

# Study on Design, Synthesis and Performance Control of New Electrode Materials for High Energy Density Lithium Ion Batteries

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## Abstract

In view of the limitations of traditional electrode materials for lithium-ion batteries, such as  $\text{LiCoO}_2$ ,  $\text{LiMn}_2\text{O}_4$  and  $\text{LiFePO}_4$ ,  $\text{Li}[\text{Ni}_x\text{Mn}_{1-x-y}\text{Co}_y]\text{O}_2$ , a lithium-rich manganese-based ternary composite, was explored in this paper, and carbon nanotubes (CNTs) were introduced for surface modification to improve the electrochemical performance of the materials. The composite was synthesized by coprecipitation method and calcined at 800-900 °C for 4-6 hours to form the final material. Performance control includes surface modification, doping modification and coating treatment to optimize conductivity, structural stability and cycle stability. The analysis through X-ray diffraction (XRD) and scanning electron microscopy (SEM) indicates that the synthesized material exhibits a well-defined crystalline structure and favorable micro-morphological characteristics. Electrochemical evaluations demonstrate that this material possesses a significant specific capacity, alongside robust cycling stability and superior rate capability. Discussions on the underlying mechanisms highlight how adjusting elemental ratios, incorporating dopants, and applying surface modifications can enhance material performance. This research successfully fabricated lithium-rich manganese-based ternary composite materials with outstanding electrochemical attributes, thereby offering both theoretical insights and technical foundations for advancing high energy density lithium-ion batteries.

## Keywords

Lithium Ion Batteries; Electrode Materials; Design, Synthesis and Performance Control.

## 1. Introduction

Traditional electrode materials for lithium-ion batteries, such as  $\text{LiCoO}_2$ ,  $\text{LiMn}_2\text{O}_4$  and  $\text{LiFePO}_4$ , have met the market demand to some extent, but there are still many limitations in energy density, cycle stability and cost. For example,  $\text{LiCoO}_2$  has high material cost and limited resources;  $\text{LiMn}_2\text{O}_4$  material has poor cycle stability and rapid capacity attenuation [1-2]. While  $\text{LiFePO}_4$  material has good safety and low cost, but its energy density is relatively low.

To address the limitations of conventional materials, researchers are actively investigating novel electrode materials for lithium-ion batteries. Over the past few years, significant advancements have been observed in the development of new materials, including lithium-rich manganese-based compounds, high-voltage spinel cathodes, and silicon-based anodes [3-4]. These new materials have excellent performance in energy density, cycle stability and rate performance, which makes it possible to further improve the performance of lithium-ion batteries. However, the design, synthesis and performance control of new electrode materials still face many challenges [5]. How to design a material structure with excellent electrochemical performance, how to choose a suitable synthesis method to prepare high-quality materials, and how to further optimize the electrochemical performance of materials by means of performance regulation are all urgent problems to be solved at present.

This paper delves into the development of high-performance electrode materials with original intellectual property by thoroughly examining the design, synthesis, and performance optimization of novel high-energy density lithium-ion battery electrodes. Through this exploration, the study offers both theoretical insights and technical support aimed at enhancing lithium-ion battery performance. The findings presented herein hold academic significance and contribute substantially to fostering the sustainable advancement of the lithium-ion battery industry.

## 2. Experimental Part

### 2.1. Material Preparation

The raw materials and specifications required for this experiment are shown in Table 1 below:

**Table 1.** Experimental raw materials and specifications

Raw material name	Specifications and Description
Lithium source	Lithium Hydroxide ( $\text{LiOH}\cdot\text{H}_2\text{O}$ ), purity $\geq 99.0\%$ , particle size $\leq 100$ mesh.
Manganese source	Manganese Acetate ( $\text{Mn}(\text{CH}_3\text{COO})_2\cdot 4\text{H}_2\text{O}$ ), purity $\geq 99.5\%$ .
Nickel source	Nickel Nitrate ( $\text{Ni}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ ), purity $\geq 98.0\%$ .
Cobalt source	Lithium Cobalt Oxide ( $\text{LiCoO}_2$ ), purity $\geq 99.0\%$ , used as a doping element.
surfactant	Polyvinylpyrrolidone (PVP), molecular weight approximately 50000, used to control material morphology.
solvent	Deionized Water, resistivity $\geq 18.2\text{M}\Omega\cdot\text{cm}$ .
Surface modifier	Carbon Nanotubes (CNTs), length 10-30 $\mu\text{m}$ , diameter 10-20nm, used to improve material conductivity.
Doped element source	Aluminum Oxide ( $\text{Al}_2\text{O}_3$ ) nanopowder, purity $\geq 99.9\%$ , used for doping modification.

### 2.2. Electrode Material Design

The new electrode material designed in this study is a lithium-rich manganese-based ternary composite, and its chemical composition can be expressed as  $\text{Li}[\text{Ni}_x\text{Mn}_{1-x-y}\text{Co}_y]\text{O}_2$  (where X and Y are in a specific ratio and N is a small amount of cobalt doped), and CNTs are introduced for surface modification [6]. The design concept focuses on three aspects: firstly, by optimizing the ratio of Ni, Mn and Co, the specific capacity and voltage platform of the material can be improved to achieve high energy density; Secondly, a small amount of cobalt doping is introduced to enhance the structural stability and reduce the capacity attenuation during the cycle to ensure good cycle stability; Finally, CNTs are added to the surface of the material to improve the electron transmission efficiency and reduce the internal resistance, thus obtaining excellent conductivity.

### 2.3. Synthesis Step

The lithium-rich manganese-based ternary composite material is synthesized by coprecipitation method [7], and the specific steps are as follows:

(1) Dissolving lithium hydroxide in deionized water to prepare a lithium salt solution with a certain concentration. Manganese acetate, nickel nitrate and lithium cobaltate were dissolved in deionized water to prepare corresponding metal salt solutions. PVP was dissolved in deionized water as surfactant solution.

(2) Under the condition of stirring, the lithium salt solution is slowly dropped into the mixed metal salt solution, and PVP solution is added at the same time to control the precipitation morphology. Adjust the pH value of the reaction system to a suitable range, and keep stirring at

a constant temperature for a period of time, so that metal ions and hydroxide ions can fully react to form coprecipitates.

(3) Filtering the coprecipitate, and washing with deionized water for many times to remove residual impurities and ions.

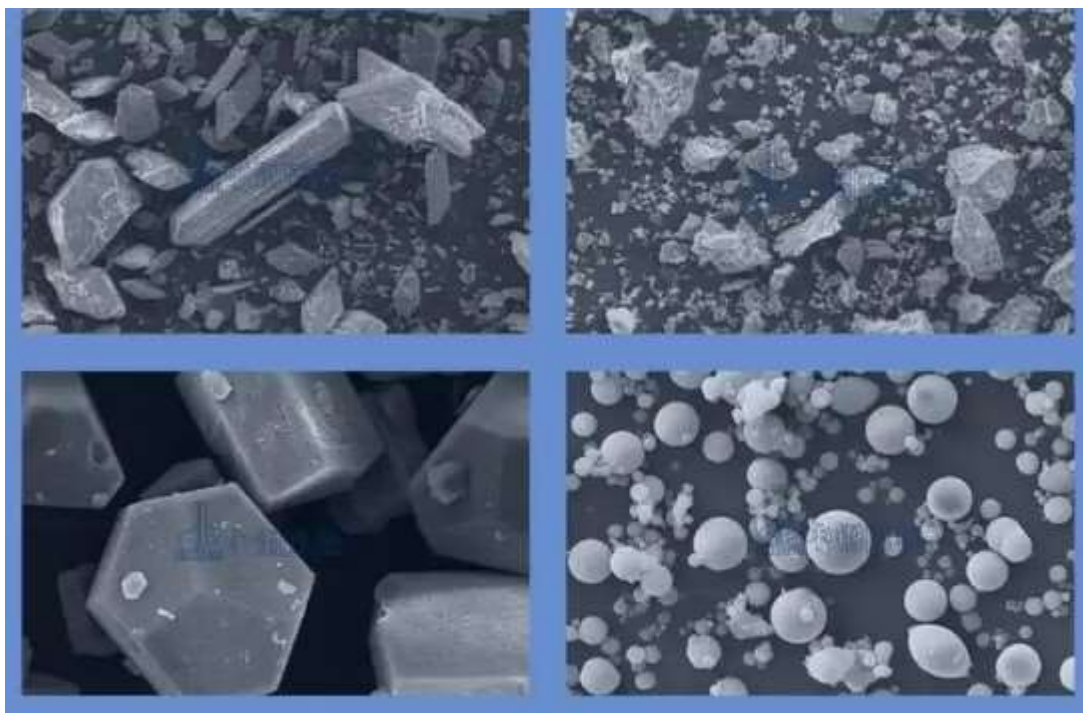
(4) Dry the washed precipitate in an oven to a constant weight. Place the dried precursor in a high-temperature furnace and calcine it in an oxygen atmosphere. The calcination temperature is set at 800-900 °C and the holding time is 4-6 hours to form a lithium rich manganese based ternary composite material.

(5) The calcined composite material was mixed with appropriate amount of CNTs, and CNTs were uniformly dispersed on the surface of the material by ball milling or mechanical stirring.

## 2.4. Performance Regulation

The material properties were optimized by surface modification, doping modification and coating treatment. Adding CNTs to the surface of the material can improve the conductivity and reduce the internal resistance, thus improving the electrochemical performance; In the synthesis process, a small amount of alumina nano-powder was introduced as doping element to enhance the structural and cyclic stability, and the doping ratio of cobalt element was adjusted to optimize the electrochemical performance, including improving the specific capacity and reducing polarization. In addition, a thin and dense oxide layer  $Al_2O_3$  is coated on the surface of the material to isolate the direct contact between the material and the electrolyte, thereby reducing side reactions and further improving the stability of the material.

## 2.5. Characterization Method



**Fig. 1** electrode materials

A variety of characterization methods are adopted: X-ray diffraction (XRD) analysis is used to confirm the successful synthesis of materials and the incorporation of doping elements into the crystal lattice, and the crystal structure and phase composition are determined by diffraction peak characteristics; Scanning electron microscope (SEM) was used to observe the microstructure, particle characteristics and modification of CNTs. In electrochemical performance test, parameters such as specific capacity, cyclic stability and rate performance

are obtained by charge-discharge and cyclic voltammetry (CV) test, so as to evaluate the practical application potential of materials and provide basis for optimizing material design and synthesis process.

### 3. Results and Discussion

#### 3.1. Structural Characterization

The diffraction pattern of Li-rich Mn-based ternary composites was obtained by XRD analysis. The clear diffraction peaks in the spectrum show that the material has a good crystal structure, and the positions of the diffraction peaks are in line with expectations, which confirms the successful synthesis of  $\text{Li}[\text{Ni}_x\text{Mn}_{1-x-y}\text{Co}_y]\text{O}_2$ . At the same time, no obvious impurity peak was observed, indicating that the doping elements aluminum and cobalt have been effectively integrated into the crystal lattice and no independent phase has been formed. In addition, the intensity and width of diffraction peak also show that the material has high crystallinity and small grain size, which is beneficial to the diffusion of lithium ions and the improvement of electrochemical properties.

The SEM observation results show that the lithium-rich manganese-based ternary composite presents uniform particle morphology, moderate particle size and uniform distribution. CNTs are tightly coated on the surface of the material, forming a good conductive network, which is helpful to improve the electron transmission efficiency of the material. At the same time, no obvious agglomeration phenomenon was observed, which indicated that PVP surfactant effectively controlled the morphology of the material during the synthesis process.

#### 3.2. Electrochemical Performance

The results of electrochemical performance test show that lithium-rich manganese-based ternary composites show excellent electrochemical performance. In the charge-discharge test, the material shows a high specific capacity, and the capacity retention rate is high after many cycles, which shows that the material has good cycle stability. In addition, the rate performance test also shows that the material can maintain a high specific capacity under different current densities, showing good rate performance.

The CV test provided deeper insights into the material's electrochemical reaction process. Distinct redox peaks were evident in the CV curve, with a symmetrical peak shape indicating that the material undergoes reversible electrochemical reactions. Additionally, the small potential difference between the redox peaks suggests minimal polarization, which is advantageous for enhancing the material's energy efficiency and power density.

#### 3.3. Discussion on Mechanism

By optimizing the ratio of Ni, Mn and Co, the specific capacity and voltage platform of the material were successfully improved. The introduction of Ni element improves the specific capacity of the material, while the synergistic effect of Mn and Co elements stabilizes the crystal structure of the material and improves the voltage platform. This enables the material to store and release more energy during charging and discharging, thus achieving high energy density. The introduction of a small amount of cobalt doping enhances the structural stability of the material. The doping of cobalt is helpful to stabilize the layered structure of the material and reduce the phase transition and capacity attenuation during cycling. At the same time, cobalt can also improve the electronic conductivity of the material and further improve the electrochemical performance. The conductivity of the material was successfully improved by adding CNTs to the surface of the material. CNTs form a good conductive network, which improves the electron transmission efficiency and reduces the internal resistance. This enables the material to respond to the current change more quickly during the charging and discharging

process, thus improving the power density and rate performance. The doping of alumina nano-powder also improves the cyclic stability of the material to some extent. As an inert phase, alumina can stabilize the crystal structure of the material, and reduce the side reaction and capacity attenuation during the cycle. At the same time, alumina can also be used as a channel for lithium ion diffusion to promote the rapid diffusion of lithium ions and further improve the electrochemical properties of materials.

In this study, lithium-rich manganese-based ternary composites with excellent electrochemical properties were successfully prepared by optimizing material composition, improving synthesis process and performance control means. This material has a broad application prospect in high energy density lithium ion batteries.

#### 4. Conclusion

By optimizing the ratio of Ni, Mn and Co, introducing a small amount of cobalt doping and adding CNTs on the surface of the material, the specific capacity and voltage platform of the material were significantly improved, and the structural stability and electronic conductivity of the material were enhanced. In addition, the electrochemical properties of the materials were further optimized by means of surface modification, doping modification and coating treatment, including improving cycle stability, rate performance and energy efficiency. The experimental results show that the prepared lithium-rich manganese-based ternary composites have good crystal structure, uniform particle morphology and good conductive network. The electrochemical performance test shows that the material exhibits high specific capacity, excellent cycle stability and rate performance. The CV test further demonstrated that the material exhibits excellent electrochemical reversibility and minimal polarization, both of which are conducive to enhancing energy efficiency and power density. Incorporating the Ni element boosts the material's specific capacity, whereas the combined influence of Mn and Co elements contributes to stabilizing the crystal structure and elevating the voltage platform. Cobalt doping strengthens structural stability, mitigating phase transitions and capacity fade during cycling. Meanwhile, the inclusion of CNTs enhances conductivity and lowers internal resistance, thereby improving power density and rate performance. The doping of alumina nano-powder also improves the cycle stability of the material to some extent and promotes the rapid diffusion of lithium ions.

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