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Advancements in Material Optimization for High-Performance Battery Technologies: Structural Enhancements and Electrochemical Innovations

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Abstract. With the increasing demand for high-performance batteries, material optimization and innovation have become key factors in improving battery performance. This paper summarizes the latest research progress in structural optimization and electrochemical performance enhancement of current sodium-ion batteries, zinc-ion batteries, aqueous batteries, and organic flow batteries. It focuses on introducing the optimization of battery materials via methods such as structural regulation, defect engineering, coating technology, and 3D printing, thereby enabling higher energy density, better long-cycle stability, and faster charge-discharge rates. This paper also discusses the application prospects of novel materials (e.g., hard carbon, vanadium-doped materials, and covalent organic frameworks in batteries) and provides an outlook on future research directions. This study finds that multi-dimensional material optimization strategies (e.g., the synergy between defect engineering and interfacial coating, and 3D printing-based structural customization) can enable batteries to achieve long-cycle stability under high-rate conditions (e.g., vanadium-based cathodes maintain 99% of their initial capacity after 2300 cycles, and hard carbon anodes retain 87% of their capacity after 1000 cycles at 1000 mA g^{-1}). Meanwhile, the application of novel systems such as biomass-derived hard carbon and modified vanadium-based materials can effectively balance the requirements of high energy density and low cost for batteries.

Keywords: Structural optimization, Material innovation, Defect engineering, Aqueous zinc-ion batteries, Interface engineering

1. Introduction

With the growing global energy demand and the widespread application of renewable energy technologies, batteries, as the core technology for energy storage, are facing higher performance requirements. Particularly in fields such as electric vehicles, renewable energy storage, and portable devices, the demand for batteries with high energy density, long cycle life, and high power density is constantly increasing. However, traditional lithium-ion batteries (LIBs) have issues such as scarce lithium resources and safety hazards. Therefore, the development of low-cost, high-efficiency, and safe alternative batteries, such as sodium-ion batteries (SIBs), zinc-ion batteries (ZIBs), and aqueous batteries, has become the focus of current research [1,2]. The enhancement of battery performance relies on the optimization and structural design of electrode materials. Through approaches such as structural optimization, introduction of defect engineering, adoption of surface coating technology, and emerging manufacturing technologies (e.g., 3D printing), significant improvements can be achieved in the electrical conductivity, ionic conductivity, and stability of battery materials. This paper will focus on discussing various strategies for improving battery performance through material innovation and structural optimization and will also introduce the application of novel materials in new energy batteries.

2. Material optimization strategies

2.1. Structural optimization and defect engineering

Structural optimization of battery materials serves as the foundation for enhancing battery performance. By controlling the crystal structure of materials or introducing oxygen vacancy defects via defect engineering and other approaches, the electronic and ionic conductivity of materials can be improved. Vanadium-based oxides are typical multivalent materials, and their layered structure endows them with excellent chemical performance in SIBs and ZIBs. Studies have shown that vacancy-rich sodium vanadate materials exhibit excellent performance when applied in aqueous ZIBs; after the introduction of oxygen vacancies and defects, the ionic conductivity and stability of the material are both enhanced. Similarly, studies have found that defect engineering can improve the reversibility and cycling stability of battery cathode materials [1]. Furthermore, the intercalation of Cu^{2+} into layered vanadium oxides can optimize the coordination environment of vanadium atoms and enhance the electrochemical activity of the material. The introduction of Cu^{2+} can also enhance the electronic conductivity and ion diffusion capability of layered vanadium oxides, thereby significantly improving its application effect in zinc storage [3].

2.2. Coating technology

Coating technology improves the electrical conductivity and stability of electrode materials by forming a thin film on the surface of electrode materials. For instance, poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) coating is applied to lithium nickel cobalt aluminum oxide ($LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$, NCA) cathode materials to optimize the electrode interface. The PEDOT:PSS coating can significantly improve the electrical conductivity of the electrode, slow down surface cracking, and prevent electrolyte erosion, ultimately enhancing the cycle life and capacity retention of the battery. Research results show that after 200 charge-discharge cycles at a voltage window of 2.7–4.3 V and a rate of 1 C, the NCA coated with PEDOT:PSS still maintains a capacity retention rate of 83.58%, which is significantly better than that of uncoated samples. Coating technology not only enhances the electrical conductivity of electrode materials but also effectively inhibits capacity degradation caused by surface cracking [4]. This method is also applicable to cathode materials of SIBs and ZIBs, contributing to the enhancement of battery performance.

2.3. 3D printing technology

With the development of 3D printing technology, its application in battery material preparation has also attracted increasing attention. 3D printing can precisely control the shape, pore size, distribution and connectivity of materials, which not only optimizes the dual ion and electron transport pathways of batteries, but also improves volumetric energy density and power density. 3D printing technology enables the design and fabrication of complex electrode structures (e.g., hierarchical porous architectures, carbon microlattices, etc.) and can precisely improve the porosity of sodium-ion battery electrodes (usually optimized to 30%-70%), further reducing ion transport resistance and optimizing ion transport pathways, thus improving the charge-discharge efficiency and cycling stability of batteries [2]. Sodium battery electrodes prepared via 3D printing exhibit excellent electrochemical performance, especially maintaining stable capacity output even under high-rate discharge scenarios, and still possessing high energy density and longer service life during long-term cycling, effectively solving the problems of single electrode structure and high interfacial impedance in traditional fabrication processes.

2.4. Design of experiments for material optimization

For the disordered rock-salt (DRX) cathodes of LIBs, solid-state synthesis combined with statistical Design of Experiments (DoE) can systematically quantify the coupling relationships between conductive phase type or content, first-cycle discharge capacity, capacity retention after 50 cycles (CR50), and rate capability without altering the host lattice. The study initially designed 9 sets of experiments using the Taguchi method. Results show that samples using Super C65 exhibit overall lower capacity and poorer rate capability; moreover, the energy storage efficiency is low at low content, and although increasing the content can recover part of the capacity, the retention rate remains unsatisfactory. When graphite is used as the conductive phase, higher first-cycle capacities (approximately 118.9–171.6 mAh g^{-1}) can be obtained, and the retention rate increases with the increase in content. The combination with multi-walled carbon nanotubes (MWCNTs) is generally optimal; however, when the content is 10 wt%, the retention rate is still only 40.2 ± 6.7%. Nevertheless, electronic conduction and microstructure mismatch remain bottlenecks [5]. It can be concluded that placing DoE in the collaborative optimization process of synthesis, electrode texture, and electrical contact in advance can quickly identify the sensitive factors affecting capacity, retention rate, and rate capability, providing a quantitative basis for the large-scale preparation and formula standardization of DRX cathodes.

2.5. Raw material and process chain optimization

Electrolytic manganese dioxide (EMD), as an important raw material precursor for alkaline manganese batteries and $LiMn_2O_4$ (LMO) cathodes, exhibits a "raw material → cathode → battery" chain amplification effect of its structure on the final battery performance. In the industrial electrolysis of EMD using traditional Ti anodes, the easy formation of TiO_2/TiO passive films leads to high cell voltage and a narrow operation window (e.g., difficulty in adapting to high acidity/high current density), which limits the adjustability and consistency of the EMD structure. After introducing the TiMn/Ti alloy anode, due to its lower oxygen affinity and stronger anti-passivation ability, the anodic overpotential can be significantly reduced and the process parameter space can be expanded. This enables the acquisition of EMD with increased Mn (III) content, more 1×2 tunnels (R phase), and elevated structural water under relatively high current density and acidity. Such structural characteristics can be further translated into performance enhancement of alkaline manganese batteries; moreover, LMO synthesized based on EMD with high Mn (III) content (e.g., EMD prepared at 90 $A \cdot m^{-2}$) can achieve a high capacity of 122 $mAh \cdot g^{-1}$ at a rate of 0.1 C within the voltage range of 3.0–4.3 V. Mechanistically, compared with 1×1 tunnels, 1×2 tunnels are more conducive to fast proton migration, thereby enhancing discharge kinetics (though excessive structural water will reduce discharge performance). Starting from the raw material end of the electrode, this study supplements an important perspective of "process chain optimization (also material optimization)" through a complete causal chain: "TiMn/Ti anode — electrolysis parameters (acidity/current density) — EMD crystal phase (1×2/1×1 tunnels)/valence state (Mn (III)/Mn (IV)) — DFT thermodynamic verification — battery performance" [6].

3. Application of novel materials

3.1. Hard carbon materials

Hard carbon materials, especially biomass-derived hard carbon, have become ideal materials for sodium-ion battery anodes due to their excellent cycling stability, high sodium storage capacity, and low cost. Studies have shown that olive shell-derived hard carbon materials optimize the material's pore structure, degree of graphitization, and surface chemical properties by synergistically regulating the carbonization temperature and pre-carbonization (pretreatment) strategy, thereby systematically enhancing the electrochemical performance of batteries. Among these parameters, 1300 °C is the optimal carbonization temperature; at this temperature, the material achieves a balance between the degree of graphitization and interlayer spacing (approximately 3.79 Å), which not only improves electrical conductivity to optimize rate capability but also ensures the unobstructed Na^+ insertion/extraction pathways. Additionally, the air-atmosphere pre-carbonization strategy can introduce more oxygen-containing functional groups (e.g., C-O, C=O) and microporous structures, thereby further increasing sodium storage active sites. Notably, the OSHC-Air electrode treated with air pre-carbonization and calcined at 1300 °C exhibits more excellent comprehensive performance: it retains 87% of its capacity after 1000 cycles at a high current density of 1000 mA g^{-1}. Meanwhile, this structural optimization not only provides more sodium ion storage sites through micropores and oxygen-containing functional groups but also alleviates the diffusion resistance of sodium ions under high rates via moderate graphitization and reasonable interlayer spacing, enabling the material to simultaneously possess high sodium storage capacity (a reversible capacity of 324 mAh g^{-1} at 50 mA g^{-1}), excellent rate capability, and long service life. Furthermore, the sodium-ion full cell assembled based on this olive shell-derived hard carbon (PB ($Na_2Fe[Fe(CN)_6]$)//OSHC-Air) exhibits a high capacity of 216 mAh g^{-1} at 50 mA g^{-1}, which further verifies its excellent practical application potential [7].

3.2. Vanadium-based materials

Vanadium-based materials, especially vanadium oxides (e.g., $Na_{0.76}V_6O_{15}$, $V_{10}O_{24}\cdot nH_2O$), are widely used in the cathodes of aqueous zinc-ion batteries (AZIBs) due to their unique tunnel and layered structures as well as the multivalent characteristics of vanadium [1]. By optimizing the crystal structure and electronic state of vanadium oxides—especially through the introduction of oxygen vacancies and the intercalation and doping modification of external metal ions and cations (e.g., NH_4^+, Cu^{2+})—the electronic conductivity of the material and Zn^{2+} transport kinetics can be significantly improved. Vanadium oxides rich in oxygen vacancies can reduce the Zn^{2+} diffusion energy barrier and enhance electron delocalization, which not only exhibit high electrochemical activity but also inhibit vanadium dissolution, thereby achieving long-cycle stability. Additionally, after Cu^{2+} intercalation into the crystal planes of $V_{10}O_{24}\cdot nH_2O$, it can optimize the coordination environment of vanadium centers and stabilize the interlayer structure, which not only improves battery capacity but also enhances stability under low current densities and high-rate discharge performance. Researchers can precisely regulate the interlayer spacing, tunnel size, and defect density of vanadium oxides by adjusting the concentration and intercalation amount of modifying ions (e.g., NH_4^+, Cu^{2+}), thereby further enhancing their electrochemical performance [1,3].

3.3. Covalent organic frameworks

Covalent organic frameworks (COFs) have emerged as emerging materials in alkali metal chalcogenide batteries such as sodium-sulfur (Na-S) batteries due to their highly tunable pore structure, excellent chemical functionalization capability, and high specific surface area (hundreds to thousands of m^2/g). The structural characteristics of COFs endow them with multi-component compatibility in Na-S batteries: when used as a cathode material carrier, they can effectively alleviate the shuttle effect of sodium polysulfides (NaPSs) through the dual mechanisms of pore size matching (e.g., sub-nanoscale pore physical confinement of NaPSs) and chemical adsorption (e.g., binding of NaPSs by functional groups such as $-NH_2$ and $-SO_3H$); when used as a separator modification layer, they can enhance the selective transport of Li^+/Na^+ and also improve thermal stability. By adjusting the pore structure and chemical functionalization of COFs, the performance of Na-S batteries can be significantly enhanced. The tunable structure of COFs can be custom-designed according to the cathode loading and ion transport requirements of Na-S batteries, providing core support for performance optimization [8].

3.4. Cu_2O anode materials

To achieve the simultaneous realization of both energy density and power density, zinc-free zinc-ion hybrid supercapacitors (ZHS) adopt a hybrid energy storage strategy combining a battery-type anode and a capacitive cathode. The latest research involves introducing Cu_2O as the battery-type anode material in the zinc-free ZHS architecture and obtaining cuboctahedral morphologies with {100} and {111} crystal planes through solvent regulation (water-alcohol medium), thereby realizing the synergistic optimization of electric double-layer capacitance and Faradaic reactions. Research results show that, in ZHS, the anode design of replacing traditional zinc foil with battery-type materials and the control of crystal plane exposure can serve as effective approaches to enhance the energy density and durability of the system [9].

3.5. Aqueous battery material design

For aqueous proton batteries, organic-inorganic hybrid anodes (e.g., PANI/WO_3) highlight the dual requirements of "host lattice stability and synergistic electron-ion transport". Studies emphasize that the solid-phase structure should be optimized through stabilizing or expanding diffusion channels, phase control, ion doping, and synergistic effects, and an integrated analytical framework from thermodynamics to kinetics should be established to guide the rational design of high-performance electrodes [10]. In aqueous environments, the aforementioned structural and interfacial optimization also needs to achieve chemical synergy with hydrogen bonds (HB). HB in the electrolyte and host-guest materials significantly affect ion transport efficiency, electrolyte decomposition potential, viscosity, conductivity, and host-guest structure stability, thereby further altering the battery’s rate capability, energy density, and cycle life. For example, disrupting water-water HB networks can expand the electrolyte’s voltage window (inhibiting side reactions such as hydrogen evolution reaction), but it is necessary to balance conductivity and stability simultaneously [10,11]. Therefore, the optimization of hybrid systems such as PANI/WO_3 should achieve collaborative design between the solid-phase dimension and liquid-phase dimension to ultimately balance lattice stability, electron-ion transport efficiency, and aqueous environment adaptability.

4. Battery performance enhancement strategies

4.1. Improving energy density

The energy density of batteries depends not only on the structure of electrode materials but also on the design of electrolytes. By adjusting the HB interactions in electrolytes, the key performance of batteries can be optimized, but it is necessary to balance the "two-sided effects". On one hand, a complete water-water HB network can accelerate cation transport, thereby enhancing ionic conductivity; however, it triggers hydrolysis side reactions such as hydrogen evolution reaction and oxygen evolution reaction by promoting proton diffusion, which limits the electrochemical stability window of the electrolyte. On the other hand, disrupting part of the water-water HB network through concentrated electrolytes, functional additives, and artificial functional layers can significantly inhibit hydrolysis reactions and expand the electrolyte's operating voltage window to above 3 V, but it may increase the viscosity of the electrolyte, leading to a decrease in ionic conductivity. Studies have shown that by precisely regulating the type (e.g., water-cation, water-additive HBs) and strength (0.5–40 kcal mol^{-1}) of HB, it is possible to inhibit hydrolysis side reactions and widen the voltage window, while maintaining high ionic conductivity by optimizing the cation solvation structure or reducing the intermolecular HB interactions of additives. Furthermore, the synergy of HB in the electrolyte (e.g., internal interlayer HBs, external charge carrier HBs) promotes the solid-state diffusion of charge carriers such as H^+/NH_4^+, further enhancing electrode reaction kinetics. In summary, scientific hydrogen bond regulation must take into account the electrolyte-electrode synergy to improve battery energy density collectively from three aspects: "widening the voltage window", "accelerating ion transport", and "inhibiting side reactions" [11].

4.2. Extending cycle life

The cycle life of batteries is one of the important indicators for evaluating battery performance. By optimizing the structure and interface of materials and reducing side reactions between electrolytes and electrodes, the service life of batteries can be significantly extended. In SIBs, rational defect control of hard carbon anodes (e.g., reducing excessive defects via carbonization at 1200-1600℃, and covering surface defects via soft carbon coating) can balance sodium storage capacity and irreversible loss; combining pretreatment and post-treatment to optimize the structure can significantly enhance long-term stability (e.g., after sulfuric acid pretreatment and carbonization at 1300°C, bamboo-derived hard carbon still maintains a capacity of 243 $mAh\cdot g^{-1}$ after 500 cycles at a current density of 300 $mA\cdot g^{-1}$, with a capacity retention of 91.6%) [12]. Structural optimization of cathode materials can also reduce electrolyte side reactions, thereby further extending the cycle life of batteries.

4.3. Data-and-model-driven material optimization

In addition to materials and processes, the synergy between data and models is emerging as a new pillar for accelerating material optimization and device performance prediction. In the verification of dihydroxyphenazine isomers, the energy efficiency prediction error of most isomers is below 25%, and the absolute error of 1000-cycle performance prediction is less than 10%, which fully demonstrates the usability for performance evaluation of emerging materials. It is expected to connect molecular-level properties and molecular-level kinetics with battery-scale performance metrics, providing an iterative optimization loop for screening organic cathode/anode redox-active molecules with high solubility, fast kinetics, and long lifespan, thereby significantly shortening the cycle from molecular design to system verification [13].

5. Conclusion

Taking "from structural optimization to electrochemical performance enhancement" as the main thread, this paper systematically summarizes multi-system and multi-dimensional material optimization strategies: ranging from the regulation of defect engineering and coordination environment (e.g., oxygen vacancies, Cu^{2+} pillaring) to interlayer spacing, morphology, and crystal plane engineering; from interfacial conductive coatings (PEDOT:PSS) to structurally programmable 3D printing; from the process chain optimization of raw materials, precursors, and cathodes (high-quality EMD preparation via TiMn/Ti anodes) to the device-oriented new material family (biomass-derived hard carbon, COFs, Cu_2O battery-type electrodes, PANI/WO_3 hybrid anodes); and further extending to methodology and data models. The research and application of these technologies provide strong support for the improvement of battery performance. It should be acknowledged that due to differences in tested systems and characterization standards, there are still some aspects of incomplete comparability during cross-literature horizontal comparison, but this does not undermine the directional insights and contributions of each method and strategy.

Although significant progress has been made in battery material optimization at present, there are still many challenges to be addressed. Future research should establish reproducible experimental benchmarks for the actual working conditions of batteries; secondly, it is necessary to develop more high-performance and low-cost battery materials, especially exploring the application of novel multifunctional materials and advanced manufacturing technologies in batteries. In addition, the safety and environmental friendliness of batteries are also key directions for future research, which require constraining green and scalable synthesis routes while meeting performance requirements. With the development of research, battery technology is expected to achieve breakthroughs in multiple fields in the future; as structured synthesis, interface chemistry, and data intelligence continue to advance, material innovation will more rapidly drive the continuous transformation and progress of experimental performance towards engineering application, reliability, and sustainability.

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