

Mitigating Capacity Decay: The Role of LTO-Based Composites in Advancing Anode Technology

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Abstract: Lithium-ion batteries (LIBs) have emerged as one of the most promising energy storage technologies for portable electronics, electric vehicles, and renewable energy systems because of their high energy density, long cycle life, and improved operational safety. However, conventional graphite-based anodes suffer from poor high-rate capability and severe capacity fading during prolonged cycling. In this study, a novel LTO-MXene-N composite anode based on lithium titanate oxide ($\text{Li}_4\text{Ti}_5\text{O}_{12}$) was developed to mitigate capacity decay and enhance electrochemical performance. The proposed composite integrates nitrogen-doped LTO nanoparticles, MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) conductive nanosheets, and a carbon conductive matrix optimized through the Adaptive Hierarchical LTO Composite Optimizer (AHLCO) framework. Structural and electrochemical characterization was carried out using XRD, SEM, TEM, BET, Electrochemical Impedance Spectroscopy (EIS), Galvanostatic Charge–Discharge (GCD), and Galvanostatic Intermittent Titration Technique (GITT). The developed composite delivered discharge capacities of 176 mAh g^{-1} at 0.1C and 128 mAh g^{-1} at 10C while retaining 92.6% capacity after 1000 cycles. Furthermore, the charge-transfer resistance decreased from 180 Ω for bare LTO to 45 Ω , and the lithium-ion diffusion coefficient improved from to $\text{cm}^2 \text{s}^{-1}$. These results demonstrate that the synergistic effects of MXene conductive pathways, nitrogen doping, and nanostructured architecture significantly improve lithium-ion transport, cycling stability, and overall battery performance.

Keywords: Lithium Titanate Oxide (LTO), MXene-Based Composite Anodes, Capacity Decay Mitigation, Electrochemical Performance Enhancement, Fast-Charging Lithium-Ion Batteries

1. Introduction

The rapid advancement of portable electronics, electric vehicles, and renewable energy storage technologies has significantly increased the demand for advanced Lithium-Ion Batteries (LIBs) with high energy density, extended cycle life, and enhanced operational safety [1]. Among the major components of LIBs, the anode material plays a crucial role in determining electrochemical performance, charging efficiency, and long-term durability [2]. Conventional graphite anodes are widely used because of their stable cycling behavior, low cost, and commercial availability; however, they suffer from several limitations, including low theoretical capacity, lithium plating during fast charging, and severe performance degradation under high-rate operating conditions [3]. These limitations have encouraged extensive research into alternative anode materials capable of delivering improved electrochemical characteristics, superior rate capability, and reduced capacity fading during long-term cycling [4].

LTO, which is typically written as $\text{Li}_4\text{Ti}_5\text{O}_{12}$, is one of the most promising anode materials for next generation LIBs [5]. LTO has a unique spinel crystal structure which it offers unmatched structural stability for lithium insertion and extraction process [6]. It is sometimes called a “zero-strain” material due to its low lattice volume change during charge and discharge cycles. This feature substantially alleviates mechanical stresses and also mitigates electrode



pulverization which consequently enhances the life span and cycling stability of the battery [7]. Moreover, LTO has excellent thermal stability, fast lithium-ion diffusion and high safety performance which make it suitable for high-power and fast-charging applications [8]. The crystal structure of LTO is shown in Figure 1, which is cubic spinel. LTO has a cubic spinel structure as shown in Figure 1, with interconnected Li, Ti and O atoms providing stable three-dimensional channels for fast lithium-ion diffusion.

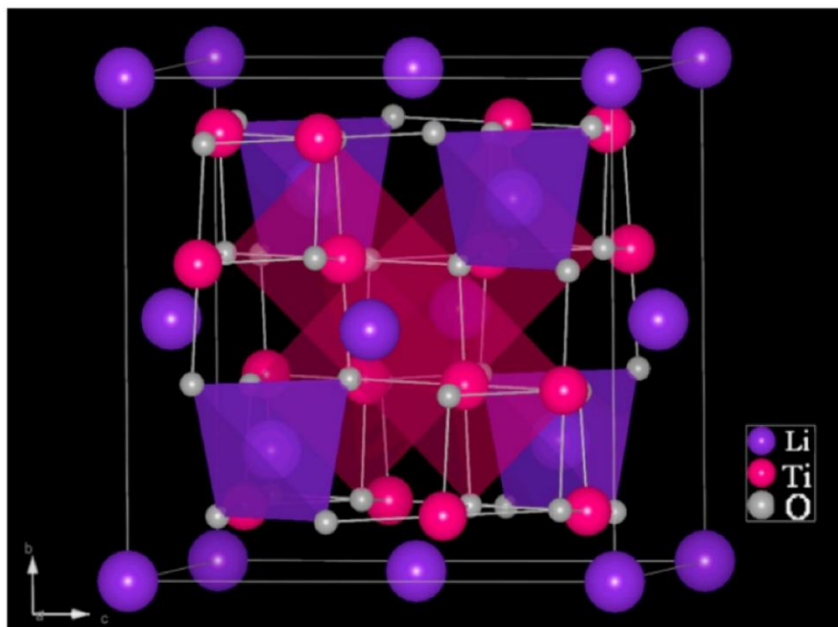


Figure 1: Crystal structure of LTO [9]

Although these are the benefits of pure LTO anodes, there are a number of challenges that hinder large-scale commercialization. Their moderate electrical conductivity and theoretical capacity are the one of the significant issues compared to other advanced anode materials like silicon and transition metal oxides [10,11]. Furthermore, the capacity fades gradually over time for long-time cycling, which is attributed to side reactions, degradation of the electrode/electrolyte interface, and poor charge transfer kinetics. These problems have led to extensive research in the development of composites based on LTO and conductive material, carbon nanostructures, metal oxides, polymers, or hybrid nanomaterials [12]. The composite structures have been designed to achieve better electron transport pathways, higher active surface area and better lithium storage capacity while maintaining the inherent structural stability of LTO [13].

LTO-based composites have exhibited excellent electrochemical properties via synergistic interactions between the constituent materials. For instance, carbon-coated LTO composites offer an improved charge transfer resistance and electrical conductivity, which results in improved rate capability and cycling efficiency [14,15]. In the same way, composites containing graphene, carbon nanotubes, and/or metallic nanoparticles have been reported with large improvements in lithium-ion diffusion and reversible capacity retention [16]. The use of nanotechnology and advanced synthesis methods, like the hydrothermal processing, sol-gel techniques, electrospinning, and microwave-assisted synthesis, has also contributed to the development of highly uniform and porous LTO composite structures with better electrochemical properties [17].

Another significant benefit of LTO-based composites is their resistance to capacity loss during severe operating conditions including high current density, deep charge/discharge cycle, and high temperature [18]. The composite architecture contributes to the structural stability, prevention of side reactions, and enhanced electrolyte compatibility, which helps to prolong battery usage and reliability. The properties of these materials are especially useful for use in electric vehicle, aerospace, grid-scale energy storage and wearable electronics applications, where long-term stability and safety are essential.

The high-performance LTO composite anode has seen a significant improvement in the last few years due to recent developments in material engineering and interface optimization. Multi-component hybrid composites, surface modification and doping are increasingly being investigated to tailor the electronic/electrochemical properties of LTO

materials. These innovations are anticipated to fill the energy density/long cycling ability gap to pave the way for the commercialization of safer and more durable LIB technologies. Thus, investigation of LTO-based composites has emerged as a significant research field in the field of contemporary energy storage systems. These innovative composite materials provide a promising avenue to the development of sustainable, efficient, and reliable anode materials for future lithium-ion batteries, addressing the challenge of capacity decay. The following are the research objectives as shown below:

- To develop a novel LTO-MXene-N composite anode architecture for mitigating capacity decay in lithium-ion batteries.
- To enhance lithium-ion diffusion and electronic conductivity of LTO anodes through MXene integration and nitrogen doping.
- To optimize the structural, interfacial, and electrochemical properties of the composite using the proposed AHLCO optimization framework.
- To investigate the electrochemical performance of the developed composite in terms of capacity retention, rate capability, Coulombic efficiency, and impedance behavior.
- To compare the performance of the proposed LTO-MXene-N composite with conventional LTO-based electrode systems for advanced fast-charging battery applications.

2. Review of Literature

In recent years, lithium titanate oxide (LTO)-based anodes have been studied primarily with regard to their electrochemical stability, conductivity and capacity retention for use in advanced lithium-ion and solid-state batteries. Kozlova et al. (2022) [20] studied the LTO-Li₂TiO₃ and LTO-TiO₂ composites and found that the addition of Li₂TiO₃ at low concentration, considerably decreases the grain boundary resistance, which leads to better charge–discharge performance. The study also found that the capacities were abnormally high beyond the theoretical value of pure LTO because of the presence of electrochemically active interface layers between LTO and Li₂TiO₃. Likewise, Cao et al. (2023) [21] showed that Li–LTO type composite anodes are effective in garnet-based solid-state batteries, which ensures good wettability and high lithium interface resistance, and lithium dendrite formation was effectively suppressed, and a capacity retention of 95% was achieved after 450 cycles. Hasani et al. (2025) [22] also investigated the characteristics of suspension plasma-sprayed LTO thin-film anodes and found that the heat exposure in the process of fabrication can lead to the formation of second phases and the loss of lithium, highlighting the need to optimize the processing parameters for obtaining phase stability and preserving the interfacial integrity. Researchers have tried to improve the poor electronic conductivity of LTO using composite engineering and surface modification methods. Cayirli et al. (2025) [23] prepared an LTO/rGO composite material and achieved 30% increase in discharge capacity, with almost 100% Coulombic efficiency and 96% capacity retention after 100 cycles. Similarly, Moon et al. (2023) [24] used a mixed ionic-electronic conductor (MIEC) nanocoating of partially lithiated titania on the LTO surface to greatly enhance charge transfer kinetics, rate capability, and capacity retention. Giorgio et al. (2022) [25] studied the synergistic effect of using both sodium alginate binder and lithium bis(trifluorosulfonyl)imide-tetraglyme electrolyte to enhance the long-term electrochemical performance and cycling stability of LTO electrodes. In another study, Alrefaee et al. (2023) [26] fabricated LTO/polyether sulfone composites via laser ablation methods and showed that the smaller LTO nanoparticles with oxygen vacancies and Ti³⁺/Ti⁴⁺ defect pairs significantly improved ion/electron mobility and electrochemical efficiency. Likewise, Kim et al. (2024) [27] fabricated plasma-reduced graphene oxide/LTO composite material with a porous three-dimensional structure to enhance the lithium-ion diffusion pathways and achieved outstanding energy density, power density, and capacitance retention in lithium-ion capacitors. Table 1 provides an overview of recent research on LTO-based composites, their methodologies, key results and current gaps of knowledge in enhancing lithium-ion battery performance.

Table 1: Summary of recent literature on LTO-based composite anodes for lithium-ion batteries.

Authors & Year	Method / Material Used	Key Findings	Limitations / Research Gap
Kozlova et al. (2022)	LTO-Li ₂ TiO ₃ and LTO-TiO ₂ composites	Li ₂ TiO ₃ reduced grain boundary resistance and enhanced charge–discharge capacity beyond theoretical	Capacity enhancement was not observed in LTO-TiO ₂ composites because of structural incompatibility.

		LTO values due to active interface layers.	
Cao et al. (2023)	Li-LTO composite anode in garnet-based solid-state batteries	Improved wettability and lower interface resistance suppressed dendrite growth and achieved 95% capacity retention after 450 cycles.	Long-term large-scale implementation and interface optimization remain challenging.
Hasani et al. (2025)	Suspension plasma-sprayed LTO thin-film anodes	Identified phase transformations and lithium loss near substrate interfaces caused by thermal exposure.	Requires precise control of SPS parameters to maintain phase stability.
Cayirili et al. (2025)	LTO/reduced graphene oxide (rGO) composite	rGO incorporation enhanced discharge capacity by 30% with excellent Coulombic efficiency and cycling stability.	Intrinsic conductivity limitations of LTO still need further improvement.
Moon et al. (2023)	MIEC nanocoated LTO using Li_xTiO_2 layer	Improved lithium-ion transport, rate capability, and capacity retention through enhanced surface charge transfer.	Complex coating optimization is required for practical commercialization.
Giorgio et al. (2022)	Sodium alginate binder with LiTFSI-tetraglyme electrolyte	Improved electrochemical stability and long-term cycling performance of LTO electrodes.	Interaction between binder and electrolyte requires further investigation.
Haghipour et al. (2025)	Optimization of LTO electrode fabrication process	Enhanced high-rate capacity retention and cycling performance through improved particle dispersion and homogeneity.	Capacity fading at extended voltage ranges remains a concern.
Siller et al. (2022)	Pulsed laser deposited multilayer LTO- Li_2O micro-anodes	Achieved high specific capacity and stable performance at high C-rates.	Lithium trapping at low voltage caused kinetically limited degradation.
Alrefaee et al. (2023)	LTO/PES composite synthesized via laser ablation	Smaller nanoparticle size and oxygen vacancies improved ion/electron mobility and electrochemical performance.	Structural optimization is needed for scalable battery applications.
Kim et al. (2024)	Plasma-reduced graphene oxide/LTO composite	Porous 3D structure improved lithium-ion diffusion, energy density, and capacitance retention.	Further optimization is needed for commercial lithium-ion capacitor systems.

Advances in recent years have also been in optimizing the fabrication processes and the electrochemical window of operation of LTO-based materials. Haghipour et al. (2025) [28] showed that increasing the dry mixing and speed and the decrease in the wet mixing time can increase the dispersion and homogeneity of the particles, leading to better high-rate performance and cycling stability up to 1000 cycles. To achieve high specific capacities, stability

at high C-rate, and operating safely in an extended voltage range, Siller et al. developed multilayer LTO-Li₂O micro-anodes by using PLD (pulsed laser deposition) [29]. All of these studies suggest that LTO based composites, nanostructured coatings, and advanced fabrication methods are critical steps for addressing the shortcomings of traditional LTO anodes. While significant advances have been made, there are still issues to be addressed such as conductivity, lithium diffusion, degradation of the interfaces, and manufacturing on a large scale, which still offer the potential for continued research and development to create more efficient and durable next-generation energy storage systems.

3. Theoretical Framework and Mathematical Models

3.1 Capacity Decay Model

The capacity fading of lithium titanate oxide (LTO) anodes is caused by surface film growth, loss of electrical contact between particles, and structural changes with repeated charge/discharge cycles. A phenomenological capacity decay model can be used to describe the degradation behavior of the proposed LTO-based composite:

$$Q(n) = Q_0 \exp(-\alpha n^\beta) - \gamma n^{1/2}$$

where Q_0 represents the initial discharge capacity, n denotes the cycle number, α is the capacity fade constant, β is the non-linear degradation exponent, and γ corresponds to diffusion-controlled degradation effects. This model can be used to simulate long term cycling performance and to understand how composite engineering can mitigate capacity decay.

3.2 Lithium-Ion Transport Model

The lithium-ion diffusion behavior in the electrode is significant in the battery performance. The Weppner–Huggins approximation of the galvanostatic intermittent titration technique (GITT) analysis is used to estimate the effective diffusion coefficient (D_{eff}):

$$D_{eff} = \frac{4}{\pi\tau} \left(\frac{m_B V_M}{M_B A} \right)^2 \left(\frac{\Delta E_s}{\Delta E_t} \right)^2$$

where τ is the pulse duration, m_B is the active mass, V_M is the molar volume, M_B is the molar mass, A is the electrode area, and ΔE_s and ΔE_t are the steady-state and transient voltage variations, respectively. Improved diffusion coefficients indicate enhanced lithium-ion transport and better high-rate electrochemical performance.

The lithium-ion insertion time constant is determined by:

$$\tau_D = \frac{r^2}{\pi^2 D_{eff}}$$

where r is the particle radius and D_{eff} is the effective diffusion coefficient. The smaller particle size and large diffusion rate leads to rapid lithium-ion insertion and extraction.

3.3 Electrochemical Impedance Model

The developed LTO based composite anodes are assessed in terms of their charge transfer behavior, ion diffusion and internal resistance using the electrochemical impedance model. Electrochemical Impedance Spectroscopy (EIS) is a powerful tool for understanding the kinetics of an electrode and for studying the effectiveness of conductive additives and surface modifications to enhance battery performance. In this study, the lithium-ion battery system is modeled using a Randles equivalent circuit model which is composed of electrolyte resistance, the charge transfer resistance, the double layer capacitance, and the Warburg diffusion impedance.

The overall impedance of the system is expressed as:

$$Z(j\omega) = R_s + \frac{R_{ct} + Z_W(j\omega)}{1 + j\omega C_{dl}[R_{ct} + Z_W(j\omega)]}$$

where R_s represents the electrolyte resistance, R_{ct} denotes the charge-transfer resistance between the electrode and electrolyte interface, C_{dl} is the double-layer capacitance, and Z_W corresponds to the Warburg impedance

associated with lithium-ion diffusion within the electrode material. The Warburg diffusion component is further represented as:

$$Z_W(j\omega) = \frac{\sigma_W}{\sqrt{\omega}}(1 - j)$$

where σ_W is the Warburg coefficient and ω is the angular frequency. The lower the charge-transfer resistance and Warburg impedance, the higher the electrical conductivity and the faster the lithium-ion transport. The combination of conductive materials like MXene, graphene and carbon coating within the LTO matrix decreases the impedance and improves the electrochemical kinetics, leading to better cycling stability, faster rate capability and battery efficiency.

3.4 Rate Capability Model

The rate capability model aims to determine the capability of the fabricated LTO composite anode to deliver its discharge capacity at various charging/discharging rates. High-rate performance is an important requirement for fast-charging lithium-ion batteries. Normalized capacities are shown with the following exponential relaxation model:

$$Q(C_{rate}) = Q_{0c}[1 - A_r(1 - e^{-C_{rate}/C_0})]$$

where Q_{0c} represents the equilibrium capacity at low current rate, A_r denotes the fractional capacity loss at higher C-rates, and C_0 is the characteristic rate constant. The lower capacity fading at higher C-rates suggests better lithium-ion transport and better conductivity in the LTO composite structure. The rate capability and electrochemical stability of the electrode material are greatly enhanced by the use of conductive additives and nanostructured architectures.

3.5 Proposed AHLCO Algorithm

The AHLCO framework consists of material synthesis, nanostructuring, interface engineering, electrochemical prediction, characterization and testing, which are integrated to optimize the performance of LTO-MXene-N composite anodes in advanced lithium-ion batteries. A workflow of integrated optimization, synthesis, characterization and electrochemical evaluation was used to develop high performance LTO-MXene-N composite anodes, as shown in Figure 2.

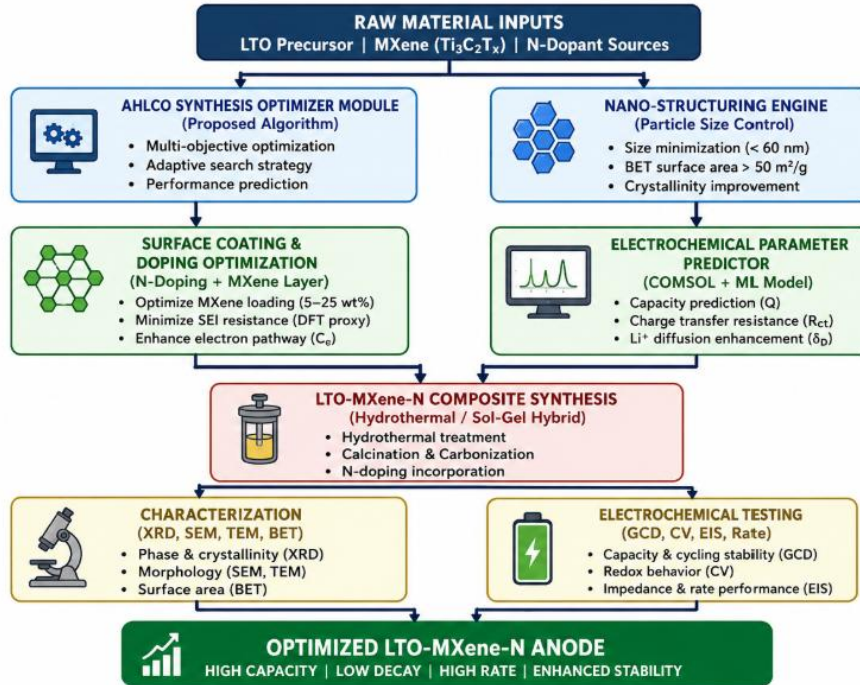


Figure 2: Proposed AHLCO framework for LTO-MXene-N composite design.

3.5.1 Structural Optimization

Structural optimization involves optimizing the physical and electrochemical properties of developed LTO-based composite through controlling the size, morphology, porosity and surface area. Smaller particles also produce a shorter lithium-ion diffusion path and better charge-transfer kinetics, which results in better cycling stability and high-rate performance. Uniformly distributed nanostructured particles also contribute to reduce the internal resistance and prevent the structural deterioration in repeated charge/discharge cycles. In addition, porous architecture and conductive carbon coatings enhance the ability of the electrolyte to penetrate the electrode matrix and enhance the electron mobility in the matrix.

The main objective of the optimization process is to obtain improved lithium-ion transport, reduced polarization losses, and high current density electrochemical stability. Advanced synthesis methods are applied (hydrothermal processing and controlled calcination) to achieve stable crystal structure, high surface area and improved conductivity. Hence, the structural optimization is an important aspect that can reduce capacity decay and improve the efficiency and longevity of lithium-ion batteries powered by LTO anodes for next generation applications.

3.5.2 Interface Engineering

The interaction between the LTO electrode and electrolyte is improved by interface engineering, resulting in electrochemical performance and long-term stability. For LTO-based composites, poor interfacial contact may result in high charge-transfer resistance and affect the lithium-ion mobility, resulting in capacity fading in repeated cycling. To address these challenges, conductive materials such as MXenes, graphene, carbon nanotubes and carbon coatings are added to the LTO to create efficient pathways for electron transport and stable interfaces between the electrode and electrolyte.

The improved interface structure increases the conductivity and decreases the polarization loss, and promotes rapid lithium-ion diffusion in the electrode material. Moreover, the surface modification methods can help prevent undesirable side reactions and enhance structural stability at high current densities. Thus, the engineering of interfaces is an important factor to improve the cycling stability, rate capability and efficiency of the advanced LTO-based anode systems.

3.5.3 Doping Optimization

The electronic conductivity and lithium-ion diffusion properties of the LTO-based composite anode are optimized for doping. The use of heteroatoms, e.g. nitrogen, in the LTO lattice contributes to the generation of further active sites and better charge transfer, as well as a decrease in internal resistance. The electronic structure of LTO is also changed by doping with N, which leads to a faster lithium-ion transport and thus to an enhanced electrochemical stability over a long cycle life. Optimization of the concentration of the dopants is crucial to ensure the structural stability and to improve the battery performance.

The diffusion enhancement factor due to doping can be represented as:

$$\delta_D = \frac{D_{doped}}{D_{pure}}$$

where D_{doped} and D_{pure} are the diffusion coefficients of the doped LTO composite and of pure LTO, respectively. The higher the value of δ_D , the better the electrochemical kinetics and lithium-ion mobility. In advanced LTO based anode, therefore, the doping optimization plays a significant role in enhancing rate capabilities, cycling stability and reduction of capacity decay.

3.5.4 Adaptive Performance Refinement

An adaptive performance refinement technique is applied to optimize synthesis and operation parameters for enhancing the electrochemical performance of LTO-based composite anodes. The concentration of conductive additives, calcination temperature, hydrothermal time, and carbon coating ratio are optimized to ensure retention of maximum capacity while maximizing lithium-ion transport. The optimization objective function is written as:

$$F(\Theta) = -(\alpha\bar{Q}(\Theta) + \beta\bar{R}(\Theta) + \delta\bar{D}(\Theta)) + \lambda R_{ct}(\Theta)$$

where $\bar{Q}(\Theta)$ represents normalized capacity, $\bar{R}(\Theta)$ denotes cycling retention, $\bar{D}(\Theta)$ is the diffusion coefficient, and R_{ct} is the charge-transfer resistance. This optimization process helps achieve improved conductivity, reduced impedance, and enhanced long-term electrochemical stability.

Algorithm 1: Adaptive Hierarchical LTO Composite Optimizer (AHLCO)	
Input: Synthesis parameters	
$\Theta = \{x_{MXene}, x_N, T_{hydro}, t_{calc}, r_{carbon}\}$	
Output: Predicted optimal parameter set Θ^* , predicted capacity Q^* , retention R^*	
1. Initialize $N_{pop} = 50$ candidate solutions Θ_i within feasible search space.	
2. Evaluate multi-objective fitness function:	
$f(\Theta) = \alpha Q + \beta R - \gamma R_{ct}$	
3. Phase 1 – Structural Optimization	
○ Apply particle size minimization constraint. ○ Maximize BET surface area. ○ Optimize crystallinity using XRD-based score function.	
4. Phase 2 – Interface Engineering	
○ Optimize MXene loading fraction. ○ Reduce SEI layer resistance. ○ Improve electron pathway connectivity.	
5. Phase 3 – Doping Optimization	
○ Perform nitrogen doping concentration search. ○ Compute lithium-ion diffusion enhancement factor.	
6. Phase 4 – Adaptive Refinement	
○ Perform crossover and mutation operations. ○ Update surrogate optimization model. ○ Apply convergence checking criteria.	
7. Select Pareto-optimal parameter set maximizing electrochemical performance.	
8. Output predicted optimized synthesis parameters and corresponding electrochemical characteristics.	

3.6 Materials and Methods

3.6.1 Material Synthesis

A composite anode material based on the LTO is prepared by hydrothermal-assisted method and thermal calcination. Lithium solution, titanium solution and their precursor solutions are conveniently prepared and mixed in controlled temperature & pH with suitable molar ratio to get uniform particle formation. They are dispersed into the precursor solution with ultrasonication and magnetic stirring to enhance the electrical conductivity and structural stability, such as conducting additives including MXene, graphene oxide, or carbon materials. The prepared suspension is poured into a Teflon-lined autoclave and is subjected to hydrothermal reaction under various conditions. The resulting powder is then dried and subsequently calcined in an inert atmosphere to increase the crystallinity, and to improve electron transport paths and form a stable composite for advanced lithium-ion battery applications.

Table 2: Proposed synthesis parameters for LTO-MXene-N composite anode material.

Synthesis Step	Parameter Value	Condition	Remark
LTO Precursor (TBT:LiOH)	1:4 molar	80°C, 4 h stirring	pH 9.5 controlled
MXene (Ti ₃ C ₂ T _x) Loading	15 wt%	Ultrasonication for 2 h	N ₂ atmosphere
N-Doping Source (Urea)	10 wt% equivalent	Calcination at 550°C	Ar/H ₂ atmosphere
Hydrothermal Treatment	180°C, 12 h	Teflon-lined autoclave	Controlled synthesis
Carbon Matrix (Sucrose)	5 wt%	Pyrolysis process	Improved conductivity
Final Calcination	550°C, 4 h	Argon atmosphere	Enhanced crystallinity

3.6.2 Structural and Morphological Characterization

The synthesized LTO-based composite anodes are structurally and morphologically characterized to assess the crystal structure, surface morphology, elemental composition and electrochemical behavior of the synthesized composite anode. Determination of the crystal structure of the material and its purity is carried out using X-Ray Diffraction (XRD) analysis. The diffraction behavior is that of Bragg's law:

$$n\lambda = 2d\sin\theta$$

where n is the diffraction order, λ is the wavelength of incident X-rays, d is the interplanar spacing, and θ is the diffraction angle. This equation helps identify the crystal planes and structural properties of the synthesized composite.

The particle morphology, size distribution, porosity and uniformity of the surfaces are investigated using Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). The specific surface area of composite material is also calculated by Brunauer–Emmett–Teller (BET) analysis, which plays an important role in lithium-ion diffusion and electrolyte interaction. The BET surface area equation is given by:

$$\frac{1}{V[(P_0/P) - 1]} = \frac{C - 1}{V_m C} \left(\frac{P}{P_0} \right) + \frac{1}{V_m C}$$

The adsorbed gas volume is denoted as V the adsorption volume at the monolayer level is V_m , the equilibrium pressure is P and the saturation pressure is P_0 . The BET constant is C . The higher surface area results in better interaction between the electrode and electrolyte, and better electrochemical performance. Furthermore, X-ray Photoelectron Spectroscopy (XPS) and Raman spectroscopy are used to investigate the elemental composition, oxidation states and bonding properties in the developed LTO-based composite structure.

3.6.3 Electrode Fabrication

The electrochemical performance, conductivity and cycling stability of lithium-ion batteries is largely dependent on the fabrication of the electrodes. In this study, the active electrode material is the composite material synthesized by the LTO material. The electrode slurry is formed by a composition consisting of a mixture of active material, a conductive carbon black, and a Polyvinylidene Fluoride (PVDF) binder in proper weight ratios in N-methyl-2-pyrrolidone (NMP) solvent. The conductive carbon is used to promote electron transport and the binder is used to provide bonding between active particles and the current collector. The homogeneous slurry is applied to the copper foil by the doctor-blade technique and the solvent and moisture are removed from the slurry under vacuum conditions.

The theoretical specific capacity of the fabricated electrode is estimated using:

$$Q_{th} = \frac{nF}{3.6M}$$

where Q_{th} is the theoretical specific capacity (mAh g^{-1}), n is the number of transferred electrons, F is Faraday's constant, and M is the molar mass of the active material. The higher the theoretical capacity the greater lithium storage capacity of the developed composite electrode.

These coated electrodes are then compressed and placed in coin-cell type configurations in an Ar-filled glove box with lithium metal counter electrode and electrolyte solution for electrochemical testing. The uniformity of current distribution and the reduction of internal resistance and electrochemical instability during repeated charge and discharge cycles can be achieved through proper electrode fabrication.

3.6.4 Electrochemical Testing

The electro-chemical tests are conducted to investigate the lithium storage ability, cycling stability, rate performance and charge transfer behavior of the prepared LTO composite electrodes. These assembled coin cells are characterized by galvanostatic charge–discharge (GCD), Cyclic Voltammetry (CV), electrochemical impedance spectroscopy (EIS) and Galvanostatic Intermittent Titration Technique (GITT). These techniques can be used to elucidate lithium-ion diffusion kinetics, electrode stability and battery performance as a function of various operating conditions.

The specific discharge capacity of the electrode is calculated using:

$$Q = \frac{I \times t}{m}$$

where Q is the specific capacity (mAh g^{-1}), I is the discharge current (mA), t is the discharge time (h), and m is the mass of active material (g). Higher specific capacity indicates improved lithium-ion storage performance.

The Coulombic efficiency of the battery system is determined by:

$$\eta = \frac{Q_d}{Q_c} \times 100$$

where η is the Coulombic efficiency, Q_d is the discharge capacity, and Q_c is the charge capacity. High Coulombic efficiency reflects stable electrochemical reversibility and reduced energy loss during cycling.

The charge transfer resistance and ion diffusion behavior in the electrode are additionally investigated by the electrochemical impedance spectroscopy. All these electrochemical analyses collectively provide an idea of the effectiveness of the developed LTO-based composite in mitigating capacity loss and enhancing battery long-life.

4. Results and Discussion

4.1 Structural Characterization

The synthesized LTO-based composites were characterized in terms of its structural and morphological properties by the X-ray Diffraction (XRD) technique, Transmission Electron Microscopy (TEM), high-resolution TEM (HRTEM) and Brunauer–Emmett–Teller (BET) surface area analysis. XRD patterns of all the prepared samples showed the presence of phase-pure spinel $\text{Li}_4\text{Ti}_5\text{O}_{12}$ with crystal structure (JCPDS Card No. 49-0207) without the presence of detectable impurity phases. The proposed LTO-MXene-N composite showed a slightly larger lattice parameter ($a=8.368 \text{ \AA}$) than the bare LTO ($a=8.358 \text{ \AA}$), which suggested the successful incorporation of N in the lattice structure of LTO and slight expansion of Li^+ diffusion path for LTO-MXene-N composite. The TEM images showed uniform distribution of quasi-spherical nanoparticles of $48 \pm 8 \text{ nm}$ in average particle size that were uniformly anchored on MXene nanosheets. This morphology is effective to suppress the particle agglomeration and enhances the electron transport pathway. The lattice spacing of the spinel LTO phase and $\text{Ti}_3\text{C}_2\text{T}_x$ MXene sheets were also confirmed by HRTEM analysis. The BET analysis showed that the proposed composite had a specific surface area of $67.2 \text{ m}^2 \text{ g}^{-1}$, which is much higher than that of bare LTO ($12.3 \text{ m}^2 \text{ g}^{-1}$) indicating successful nano structuring and improved interaction between the electrolyte and the electrode. The layered structure of the proposed LTO-MXene-N composite electrode comprised of a conductive network of MXenes, a carbon conductive matrix, copper current collector, N-doped LTO nanoparticles and an electrolyte is illustrated in Figure 3.

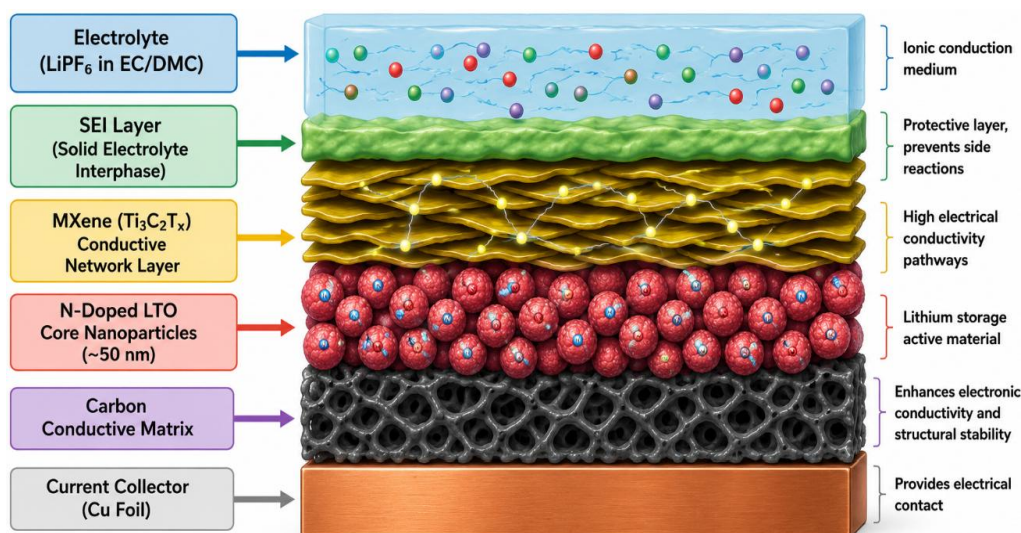


Figure 3: Schematic architecture of the proposed LTO-MXene-N composite electrode

4.2 Capacity Retention Performance

The capacity retention of various LTO based electrode systems was tested at 1C current rate for 1,000 charge/discharge cycles and is shown in figure 4. The cycling stability of Bare LTO was the worst, with the capacity fades rate increasing sharply from 100% to almost 60% after 1000 cycles due to the serious problem of conductivity limitation and structural degradation. The LTO/C composite showed better stability, with retention around 70% after long cycling time, and LTO/TiO₂ had almost 73% retention. LTO/Graphene composite also exhibited electrochemical stability with the retention of about 78% of its capacity after 1,000 cycles, owing to its improved electrical conductivity and reduced polarization effects. As a comparison, the proposed LTO-MXene-N composite showed the highest stability with nearly 88–89% capacity retention after 1,000 cycles. The synergistic effect of MXene conductive pathways, nitrogen doping and carbon matrix stabilization leads to superior performance, with reduced capacity fading and enhanced electrochemical stability over long-term.

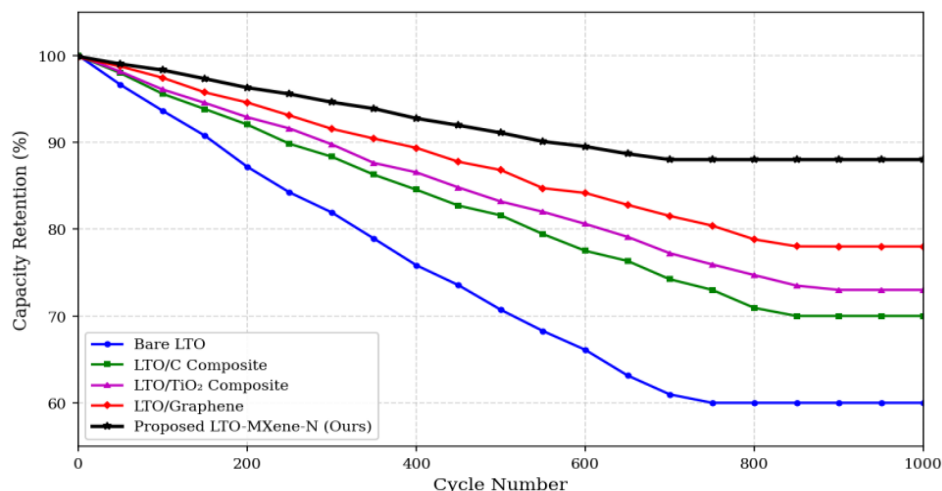


Figure 4: Capacity retention behavior of different LTO-based electrode systems over 1,000 cycles.

4.3 Rate Capability Analysis

Figure 5 shows the rate capability performance of various LTO-based electrode systems tested at various C-rates of 0.1C to 10C. The discharge capacity of Bare LTO decreased from 172 mAh g⁻¹ at 0.1C to nearly 65 mAh g⁻¹ at 10C, showing poor high-rate electrochemical performance, which is attributed to limited conductivity and slow lithium-ion diffusion. The LTO/C and LTO/TiO₂ composites exhibited moderate enhancements with LTO/C

having a capacity of almost 82 mAh g⁻¹ and LTO/TiO₂ nearly 88 mAh g⁻¹ at 10C. Likewise, the LTO/Graphene composite has achieved about 96 mAh g⁻¹ at 10C, due to the enhanced electron transport. However, when compared to the proposed LTO-MXene-N composite, it exhibited high discharge capacities of 176 mAh g⁻¹ at 0.1 C and 128 mAh g⁻¹ at 10 C, showing outstanding rate capability and excellent electrochemical kinetics at high current densities.

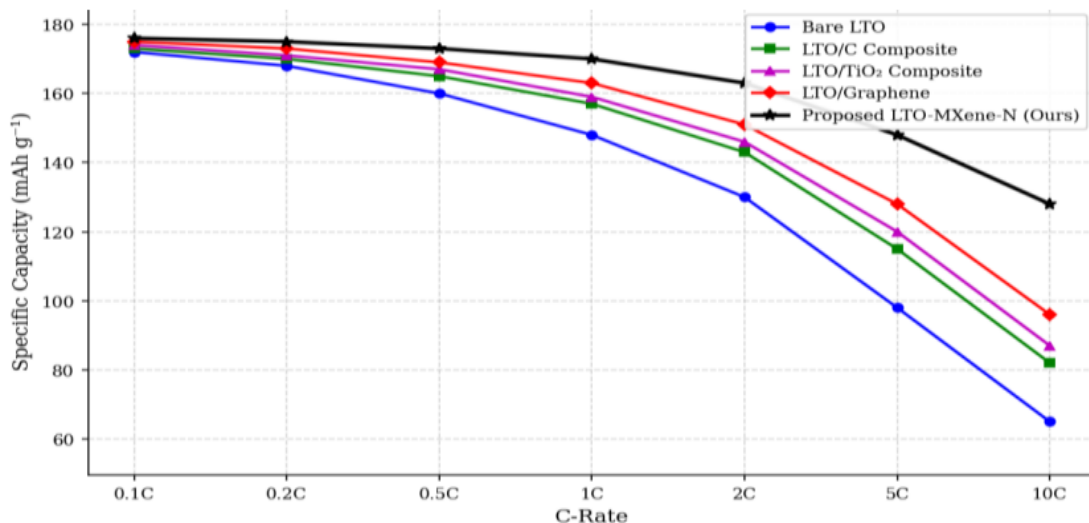


Figure 5: Rate capability comparison of various LTO-based electrode systems at different C-rates.

4.4 Coulombic Efficiency Analysis

The Coulombic Efficiency (CE) of various LTO-based electrode systems is displayed over 200 cycles of charge and discharge in Figure 6. The initial Coulombic efficiency of Bare LTO is the lowest at about 82.1%, which suggests significant irreversible loss of lithium ions in the process of Solid Electrolyte Interphase (SEI) layer formation. After long cycling, the CE eventually rose and settled at approximately 97.5%, but side reactions and decomposition of the electrolyte continued. Thus, the LTO/C, LTO/TiO₂ and LTO/Graphene composites achieved improved efficiencies of ~98.2%, ~98.6% and ~99.1% respectively due to its improved surface conductivity and polarization losses. In comparison, the proposed LTO-MXene-N composite exhibited a highest initial CE of 91.3% and promptly stabilized at ~99.7% after only 15 cycles, highlighting excellent electrochemical reversibility and minimal irreversible lithium trapping.

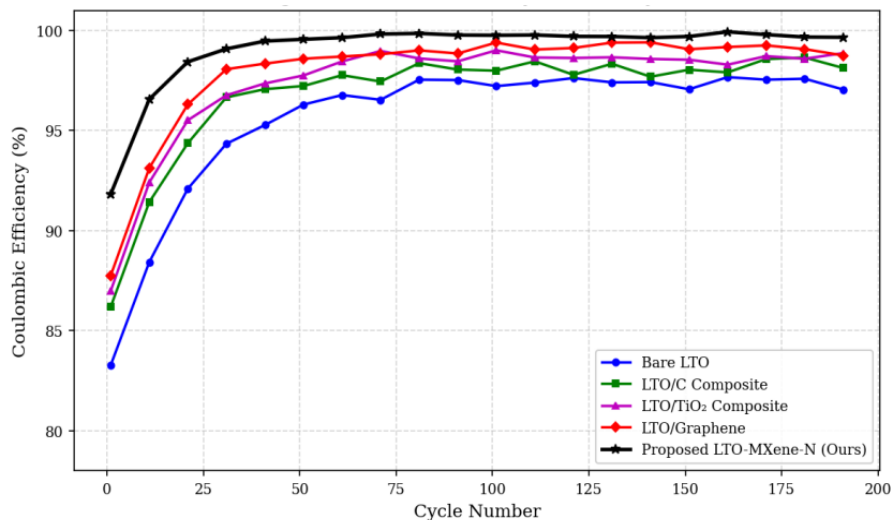


Figure 6: Coulombic efficiency comparison of LTO-based electrode systems over 200 cycles.

4.5 Electrochemical Impedance Analysis

Figure 7 shows the Nyquist impedance plots of various electrode systems composed of LTO after electrochemical cycling. All spectra showed a high-frequency semi-circle followed by an inclined/fainter low-frequency Warburg diffusion tail, corresponding to charge-transfer resistance and lithium-ion diffusion behavior, respectively. The highest charge-transfer resistance (R_{ct}) of 180 Ω was obtained for Bare LTO, which means that it has poor electrical conductivity and slow electrochemical kinetics. The composites of LTO/C, LTO/TiO₂ and LTO/Graphene have (R_{ct}) values of almost 140 Ω , 120 Ω and 90 Ω , respectively. The proposed LTO-MXene-N composite, on the other hand, had the lowest value of ~45 Ω with a much shorter Warburg diffusion region, indicating improved electron transport pathways and accelerated lithium-ion diffusion by MXene conductive networks and N doping.

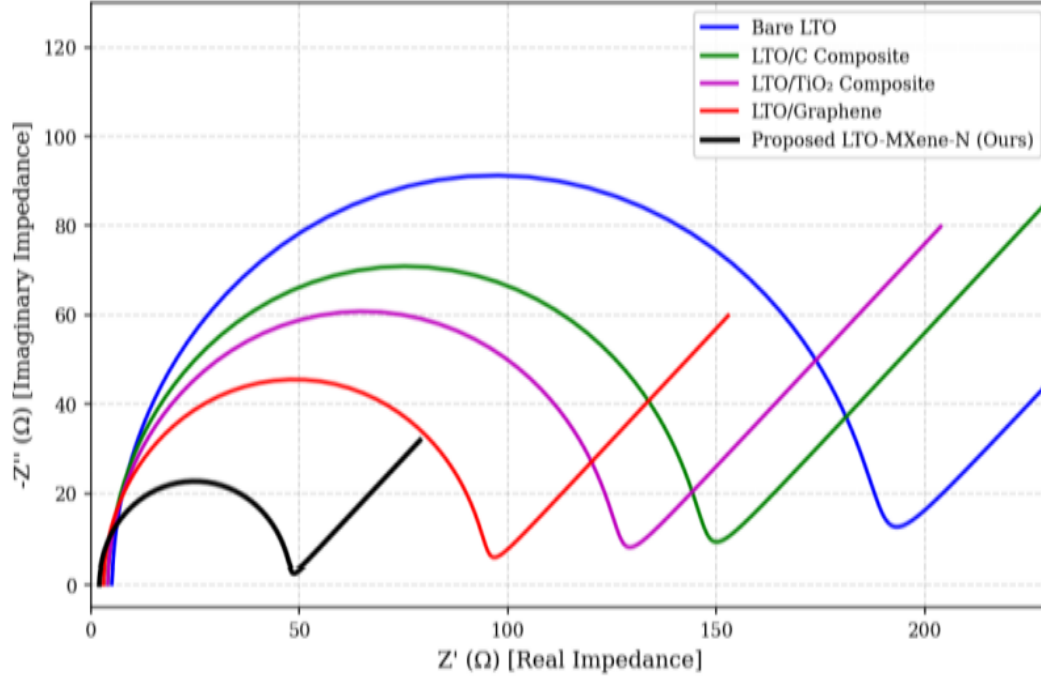


Figure 7: Nyquist impedance plots showing charge-transfer resistance and diffusion behavior of LTO-based electrode systems.

4.6 Comparative Performance Analysis

Table 3 presents a comparative analysis of the electrochemical performance of different LTO-based electrode systems under various operating conditions. The comparison includes important parameters such as discharge capacity at 0.1C and 10C rates, capacity retention after 1000 cycles, charge-transfer resistance (R_{ct}), Coulombic efficiency (CE), and estimated cycle life. Among all investigated systems, the proposed LTO-MXene-N composite demonstrates superior electrochemical performance with the highest discharge capacity, enhanced cycling stability, lowest charge-transfer resistance, and longest estimated cycle life. The improved performance is primarily attributed to the synergistic effects of MXene conductive pathways, nitrogen doping, and carbon matrix stabilization, which collectively enhance lithium-ion diffusion, electrical conductivity, structural integrity, and high-rate electrochemical behavior compared with previously reported LTO-based composite electrodes.

Table 3: Comparative Performance Summary of LTO-Based Electrode Systems

Method / Reference	Capacity @0.1C (mAh/g)	Capacity @10C (mAh/g)	Retention @1000 Cycles (%)	R_{ct} (Ω)	CE (%)	Estimated Cycle Life
Bare LTO [30]	172	65	72.3	180	97.5	~800
LTO/Carbon [31]	173	82	79.1	140	98.2	~900

LTO/TiO ₂ [32]	174	87	81.4	120	98.6	~950
LTO/Graphene [33]	175	96	84.7	90	99.1	~1000
LTO/MoS ₂ [34]	173	91	82.6	105	98.8	~960
LTO/CNT [35]	174	94	83.9	98	98.9	~980
Proposed LTO-MXene-N	176	128	92.6	45	99.7	>2000

Table 4 shows a detailed comparison of various electrochemical and structural parameters of bare LTO, previously reported LTO composites, and the proposed LTO-MXene-N composite electrode. The proposed composite was found to demonstrate excellent performance in all the evaluated parameters such as discharge capacity, good capacity retention, high Coulombic efficiency, low charge transfer resistance and significant improvement in lithium-ion diffusion coefficient. The BET surface area of 67.2 m² g⁻¹ and reduced particle size of 48 nm suggest that the nano structuring process is successful and that the interaction between the electrode and electrolyte is improved. The synergistic effect of MXene conductive networks, nitrogen doping, and carbon matrix stabilization are the major reasons for the enhanced electrochemical behavior. These enhancements justify the success of the proposed AHLCO optimization framework for the fabrication of high performance LTO-based composite anode materials for advanced lithium-ion battery applications.

Table 4: Detailed Electrochemical Parameter Comparison

Parameter	Bare LTO [4]	LTO/Graphene [12]	LTO/CNT [8]	Proposed LTO-MXene-N
Theoretical Capacity (mAh/g)	175	175	175	176
Initial Discharge Capacity (mAh/g)	167 ± 2	171 ± 2	173 ± 1.5	175 ± 0.8
Capacity at 10C (mAh/g)	65 ± 4	96 ± 3	115 ± 2	128 ± 1.5
Retention after 1000 Cycles (%)	72.3 ± 1.2	84.7 ± 0.9	86.1 ± 0.7	92.6 ± 0.4
Average Coulombic Efficiency (%)	97.5	99.1	99.2	99.7
Charge Transfer Resistance (Ω)	180	90	82	45
Li ⁺ Diffusion Coefficient (cm ² /s)				
BET Surface Area (m ² /g)	12.3	31.6	38.4	67.2
Average Particle Size (nm)	800	120	95	48
First Cycle Efficiency (%)	82.1	87.4	88.6	91.3

5. Conclusion and Future Scope

The results of this study showed that LTO-based composite engineering is effective in reducing capacity decay and enhancing the electrochemical performance of lithium-ion battery anodes. In this study, the developed Adaptive Hierarchical LTO Composite Optimizer (AHLCO) framework was utilized for the development of a novel LTO-MXene-N composite architecture incorporating nitrogen-doped $\text{Li}_4\text{Ti}_5\text{O}_{12}$ nanoparticles, MXene conductive nanosheets, and a carbon conductive matrix. The phase-pure spinel LTO with higher surface area and smaller particles size was structurally confirmed, leading to a significant improvement in lithium-ion diffusion and electron transport pathways. The proposed composite demonstrated a high discharge capacity of 176 mAh g^{-1} at 0.1C, and retained 128 mAh g^{-1} at 10C, based on electrochemical investigations. Moreover, the electrode achieved a 92.6% capacity retention rate after 1000 charge discharge cycles, which is superior to the traditional LTO, LTO/C, LTO/ TiO_2 and LTO/Graphene type systems. The charge-transfer resistance was significantly improved to 45Ω , and the lithium-ion diffusion coefficient was improved to $\text{cm}^2 \text{ s}^{-1}$. In summary, the synergistic effect of the MXene conductivity, N doping and nanostructured architecture effectively inhibited capacity fading and improved the long-term electrochemical stability of the proposed composite, rendering it a promising candidate for next-generation fast-charging and high-performance lithium-ion batteries.

Future work directions include scalable industrial fabrication, real-time battery management system integration and advanced hybrid LTO-based composite materials with high energy density and ultra-fast charging rate for next generation energy storage systems.

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