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Advances in Chemistry of Energy Storage and Conversion Materials

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Abstract

With the rapid advancement of global industrialization, the massive consumption of non-renewable energy sources such as coal, petroleum, and natural gas has triggered a series of global crises, including frequent extreme weather events and continuous ecological environment deterioration. Public environmental awareness has been growing, and calls for environmental protection and green-living initiatives are rising. Against this backdrop, China has explicitly put forward the “carbon peaking and carbon neutrality” strategic goals and vigorously developed renewable-energy industries, including solar energy, wind energy, and hydropower. Nevertheless, the inherent randomness and volatility of these energy sources have become a bottleneck for the new-energy industry, leading to mismatches between energy supply and demand. To address the above-mentioned challenges and enable renewable clean energy to better serve human society, the chemistry of energy storage and conversion materials has gained increasing importance. This paper reviews the research advances in this field, cites relevant examples, summarizes existing challenges, and provides prospects for future development.

Keywords

energy storage, energy conversion, development status, challenges, future development

1. Introduction

Energy conversion and storage represent critical challenges confronting modern society. As global energy demand keeps rising, nonrenewable energy resources on the Earth are gradually depleted. Meanwhile, centuries-long industrial-revolution activities have caused continuous natural-environment degradation. Current available renewable energy sources such as tidal energy, wind energy, and solar energy are highly dependent on local environmental conditions. Their volatility and randomness limit their large-scale deployment. Therefore, developing high-efficiency, clean, and renewable energy-conversion and-storage materials as well as improved technologies has become a shared research objective for scientists and engineers worldwide. Consequently, the chemistry of energy storage and conversion materials has emerged. This paper analyzes research progress within this discipline and sorts out major research topics and representative achievements, namely high-performance lithium-ion battery materials, electrocatalytic energy-conversion materials, and novel large-scale energy-storage systems. Existing limitations are discussed, followed by future outlooks.

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2. Subject Overview and Fundamental Principles

The chemistry of energy storage and conversion materials is an important branch of materials chemistry oriented toward energy applications. It focuses on material research for energy storage and interconversion among different energy forms.

From the perspective of reaction essence, energy storage and conversion processes rely on breaking old chemical bonds and forming new chemical bonds in chemical reactions, accompanied by charge transfer, as well as energy absorption, release, and interconversion among different forms. Researchers can tune the migration behaviors of electrons, ions, molecules, and other particles inside materials to improve energy-utilization efficiency and satisfy practical application requirements for energy storage and conversion.

Two core principles underpin this discipline: the electrochemical principle and the catalytic principle. The electrochemical principle is widely adopted in energy-storage systems, where mutual conversion and storage between electric energy and chemical energy are realized through ion insertion/extraction and charge transport at electrode-electrolyte interfaces. The catalytic principle applies to energy-conversion systems. It lowers reaction energy barriers to achieve high-efficiency energy conversion and reduce energy loss.

Based on the above principles, the core research idea of this discipline is to design rational reaction pathways and material microstructures according to target material properties or performance-optimization requirements, build ion and electron-transport channels, act as “micro-architects” for ion and electron migration, and realize controllable whole-process energy storage and optimization.

Hence, core research directions of this discipline are well-defined. Iteration of cutting-edge technologies in this field always centers on the following aspects:

First, precise design of material microstructures. Physicochemical properties of materials are highly dependent on internal atomic arrangement, crystal size, hetero-atom doping, and other structural factors. Early material synthesis largely relied on trial-and-error screening for high-performance samples. Today, the chemistry of energy storage and conversion materials has moved beyond trial-and-error-based synthesis. Guided by structural-chemistry theories and combined with micro-modification approaches, researchers optimize existing materials or develop brand-new functional materials for practical applications featuring low-energy consumption and high efficiency, which aligns with current green-low-carbon development demands.

Second, in-depth analysis of reaction mechanisms. For a long time, constrained by technical means and theoretical frameworks, improving material performance for energy storage and conversion required massive trial-and-error work. Researchers had limited understanding of phase transformations, interfacial side reactions, and actual charge-transport processes during energy absorption and release inside materials. Nowadays, advances in technologies and theories enable micro-characterization tools such as spectroscopy and in-situ electron microscopy to help researchers “directly observe” full chemical-reaction processes related to material performance. Researchers can move away from experience-driven modification toward targeted material design based on reaction mechanisms, greatly boosting material-development efficiency. In 2022, Zhao et al. reported a novel photothermal-conversion phase change material, carbon-nanotube@phase-change-materials (CNT@PCMs). This material was synthesized by introducing carbon nanotubes (CNTs) into polyethylene glycol (PEG)-based solid-solid phase-change-material (PCM) matrices. It addresses randomness and instability of solar-energy storage and conversion induced by day-night alternation, seasonal shifts, and climate variations [1]. During performance tests, especially characterization of phase-change behaviors, researchers adopted multiple micro-probing and thermodynamic measurement techniques, including X-ray diffraction (Figure 1(h)). Several conclusions were drawn: first, all samples maintained their original shapes under experimental conditions, demonstrating favorable shape stability of CNT@PCMs (1a); second, samples exhibited certain solvent resistance when immersed in N,N-dimethylformamide solvent at 60 °C for 72 h (Figure 1(b)); moreover, Figure 1(i), Figure 1(j), and attached tables indicate that carbon-nanotube content improves crystallinity and phase-change temperature of CNT@PCMs, yet excessive carbon-nanotube loading reduces heat-storage capacity. In Table 1, OC-8K represents samples with zero carbon-nanotube content, 1CNT@PCM denotes samples with 1 wt % carbon-nanotube content, and so forth.

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Figure 1: Performance test of samples with different carbon nanotube concentrations

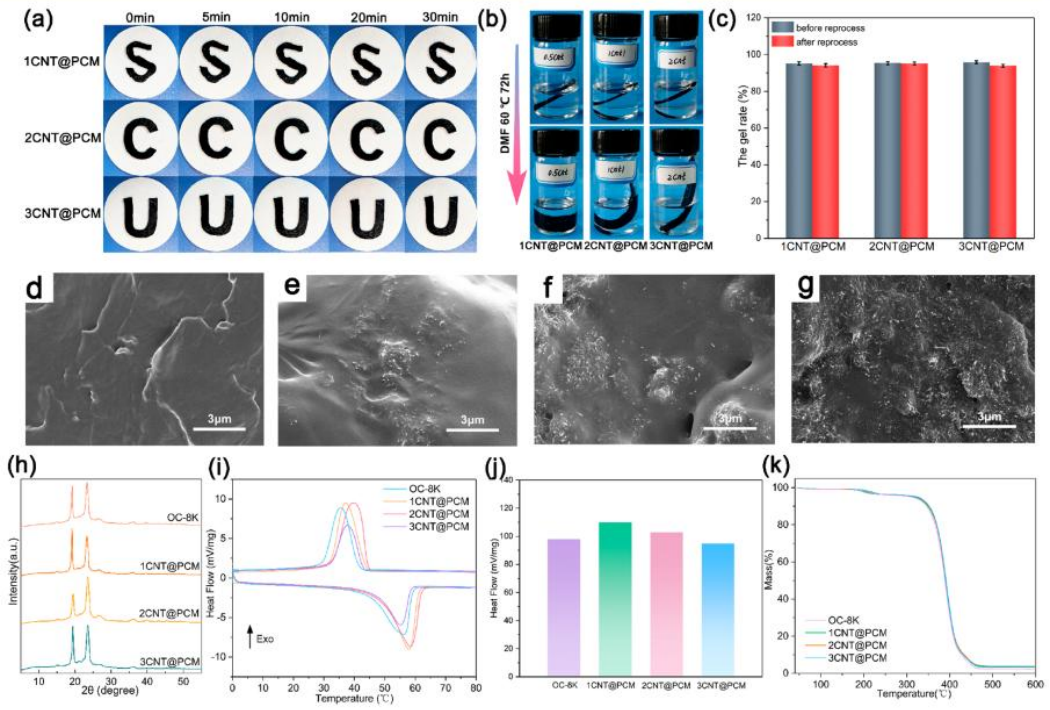


Table 1: Melting and solidification temperatures and enthalpy changes for samples with different carbon-nanotube concentrations

Sample	Melting point (°C)	Melting enthalpy ($J \cdot g^{-1}$)	Solidification temperature (°C)	Solidification enthalpy ($J \cdot g^{-1}$)
OC-8K	42.9	97.8	38.7	93.9
1CNT@PCM	48.9	110.0	43.6	107.6
2CNT@PCM	48.0	104.6	45.1	102.8
3CNT@PCM	46.4	94.9	42.8	92.0

In this way, energy transfer, absorption, and release behaviors of materials can be rapidly characterized by multiple instruments, improving research-and-development efficiency.

Third, translating laboratory-developed materials into practical industrial production. As society evolves, production requirements for materials have shifted from single-target to multi-dimensional evaluation. When evaluating a smartphone, consumers no longer only focus on basic communication functions but demand diversified features. The same logic applies to energy-storage and-conversion-materials chemistry. New materials cannot merely achieve outstanding performance in a single metric while neglecting other properties; otherwise, industrial-scale deployment cannot be realized. Researchers must balance competing performance indicators to achieve both excellent material performance and feasible mass production. Five major evaluation indicators (no priority ranking) for product development include high energy density, environmental friendliness, safety, low-cost preparation, and ultra-long cycle life.

3. Literature Review

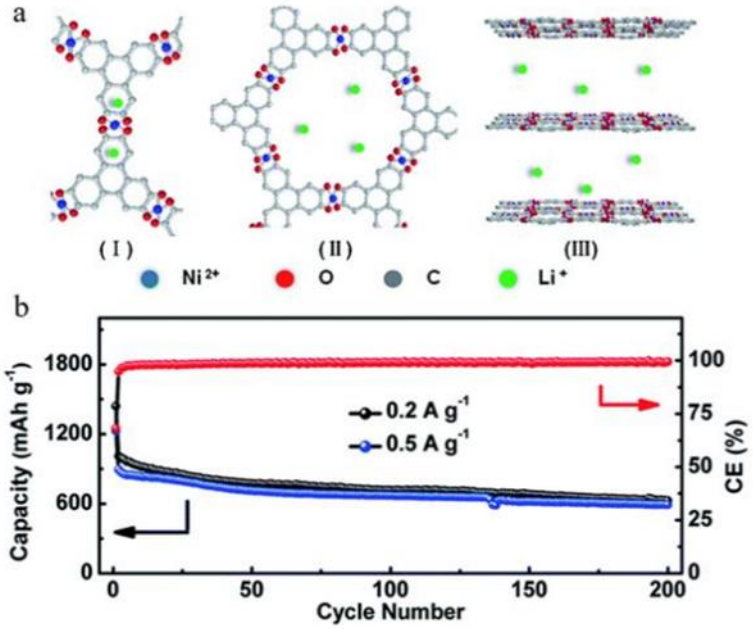
3.1 Innovations of Current High-Performance Battery Materials

As the most widely deployed electrochemical-energy-storage device, lithium-ion batteries trace their technical origins back decades. In 1972, Whittingham's team at ExxonMobil developed the first lithium-battery prototype with a TiS_2 cathode and metallic-lithium anode. As core components of modern energy-storage systems, lithium-ion batteries have achieved industrial-scale applications for decades. Thanks to high energy density, outstanding cycling stability, and low self-discharge, they have become the dominant technology in electrochemical energy storage [2,3]. Currently, lithium-ion batteries are widely used in portable electronic devices and electric vehicles. Nevertheless, widespread real-world applications impose higher

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performance requirements, such as enhanced energy-storage capacity and improved lithium-ion transport efficiency. Researchers have proposed corresponding solutions: optimizing cathode and anode materials to reduce consumption of conventional electrode materials and cut manufacturing costs. For instance, MOFs are porous coordination compounds synthesized via coordination bonding between metal ions (or metal clusters) and organic ligands. Rich redox-active metal centers and modifiable organic ligands endow MOFs with unique chemical properties, promising for energy-storage applications [4]. However, conventional MOF electrodes suffer from poor intrinsic electronic conductivity. Furthermore, intrinsic lithium-storage mechanisms of conductive M-CAT MOFs applied as lithium-ion-battery anodes remain unclear, hindering targeted structural optimization. To tackle these bottlenecks, Guo's group [5] adopted hydrothermal synthesis to leverage the structural merits of MOFs and prepare hexagonal honeycomb-shaped highly conductive porous 3D-channel Ni-CAT MOF organic-inorganic composite materials. Ni-CAT MOF with hydroquinone groups was fabricated and employed as an anode for lithium-ion batteries. In the composite matrix, three independent Li^+-storage sites are available: benzene rings, pores, and interlayer spaces. Compared with conventional anode materials, this new material makes full use of energy output at each potential, substantially boosting total energy-storage capacity. As demonstrated by detailed electrochemical tests in Figure 2, after 200 charge-discharge cycles at high current densities of 0.2 $A \cdot g^{-1}$ and 0.5 $A \cdot g^{-1}$, high reversible capacities of 626 $mAh \cdot g^{-1}$ and 592 $mAh \cdot g^{-1}$ can be retained. Compared with previously reported MOF-based anodes, Ni-CAT delivers superior rate capability and cycling performance. This work not only provides an alternative high-performance MOF anode candidate but also advances mechanistic understanding of lithium-storage behaviors in conductive M-CAT MOF systems, offering mechanistic references for future structural design of analogous MOF electrodes.

Figure 2: (a) Structural diagram of the benzenediol group in Ni-CAT MOF of metal-organic framework; (b) Effects of different current densities on the capacity of this new-type battery



Minor chemical modifications can substantially improve energy-storage performance of electrochemical devices. Modern fast-charging cell-phone batteries and cycle-life breakthroughs exceeding ten thousand cycles originate from similar strategies.

3.2 Electrocatalytic Energy Conversion

While batteries realize energy storage and utilization, electrocatalytic conversion serves as a core pathway for cross-form conversion of clean energy. Intermittent electric energy can be converted into chemical fuels for long-term energy storage and transportation.

A typical example is water electrolysis for hydrogen production. Surplus photovoltaic or wind-generated electricity can drive catalytic water splitting into hydrogen and oxygen. Hydrogen possesses ultra-high energy

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density and yields only water upon combustion; hence, it is recognized as an ultimate energy carrier. Nevertheless, conventional water electrolysis hydrogen production suffers from two major drawbacks [6]. First, energy-conversion efficiency is normally limited to 50 %-70 %. Resistive losses occur during ion transport in electrolytes; electrode polarization and water-decomposition voltage also introduce extra energy dissipation. Second, conventional water electrolysis systems rely on scarce and costly noble-metal electrodes such as platinum and palladium. Such materials are incompatible with large-scale hydrogen production and conflict with sustainable-economy requirements. To solve these challenges, Jiang et al. [7] reported an atomic-to-macroscale integrated Ni/MoO_2 electrode with abundant atomic-heterointerfaces and tri-level porous architectures for high-performance hydrogen-evolution reactions. Under industrial operating conditions (30 wt % KOH, temperature above 85 °C), a cell voltage of 1.80 V is achieved at a current density of 1 $A \cdot cm^{-2}$, corresponding to a hydrogen-production energy consumption of 4.3 kWh per standard cubic meter, with durability exceeding 1000 hours. This electrode improves water-splitting efficiency and reduces costs. Another representative technology is electrocatalytic CO_2 reduction, which converts industrial-emitted greenhouse-gas CO_2 into high-value small-molecule organic fuels and chemical feedstocks, providing new routes for greenhouse-gas mitigation [8].

3.3 Breakthroughs in Novel Large-Scale Energy-Storage Systems

Lithium-ion batteries are mainly suitable for short-duration and small-to-medium-scale energy-storage scenarios. Constrained by lithium-resource reserves, material costs, and thermal-safety risks, lithium-ion batteries alone cannot satisfy nationwide, cross-seasonal, and cross-regional long-duration energy-storage demands. Therefore, researchers keep exploring novel large-scale chemical-energy-storage systems. Sodium-ion batteries represent a promising candidate for grid-scale energy-storage applications owing to the high crustal abundance of sodium resources, low cost, and favorable low-temperature performance. As reported by Nayak's team [9], sodium-ion batteries attract extensive attention as alternatives to lithium-ion batteries. Sodium exhibits much higher crustal abundance (23 600 ppm, approximately 2.6 %) than lithium, leading to lower raw-material costs (see Table 2). Meanwhile, the self-heating temperature of sodium-ion batteries reaches 260 °C, higher than the 165 °C of lithium-ion batteries, indicating superior thermal stability and safety. Therefore, sodium-ion batteries are actively deployed for stationary-energy-storage systems and low-temperature applications. Faster ionic-transport kinetics enable sodium-ion batteries to work under harsh low-temperature conditions. In addition, aqueous-electrolyte batteries, including water electrolysis-related systems, adopt water-based electrolytes, eliminating fire-and-explosion hazards under extreme conditions. They guarantee property-and-life safety and are ideal candidates for large-scale energy-storage stations in densely populated regions.

Table 2: Comparisons of the Properties of Na and Li

Property	Na	Li
Material abundance (ppm)	23,600	20
Shannon's Ionic radii (Å)	1.02	0.76
Relative atomic mass	6.94	23.00
E° (vs SHE) (V)	-2.71	-3.04
Melting point (°C)	97.7	180.5
Desolvation energy in PC	157.3 kJ mol^{-1}	218.0 kJ mol^{-1}
Self-heating temperature	260 °C	165 °C
Price	~0.3$	~6$
Coordination preference	octahedral and prismatic	octahedral and tetrahedral
Distribution	Everywhere	70% in South America

4. Discussion

Despite rapid disciplinary development, multiple bottlenecks remain to be addressed in this cutting-edge field.

First, gaps persist in fundamental-mechanism understanding. Although in situ electron microscopy, synchrotron radiation, and other characterization techniques have been adopted, their applicable scope remains limited. Precise characterization approaches for complex dynamic interfacial chemical processes are still lacking, and key mechanistic questions require further clarification. For instance, an ideal solid-electrolyte

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interphase (SEI) for batteries should deliver high ionic conductivity, uniform lithium-ion-transport pathways and robust mechanical integrity. However, despite extensive research efforts including electrolyte engineering, most electrochemically induced SEI-formation strategies cannot realize precise control over SEI composition and structure [10]. Such challenges stem from complicated electrochemical reactions. Uncontrolled decomposition pathways hinder the formation of chemically homogeneous SEI via well-defined reaction sequences. Researchers are proposing strategies such as sequential reactions to resolve these issues.

Second, notable gaps exist between laboratory-scale achievements and industrial translation. For example, numerous research schemes for aqueous water-electrolysis batteries have been proposed, yet large-scale commercialization has not been achieved. Synthesis protocols for many new materials involve complex processes and high manufacturing costs. Long-term stability under diverse practical-environment conditions cannot be guaranteed, hindering real-world deployment beyond laboratory publications.

5. Conclusions and Outlook

Global energy-transition initiatives are gaining momentum. As a core discipline tackling energy challenges, the chemistry of energy-storage and-conversion materials faces enormous opportunities alongside prominent challenges. This paper reviews representative advances along three major research threads: high-performance battery materials, electrocatalytic energy conversion, and novel large-scale energy-storage systems. For high-performance battery materials, technological evolution started from TiS_2-based lithium-battery prototypes and progressed toward mature commercial-energy-storage technologies. Within electrocatalysis, non-noble-metal hydrogen-evolution electrodes provide feasible solutions to break reliance on noble metals and reduce hydrogen-production costs. For large-scale energy storage, sodium-ion batteries stand out as promising grid-scale energy storage candidates thanks to abundant resources and enhanced safety. Photothermal phase-change materials offer new ideas to mitigate intermittency issues of solar-energy utilization. Nevertheless, limitations remain within this research domain. On one hand, fundamental-mechanism knowledge is incomplete. Despite advances in various in situ characterization tools, competitive side reactions interfere with electrochemically generated SEI. It is difficult to simultaneously achieve high ionic conductivity, uniform lithium-ion-transport pathways, and excellent mechanical integrity. Precise tuning of interfacial composition and microstructures remains challenging, and dynamic interfacial-evolution processes cannot be fully characterized. On the other hand, clear barriers separate laboratory outputs from industrial-scale applications. Many high-performance materials require complicated synthesis workflows and suffer from high costs; long-term stability under practical operating conditions cannot be guaranteed. Substantial gaps must be closed before large-scale commercialization. To address the above-mentioned bottlenecks, future research may focus on several directions. For battery research, intrinsic electrode-energy-storage mechanisms should be further deciphered. Precise construction of ideal electrolyte-interphase layers should be promoted to move beyond limitations of spontaneous electrochemically driven film formation. Electrocatalysis research should prioritize activity-evolution mechanisms of catalysts under real industrial conditions and develop high-performance electrodes. For novel-energy-storage systems, modification strategies should be optimized to tackle low-conductivity drawbacks of polyanionic-type sodium-ion-battery cathodes. Meanwhile, coordinated development of aqueous-electrolyte energy-storage and photothermal phase-change-storage technologies should be advanced. With continuous improvement of fundamental theories, iterative upgrading of research-and-development tools, and optimization of manufacturing processes, energy-storage and-conversion materials are expected to deliver more breakthrough innovations. These advances will facilitate global energy-system transformation and realize coordinated progress of scientific innovation, industrial development, and green-low-carbon goals.

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Conflicts of Interest

The authors declare no conflict of interest.

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