural resilience ensures superior cycling stability and long-term performance longevity.

3.3 Advanced Strategies for Performance Enhancement and Optimization

To address existing limitations, such as the restacking tendency of sheets, sophisticated engineering approaches are being pursued:

1. Interlayer Engineering: The deliberate incorporation of pillaring species (e.g., carbon nanomaterials or polymer spacers) is essential to expand the interlayer spacing. This strategy is critical for accelerating Li^+ diffusion and ensuring kinetic accessibility [16].
2. Heteroatom Doping: The introduction of heteroatoms (N, S, P) is employed to further enhance intrinsic electronic conductivity and to introduce new, strategically located redox-active sites, thereby improving reversible capacity.
3. Hybridization with High-Capacity Components: The formation of composite materials utilizing the highly conductive MXene framework alongside high-capacity components (metal oxides, sulfides) represents a major step toward achieving the optimal balance between high energy density and cycling stability [17].

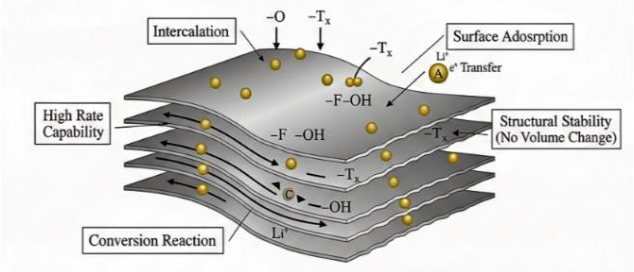

Fig. 2 Schematic overview of MXene as an anode material, illustrating multi-modal Li^+ storage

4. Mxenes as Cathode Materials and Conductive Additives

4.1 Differentiating Role and Multifunctionality

MXenes are invaluable as superior conductive additives in cathode composites. Their high electronic conductivity and flexible morphology create continuous charge transport networks, drastically reducing internal resistance. Crucially,

their tunable polar T_x surface chemistry differentiates them from traditional carbon additives, enabling favorable chemical interactions that enhance structural integrity and suppress parasite side reactions [17].

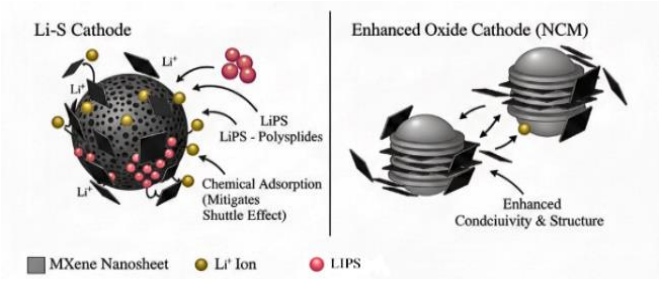

Fig. 3 Illustration of MXene as a cathode additive, depicting their role in Li-S batteries

4.2 Performance Augmentation in Hybrid Systems

The integration of MXenes leads to critical performance gains:

- Li-S Batteries: MXenes function as effective polar hosts, chemically adsorbing soluble lithium polysulfides (LiPSs) [16]. This mechanism is vital for mitigating the notorious shuttle effect, resulting in significantly improved Coulombic efficiency and cycling life, while the conductivity accelerates sluggish sulfur redox kinetics [19].
- Layered Oxide Cathodes: In materials like NCM, MXenes enhance both electronic pathways and mechanical stability. This improves rate performance and capacity retention, especially for high-current applications.

MXenes thus serve as a single, multifunctional component: a high-speed conductor, a structural reinforcer, and a chemical adsorbent, positioning them as a key enabler for advanced battery architectures [16], [19].

Table 2 Analytical comparison of key battery materials and components.

Category	Materials	Key Electrochemical Role(s)	Analytical Advantage over Alternatives	Primary Technical Challenge
Anode	$Ti_3C_2T_x$ MXene	Li^+ intercalation, surface adsorption	High conductivity, excellent rate capability, and negligible volume change	Scalability, stability in air/electrolyte
Anode	Graphite (LiC_6)	Li^+ intercalation	Low cost, excellent cycle life	Low specific capacity (< 372 mAh g^{-1})
Additive	MXene (T_x)	Electronic conduction, LiPS scavenging (in Li-S), structural reinforcement	Polar surface chemistry, superior electronic network	Cost-effective and processability
Additive	Carbon black/CNT	Electronic conduction	High purity, established industrial scale	Lack of chemical interaction/polysulfide adsorption

5. Challenges in MXENE Applications for Li-Ion Batteries

MXenes, such as $Ti_3C_2T_X$, are promising candidates for Li-ion battery (LIB) electrodes due to their high conductivity and tuneable surface chemistry. However, several challenges hinder their practical implementation. The most critical limitations are structural degradation during cycling, narrow voltage operation, restacking and aggregation of nanosheets, and scalability with cost concerns.

1. Structural Degradation during Cycling

MXenes are prone to irreversible structural and chemical modifications in the course of repeated lithiation and delithiation. They are easily oxidized and the instability of their terminations may trigger side reactions with the electrolyte, resulting in the capacity fading and short lifespan of the cycles [20]. The MXene phase can also degrade even in composites, which leads to mechanical instability and the disappearance of electrochemically active sites [21]. This degradation is still a significant challenge to long term stability of MXene-based anodes.

2. Limited Voltage Window

The second weakness is that MXenes can be used only within a limited range of potential. Most MXene anodes operate at potentials of less than -0.5-1 V vs. Li/Li^+ and have poor electrochemical behavior at higher potentials [22]. This decreases the total energy density of MXene based full cells, despite the use of high-voltage cathodes. Besides, the work outside of the stable window may cause parasitic responses, which further affect the electrode performance.

3. Restacking and Aggregation Issues

The van der Waals forces between Maxene nanosheets are quite strong to allow them to reassemble into stacked structures. Restacking decreases interlayer separation, screens ion-accessible surfaces and inhibits Li+ diffusion [23]. This leads to reduction in capacity and rate capability. This can be mitigated with some success by such strategies as carbon spacer use, pillaring agents or hybrid composites but stable, open architectures are still difficult to realize [24].

4. Scalability and Cost Concerns

Lastly, economic and safety concerns are a problem in the production of MXenes. Traditional synthesis is based on etching of the MAX phases using harmful gases such as HF, which is very dangerous during handling and also to the environmental conditions [25]. Also, the price of manufacturing high-quality MXenes is still too high, and the existing methods cannot be applicable to mass electrode production. It will be essential to develop fluoride-free etching, scalable delamination processes, and safer industrial procedures to translate MXene research into practical LIB technologies [26].

6. Strategies to Overcome Challenges

Despite their promise, MXenes face challenges such as instability, restacking, and scalability issues. Several strategies have been proposed to mitigate these limitations and enhance their performance in Li-ion batteries (LIBs).

1. Surface Functionalization

Surface chemistry has a significant impact on the MXene stability and the electrochemical properties. Oxygen or sulfur functionalization or single-atom doping (i.e. N, S, P) to suppress surface oxidation and fine-tuning Li + adsorption energy can enhance capacity and cycling life [24], [27]. In order to stabilize MXenes during repeated cycling, protective coatings with thin oxides or polymers are applied to it.

2. Interlayer Engineering

Restacking of nanosheets reduces ion-accessible surfaces and slows Li^+ transport. Expanding interlayer spacing through ion intercalation, pillaring agents, or rigid nanoparticles maintains open channels and prevents collapse. For example, silica or carbon spacers have been used to stabilize $Ti_3C_2T_x$ layers, resulting in enhanced rate capability and more uniform Li deposition [26]. Such approaches preserve active surface area and reduce diffusion barriers.

3. Composite/Hybrid Design:

Forming MXene-based composites combines the strengths of different materials. Carbonaceous frameworks (graphene, CNTs, porous carbon) act as conductive scaffolds and prevent aggregation, while conducting polymers (e.g., polypyrrole) improve flexibility and structural integrity. Similarly, hybrids with metal oxides or sulfides buffer volume changes and introduce additional Li-storage mechanisms. These designs typically achieve higher capacity, longer cycle life, and better rate performance than pristine MXenes [28].

4. Novel Synthesis Techniques:

Traditional HF-based etching of MAX phases is hazardous and difficult to scale. Recent advances include electrochemical etching in benign salts and molten salt methods, which produce MXenes with cleaner surfaces and tuneable terminal groups [29]. Such approaches reduce safety risks, lower costs, and enable scalable production—key steps toward industrial application.

7. Future Perspectives and Opportunities

In the future, MXenes will have the capability of powering various future battery platforms in seconds due to their high conductivity, tunable surfaces, and processability. MXene hosts interlayers of Li-S batteries have been chemically active with polysulfides and catalytic promotion of S redox, indicating improved area loading and reduced fade in lean-electrolyte cells[30]. MXene-based cathodes and 2D heterostructure catalysts in Li-O_2 batteries can be used to control Li_2O_2 formation, decomposition and lower charge overpotentials, providing a good roadmap to improved rate performance and cycling performance[31]. In solid-state systems, it is also advantageous to use polymer and inorganic electrolytes with small loadings interlayers of MXene that enhance ionic conductivity and interfacial contact through percolation/coordination effects, and MXene structures can be used as a conductive scaffold in all-solid-state designs[32], [33].Other than performance, commercialization is based on greener, scalable synthesis and air stability: fluorine-free, Lewis-acid molten-salt etching, replacing HF to expand chemistries and tune terminations that are important in interphase control, and recent work elucidates oxidation pathways and demonstrates that eliminating confined water as well as designing MXene-matrix interfaces significantly extend shelf-life and thermal tolerance[34], [35].

Lastly, MXene inks/films allow ultrathin, flexible/wearable micro-cells and hybrid battery-supercapacitors, although encapsulation and termination control is required to suppress oxidation due to sweat/humidity[36], [37].

8. Conclusion

This article builds a comprehensive discussion on MXene materials-based Li-ion batteries. Through the article structure and properties of MXene and its properties, MXene as anode materials in Li-ion batteries, as a cathode material and conductive additives, challenges and strategies to overcome challenges and its application are discussed. Though MXene has a enormous potential to be used in Li-ion batteries, it has some limitations like structural degradation, limited voltage window, restacking and aggregating issues and production cost. By functionalizing, changing structural design, process, and interlayer spacing drawbacks can be mitigated. So, engineers and scientists have a huge scope to work on these points. If the challenges can be addressed, MXene based Li-ion batteries have great potential to be used for energy storage.

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