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Fire-Retardant Electrospun Gel Polymer Electrolytes for Safe, High-Performance Lithium-Metal Batteries

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Abstract

Lithium-metal batteries (LMBs) offer high energy density, but safety concerns, particularly electrolyte flammability, hinder their practical application. This work presents a novel, fire-retardant gel polymer electrolyte (GPE) fabricated via electrospinning, composed of a PVDF/HFP matrix incorporating SiO_2 nanoparticles and the flame retardant additive triethyl phosphate (TEP). Electrochemical impedance spectroscopy and transference number measurements demonstrate enhanced ionic conductivity in the PVDF/HFP/SiO_2/TEP GPE compared to conventional Celgard separators. The performance of LMBs employing this GPE is evaluated in half-cells with lithium metal anodes and various cathode materials. Results confirm that incorporating SiO_2 and TEP into the PVDF/HFP matrix significantly improves fire retardancy and ionic conductivity while preserving mechanical integrity. LMBs assembled with the optimized GPE exhibit superior cycling performance and rate capability compared to those using liquid electrolytes. This study demonstrates the potential of this novel fire-retardant electrospun GPE for realizing safer, high-performance LMBs. The performance of LMBs using this GPE was tested in half-cells with lithium metal anodes and $LiFePO_4$ cathodes, with a high cathode loading of approximately 10 mg/cm^2. Incorporating SiO_2 and TEP into the PVDF/HFP matrix.

A PVDF-HFP/TEP membrane in a 1:1 ratio exhibited stability up to 120°C, whereas a membrane without TEP was stable only up to 80°C. LMBs using the 1:1 PVDF-HFP/TEP membrane demonstrated a discharge capacity of 160 mAh/g and a first-cycle coulombic efficiency of 80.2%. Additionally, the rate capability and cyclic stability were evaluated for LMBs with and without TEP.

Keywords: Solid State battery, Polymer electrolyte, Metal ion battery,

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Pseudocapacitance of Vanadium Carbide MXene in Concentrated Calcium-ion Electrolyte

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Abstract

The two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides, commonly known as MXenes, have gained significant attention as conductive redox charge storage hosts due to their redox activity combined with metallic conductivity.[1] Proton-induced pseudocapacitance is well-known for MXenes, which give rise to maximum storage capacity in protic electrolytes. In this contribution, we unlock the redox capacity of vanadium carbide (V_2CT_x) MXene in concentrated Ca-ion electrolytes. V_2CT_x MXene is known to exhibit pseudocapacitive charge storage behavior in acidic and basic medium and intercalation capacitance in neutral electrolytes due to the formation of electrical double layer by hydrated metal ions.[2] The concentrated Ca-ion electrolyte suppresses water activity and enables an expanded operational voltage window of 1.3 V, showing a specific capacity of 88 mAh g^{-1} at a current density of 0.5 A g^{-1}.[3] This extended potential range activates additional redox processes involving the V^{3+}/V^{4+} couple, as evidenced by ex-situ X-ray photoelectron spectroscopy. Further, all MXene-based symmetric V_2CT_x // V_2CT_x full device was demonstrated with an operational voltage window of 1.4 V and showing cycling stability for 10,000 charge–discharge cycles in Ca ion electrolyte.

Keywords: Vanadium carbide MXene, Pseudocapacitance, Concentrated electrolyte, Ca-ion storage.

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A Biodegradable Peptide-based Supercapacitor

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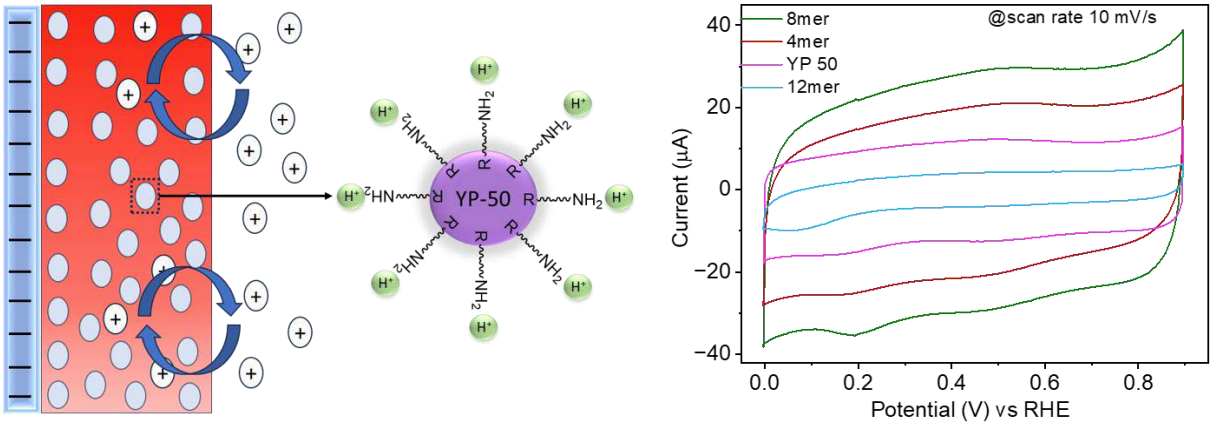
In this study, we investigated the role of amino groups in peptides for charge storage applications. The electrochemical protonation of amino groups in peptides contributes significantly to charge accumulation. Our findings reveal a complex relationship between peptide length and the number of amino groups, indicating a non-linear effect on charge storage capacity. Notably, the incorporation of peptides into a composite with the conductive carbon material YP50 enhances its electrochemical performance. Among the peptides tested, the 8-mer Peptide exhibited superior performance in cyclic voltammetry compared to the 4-mer Peptide and 12-mer Peptide analogues, highlighting an optimal balance between length and functional group density. Based on these results, we have developed a biodegradable peptide-based supercapacitor that demonstrates a performance improvement of **2-**fold over YP50 alone; the benchmark material for high-capacitance applications.



Development of High-Performance Silicon-Based n-i-p Heterojunction Photoanode for Large-Scale Photoelectrochemical Water Splitting Applications

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Abstract

With the rising global demand for sustainable energy, the production of green hydrogen through the photoelectrochemical (PEC) route has emerged as a highly promising solution. Heterojunction photoelectrodes are advantageous for PEC applications due to their ability to enhance light absorption, improve charge carrier generation, and facilitate efficient charge separation and transfer while minimizing recombination losses. In this work, a high-performance silicon-based n-i-p heterojunction photoanode with an FTO/TiO_2/Si/NiO architecture has been successfully developed using earth-abundant materials, leveraging the inherent benefits of the heterostructure design. Targeting the practical application of the photoelectrodes for solar fuel production, the heterojunction was fabricated via the industry-relevant magnetron sputtering technique, ensuring scalability and uniformity. The optimized FTO/TiO_2/Si/NiO_A configuration achieved an impressive surface photovoltage of 600 mV and delivered a photocurrent density of approximately ~0.65 mA/cm^2 at 1.23 V_{RHE} under simulated solar illumination (100 mW/cm^2), with a low onset potential of around ~0.11 V_{RHE}, attributed to the strategic selection of materials and architectural design. The photoanode also demonstrated remarkable photochemical stability, retaining over ~96% of its initial photocurrent after 10 hours of continuous operation in 1 M KOH (pH 13.5). Furthermore, the successful fabrication and demonstration of a large-area (25 cm^2) photoanode validated both the performance and the scalability of the approach, reinforcing its potential for industrial-scale PEC water splitting applications.

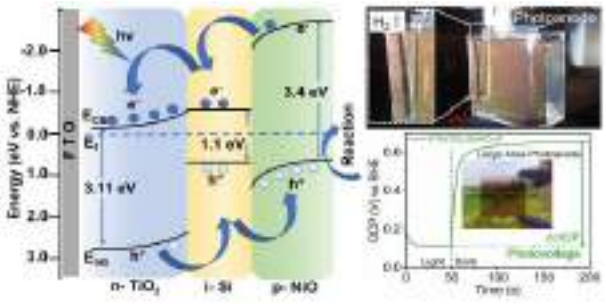

Figure 1: n-TiO_2/i-Si/p-NiO heterojunction photoanode enabling efficient water splitting with enhanced photovoltage and visible hydrogen evolution on a large-area photoanode.

Keywords: Photoelectrochemical water splitting, Si-based photoanode, *n-i-p* heterojunction, magnetron sputtering, large area device

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Unraveling the Oxygen Redox Mechanism in 'Layered' Sodium-Transition Metal Oxide Cathodes for Sodium-Ion Batteries

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Abstract

The growing demand for high energy density Li-ion and Na-ion batteries has led to significant impetus towards the development of 'layered' or even cation-disordered Li-/Na- transition metal (TM) oxide cathode materials that can utilize 'anionic redox' as an additional charge compensation mechanism beyond the TM-redox. However, the stability of 'anion redox' still remains unsatisfactory, with the mechanisms associated with this phenomenon poorly understood [1]. Against this backdrop, our work looks into the correlations between the compositional-structural-electrochemical aspects of 'layered' Na-TM-oxide based cathode materials, starting with our high Na-containing P2-structured $Na_{0\cdot84}([]_{0\cdot06}Li_{0\cdot04}Mg_{0\cdot02}Ni_{0\cdot22}Mn_{0\cdot66})O_2$ [as reported in Chem Mater (2022), 34(23), 10470-10483][2] and generating a few logical variations of the same. While Na-extraction/insertion takes place via solid-solution pathway and primarily $Ni^{2+/4+}$ redox within a potential window of 2-4 V vs. Na/Na^+, phase transformation(s), yielding either OP4/O2, is/are observed beyond 4 V, with 'anionic redox' primarily supporting the electrochemical Na-extraction/insertion, leading to reversible specific capacities of 161, 164, and 193 mAh g^{-1} upon cycling within 2–4.2, 2–4.3, and 2–4.5 V, respectively. A combination of XPS, in-situ Raman, in-situ XANES, ex-situ soft XAS, magnetic measurements and DFT-based simulations reveal a complex interplay between O-redox and transition metal over-oxidation/reduction when going beyond 4 V; thus, throwing new insights into the 'anion redox' mechanism of such 'layered' transition metal oxide-based cathode materials.

Keywords: Anionic redox, Sodium-ion batteries, cathode

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Controlled Cation Doping in Iron-Based NASICON Frameworks Toward High-Performance Sodium-Ion Batteries

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Abstract

Despite holding great promise for large-scale energy storage, the commercial viability of sodium-ion batteries (NIBs) is limited by the unavailability of high-performance cathodes. In this regard, NASICONs have gained considerable attention due to their three-dimensional Na^+ diffusion pathways, high redox potential, and exceptional structural stability. Strategies like multivalent cation doping, coupled with mixed polyanion groups, can effectively overcome the intrinsic limitations of conventional NASICON-type (pyro/fluoro)phosphate materials.[1] Herein, we prepared a phase-purified $NaFe_2PO_4(SO_4)_2$ (NFPS) cathode with high electrical conductivity and a lower Na^+ diffusion barrier *via* precisely doping Mg^{2+} at the Fe site. The optimised cathode delivered a specific capacity of 111 mAh g^{-1}(at 0.1 C) and energy density of 324 Wh kg^{-1}.[2] Despite enhanced electrochemical performance, the NFPS cathode showed limited long-term cycling life. To overcome these issues, Al^{3+} was introduced in the Fe-site *via* a solid-state reaction to form $NaFe_{1.93}Al_{0.07}(PO_4)(SO_4)_2$ (NFAPS) which delivered a specific capacity of 124 mAh g^{-1} (97.63% of its theoretical capacity) and a high energy density of 372 Wh kg^{-1}, along with extended cycling life.[3] The outstanding performance of NFAPS stems from the lowered charge transport resistance, reduced Na^+ activation energy (Ea), and enhanced Na^+ diffusion coefficient post-doping. Extending this strategy, a unique NASICON framework with the formula $NaFe_2(PO_4)(MoO_4)_2$ (NFPM) was designed, which incorporates $[MoO4]^{2-}$ transition metal oxide as the polyanion group. To further improve electrochemical performance, In^{3+} was substituted at the Fe site, promoting lattice expansion, reducing the bandgap, and enhancing Na^+ ion diffusivity. With 0.10 moles of In^{3+} doping, the NFPM samples were optimized to host sodium ions with a specific capacity of 111.85 mAh g^{-1} with reduced voltage hysteresis, along with excellent cycling stability.[4]

Keywords: Sodium-ion batteries, NASICON cathodes, Cation doping, Energy density, DFT

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Enhancing the safety and performance of Li-metal battery via a multifunctional fluoro-phosphonate-based additive

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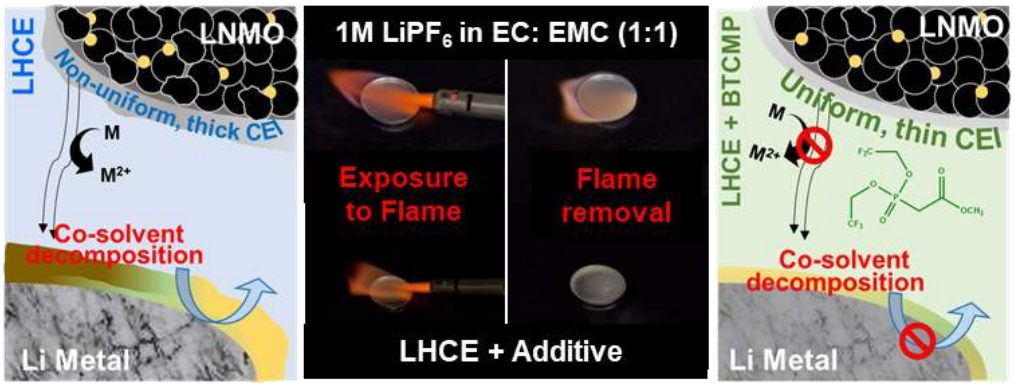
Abstract

Lithium metal batteries (LMBs) offer high energy density but suffer from interfacial instability, dendrite growth, and safety concerns. This study introduces a novel fluorinated phosphonate additive, Bis(2,2,2-trifluoroethyl)(methoxycarbonylmethyl)phosphonate (BTCMP), into a localized high-concentration electrolyte (LHCE) to address these challenges.[1] Ab initio molecular dynamics (AIMD) and Density Functional Theory (DFT) simulations revealed that BTCMP alters the solvation structure of LHCE, breaks large solvation aggregates into smaller fragments, and strengthens Li^+–(O=P) interactions, raising the LUMO levels of other solvating solvents and suppressing electrolyte decomposition. As a result, a thinner and more stable cathode electrolyte interphase (CEI) forms, as confirmed by XPS and TEM. The BTCMP-modified LHCE (LHCE+Additive) achieved 82% capacity retention with 99.5% coulombic efficiency after 200 cycles in Li||LNMO cells, significantly outperforming the pristine LHCE (47.2% retention after 150 cycles). Moreover, BTCMP imparts flame-retardant properties, enhancing safety. [1]

Keywords: CEI, Additive, Safety, Fluorinated, BTCMP



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Impact of Co-Solvents during Cointercalation at Graphite for Sodium Ion Batteries

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Abstract

Sodium ions are capable of inserting into graphite by using a solvent co-intercalation mechanism, such as that observed with diglyme (DG) electrolytes, attaining more than 2000 cycles. However, the reversible capacity is low at about 110 mAh/g, and the graphite expands and contracts significantly during charge and discharge. Aside from DG, very few stable cointercalation solvents have been studied. In 2024, our laboratory investigated the use of branched diamines such as 1,3-diaminopentane (13DAP) as a solvent which increased the reversible capacity, decreased the redox potential, and reduced the interlayer expansion at graphite (1). At the same time, the cyclability and oxidation resistance were poor compared with DG electrolytes. In this study, we explore the impact of mixed electrolytes containing two cointercalating solvents on Na ion insertion into graphite with the aim of further improving charge/discharge characteristics and cyclability.

As shown in Figure 1a-c, the charge/discharge curves and capacities in the electrolytes with a volume ratio of 1:9 and 9:1 (DG:13DAP) show no apparent impact on the cointercalatino mechanism of the primary solvent. In contrast, when the solvent ratio was changed to 7:3, 3:7, and 5:5 (Fig. 1d), we start to observe notable changes to the profile and differences in the Coulombic efficiency and cycle life. While 10% addition to DG significantly improved the cyclability of 13DAP, higher additions led to poor cycling characteristics. Molecular dynamics simulations indicated that DG molecules tend to have shorter bond distances and remain closer to Na^+ in all mixtures. Results from operando XRD show unique and dynamic behavior during cycling, with DG preferentially co-intercalating first. The implications of these mixtures for SIBs will be discussed.

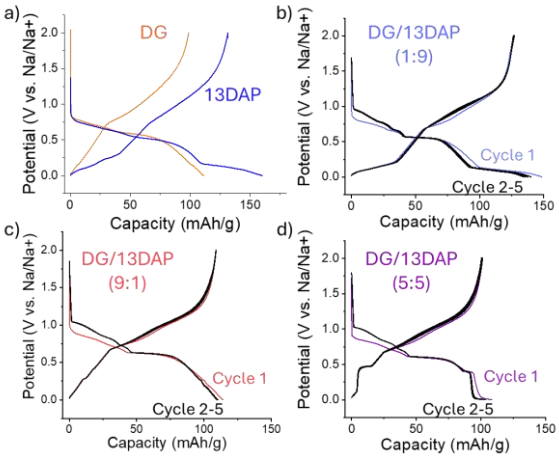

Fig. 1. Cointercalation using mixed solvents.

Keyword: Sodium ion battery, graphite, co-solvent, cointercalation, electrolyte

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Suppressing Lithium Dendrite Growth in Graphite Anodes using Potassium Additives via Interphase Engineering for Lithium-Ion Batteries

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Abstract

Over the past few years, fast-charging has become mandatory requirement for lithium-ion batteries (LIBs) in order to meet the growing demands of its usage in portable electronics and electric vehicles. However, fast charging is associated with several challenges, among which Li dendrite formation and its growth is critical as it compromises the safety of LIBs [1]. Furthermore, operating LIBs at lower temperature range results in sluggish reactions leading to Li dendrite formation, conscequently declining the overall performance of LIBs. This work addresses the aforementioned challenges by electrolyte engineering using potassium additive via additive–solvent optimisation. In this work, a systematic study was conducted by using KPF_6 salt as an electolyte additive to mitigate the dendritic growth in LIB cells [2]. Additionally, propylene carbonate (PC) solvent was used in association with KPF_6 to simultaneously mitigate Li dendrites and enhance the low-temperature electrochemical performance [3]. Although graphite exfoliation is a well known issue with PC-based electrolytes, this study demonstrates that with strategic solvent-additive optimisation effectively suppress exfoliation as well as Li dendrite growth, thereby enabling stable cycling performance of graphite|NMC 622 cell.

Keywords: Propylene Carbonate, KPF_6, Fast Charging, Li Dendrites, Graphite Exfoliation

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Al/Ti co-doping Boosts Electrochemical Performance and P3/O3 Structural Stability of Na-ion Battery Cathode

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Abstract

There has been growing research interest in layered transition metal oxides as potential cathodes for high-performance sodium-ion batteries. However, these materials suffer from detrimental phase transformations during the charge-discharge process, limiting their long-term cyclability and causing poor rate performance. Herein, Ti-Al co-doped $Na_{2/3}Mn_{2/3}Ni_{1/3}O_2$ cathode (NMAT) with an optimized P3/O3 biphasic structure is designed that effectively constrains these undesirable phase transformations and cooperative Jahn–Teller distortion, especially at lower voltages. Further, Ti/Al doping imparted excellent electrochemical properties with NMAT-10 (with the optimum 10% Al content) showed an excellent specific capacity of ~170 mAh g^{-1} at 0.1C in the 1.5-4.2 V range, and capacity retention of 83% after 300 cycles at 2C in 2.0-4.2 V. It also exhibited a much-improved rate capability with about 80% capacity at 5C relative to the capacity observed at 0.1C. These improvements in electrochemical performance are attributed to the stronger Al-O bond, which suppresses the severity of P3↔P3′↔O3 phase transformation, as confirmed by the operando synchrotron XRD studies. The practical viability of the NMAT-10 cathode is verified by fabricating a full cell using a commercial hard-carbon anode, which showed a discharge capacity of ~ 80 mAh g^{-1} at C/5 and remarkable capacity retention in the 2.0-4.2 V range. This work highlights the P3/O3 biphasic structure as an effective approach to achieving an excellent rate performance and better cycling stability in layered oxides for sodium-ion batteries.

Keywords: Na-ion batteries, P3/O3 biphasic cathode, *Operando* synchrotron XRD, Electrochemical behavior

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Computational Design and Experimental Realization of $Na_3FeV(PO_4)_3$ as a Sustainable Cathode for High-Performance Sodium-Ion Batteries

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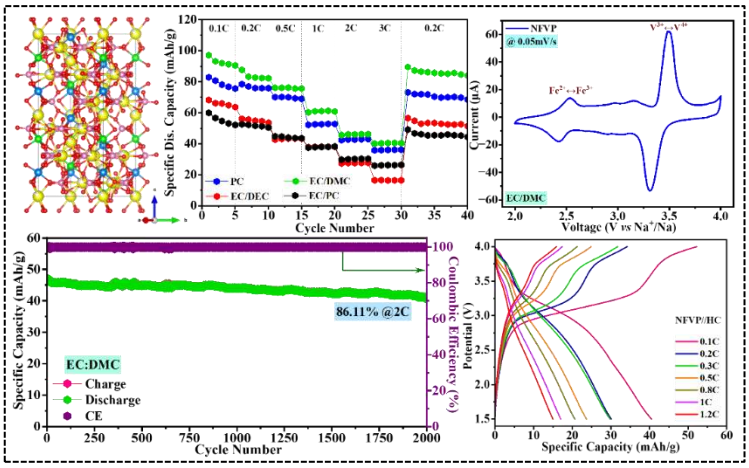
Abstract

NASICON-type materials are very promising cathodes for sodium-ion batteries (SIBs) owing to their stable 3D framework and rapid Na^+ diffusion. Although, high-voltage Na3V2(PO4)3 (NVP) is extensively investigated for good capacity (~117 mAh/g) as well as outstanding rate capability, its practical use is limited because of the expensive and toxic vanadium. Hence, replacing V with Fe in Na3FeV(PO4)3 (NFVP) presents a more sustainable composition with dual redox activity while maintaining high voltage [1,2]. Herein, phase-pure NFVP was synthesised via a facile sol-gel method, delivering a specific capacity of 108.43 mAh/g and 317 Wh/kg of energy density at 0.1C. Further, it demonstrated excellent rate capability with outstanding retention of 95.24% over 100 cycles and 86.11% over 2000 cycles at 0.5C, and 2C, respectively. To investigate its practical applicability, NFVP//HC full cell configuration was fabricated, which delivered specific capacity of 54 mAh/g and energy density of 114 Wh/kg at 0.1C. Additionally, the post-cycling analysis and detailed computational study provided crucial insights into structural stability, kinetics, and sodium-ion transport mechanisms of NFVP, highlighting its strong potential as a cathode material for future commercialisation of SIB systems.

Keywords: NASICON compound, Electrolyte compatibility, Multi-redox activity, Sodium-ion battery, Full cell configuration.



Caption: Electrochemical performance of NFVP cathode in various electrolytes showing charge–discharge profiles, cyclic voltammetry, cycling stability, and rate capability of NFVP//HC full cell

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The Importance of Chemical Reactions in the Charging Process of Lithium-Sulfur Batteries

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Abstract

The underlying mechanism of lithium-sulfur (Li-S) batteries is still not fully established because it involves a series of both chemical and electrochemical reactions as well as the formation of soluble polysulfide intermediates. To improve the mechanistic understanding of Li-S batteries, we investigate chemical reactions between the Li_2S cathode and more oxidized sulfur species, such as S_8 and polysulfides, during the electrochemical charge of the battery. By combining electrochemistry with X-ray absorption spectroscopy, we show that chemical reactions and, in particular, the resulting accumulation of solution species in the electrolyte are essential to oxidize Li_2S at a low overpotential. Additionally, by efficiently separating the anode and cathode compartments of a battery with a lithium ion-exchanged Nafion interlayer, we establish the adverse effect of the anode on the buildup of solution intermediates. In the absence of the interlayer, polysulfide intermediates can diffuse through the separator and react at the anode's surface, while the addition of the interlayer allows the intermediates to accumulate in the separator of the cathode compartment and facilitate the oxidation of Li_2S.

Keywords: Lithium-sulfur batteries, Polysulfides, Nafion layer, X-ray absorption spectroscopy.

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ACEPS-13, January 11-14, 2026, Bengaluru, India

In-Situ Synthesized Gel Polymer Electrolyte for Long-Life Sodium-Ion Batteries

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Abstract

We present a solid-state sodium-ion conducting gel polymer electrolyte (GPE), in-situ synthesized directly on sodium metal or electrode surfaces, as a promising alternative to conventional liquid and ceramic electrolytes for high-performance sodium-ion batteries (SIBs). The GPE is fabricated through a straightforward protocol involving in-situ polymerization of a liquid electrolyte (LE) and polymer precursor (PP) mixture within a highly porous electrospun polyacrylonitrile (PAN) membrane pre-mounted on either Na metal or suitable electrodes. The membrane's high porosity enables significant LE entrapment (~60 vol%), which upon polymerization forms a robust, thermally and mechanically stable amorphous gel.

The resulting GPE exhibits high ionic conductivity (~1 mS cm^{-1}, comparable to LE), a high Na^+ transference number (0.63), a wide electrochemical stability window (up to 5.2 V vs. Na^+/Na), and excellent interfacial compatibility. Importantly, the chemically stable GPE effectively suppresses dendrite growth, enabling sustained Na plating/stripping for hundreds of cycles at various current densities with low overpotentials. Electrochemical impedance spectroscopy (EIS) studies reveal that, unlike LE which shows unstable solid–electrolyte interphase (SEI) evolution over ~1 month, the GPE supports long-term stable SEI growth lasting over ~2 months.

In half cells ($Na||Na_3V_2(PO_4)_3$) and symmetric NVP||NVP configurations, the GPE delivers outstanding cycling stability with consistent performance at 1C for 500–1000 cycles at room temperature. Furthermore, its compatibility with emerging Sn-based alloy anodes—considered viable alternatives to hard carbons—demonstrates the versatility and broad applicability of the GPE for future SIB technologies.

Keywords (max 5): Sodium-ion batteries (SIBs), Gel polymer electrolyte (GPE), Electrospun PAN membrane, Stable SEI formation, Sn-based alloy anode

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Impact of Air Stability through Alkaline Earth Metal Doping on P2-$Na_{0.67}Fe_{0.5}Mn_{0.5}O_2$

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Abstract

Na-ion batteries (NIBs) are considered as promising energy sources alongside Li-ion batteries owing to their low cost, abundant and widely available resources. For the positive electrode, P2-type layered transition metal oxides (*i.e.* P2-Na_xTMO_2, TM=transition metal) have garnered significant interest due to their excellent rate capability and cycling performance. Our group reported P2-type $Na_{2/3}[Fe_{1/2}Mn_{1/2}]O_2$ (P2-NFM) as a promising positive electrode for NIBs with a high reversible capacity of 190 mAh g^{-1}.[1] However, improving air and moisture stability remains an important challenge for practical use of P2-NFM. P2-Na_xTMO_2 often undergo structural transformation by reacting with air, *e.g.* CO_2 and H_2O, which will increase battery manufacturing costs. To improve the stability of P2-NFM, we are exploring and comparing the doping effects of alkaline earth metals (AEMs) such as Ca^{2+}, Mg^{2+}, Sr^{2+} and Ba^{2+}.

We recently found that Ca^{2+}-doping significantly improves air stability by forming a thin Ca-rich surface layer that acts as a protective barrier against Na^+/H^+ exchange and surface degradation. In this study, we are expanding towards other AEMs as prospective dopants to improve air stability. As shown in the X-ray diffraction (XRD) patterns in Fig. 1, undoped P2-NFM undergoes structural changes after 2 days of air exposure at 65% relative humidity with the emergence of impurity phases such as hydrated products and sodium bicarbonate ($NaHCO_3$). In contrast, Ca-doping maintains the original P2 phase without any secondary peaks. Doping with other AEMs shows varying degrees of structural change and growth of impurities. At the same time, electrochemical analysis of the air exposed materials showed that AEM-doped samples generally retained high charge/discharge capacities compared to undoped NFM especially with Ca showing the most promising improvement. This study provides a comparative outlook of using AEMs as dopants to enhance the ambient stability of P2-type layered oxides.

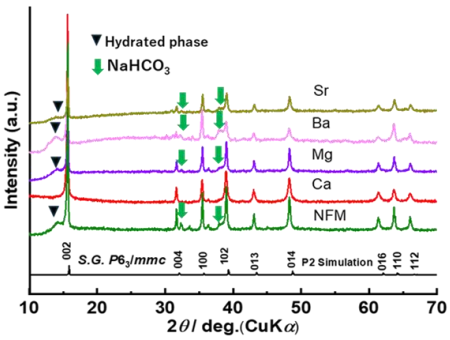

Fig. 1. X-ray diffraction (XRD) pattern after air exposure for 2 days under 65% RH

Keyword: Sodium ion battery, P2 type positive electrode, alkaline earth metal doping, air stability

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Investigation of the Layered Structure and Electrochemical Behaviour of $Na_{2-x}Li_xMn_3O_7 \cdot yH_2O$

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Abstract

Manganese-based cathodes are promising owing to their natural abundance, structural versatility, and tunable redox properties.[1] $Na_{2-x}Li_xMn_3O_7 \cdot yH_2O$ is a novel layered manganese oxide synthesized for the first time via a soft-chemistry ("*chimie douce*") using $Na_2Mn_3O_7$ as the starting phase. The composition was confirmed through atomic absorption spectroscopy (AAS). Thermogravimetric analysis (TGA) and *operando* high-temperature X-ray diffraction (XRD) were used to investigate thermal stability. A dehydrated phase was also synthesized under varied conditions and found to match structure reported by the Zhou group.[2] Electrochemical performance was evaluated for both hydrated and dehydrated phases in the 2–4 V range. Structural and mechanistic changes during cycling were studied using various characterizations like *in-situ* and ex situ diffraction, Raman spectroscopy, electron microscopy, magnetic measurements and electrochemical analyses. The structure and electrochemical properties of these manganese oxide phases will be elaborated.

Keywords: Na-ion batteries, Cathodes, Layered structure, Manganese Oxides, *Chimie Douce*

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Screen printed MEAs incorporating carbon nanotube-structures as structural additives to enhance electrocatalytic performance

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Abstract

Hydrogen PEMFCs are a promising green technology for combating global warming. We have just published a screen-printing method for MEA production, but the output power must be improved [1]. There have been reports that the use of carbon nanotubes (CNTs) improves the specific activity of catalysts for spray-coated MEAs.[2] In this study, we focused on carbon nanotube-structures (CNSs) for the screen-printing paste. Unlike conventional CNTs, CNSs feature a cross-linked structure formed by branched nanotubes, exhibiting high dispersibility (Fig. 1). The I-V results (Fig. 2) show that PEMFCs prepared with ink containing 3% CNSs generate higher current across the entire potential range compared to their CNSs-free counterpart. In particular, the incorporation of CNSs significantly enhanced the electrochemical surface area (ECSA),indicating improved electrocatalytic performance. This enhancement could be attributed to a more favorable catalyst layer structure promoted by the presence of CNSs. These results suggest that incorporating CNSs into the catalyst layer is a promising approach to improve platinum utilization in screen printed MEAs.

Keywords: Carbon nanotube-structures, Screen-printing, PEMFCs

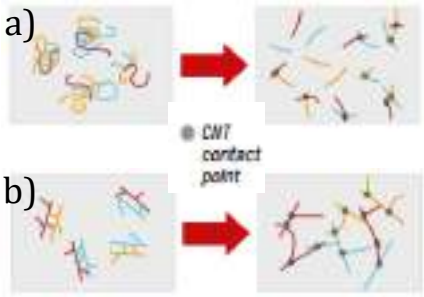

Figure 1. Dispersion difference between a) CNTs and b) CNSs.

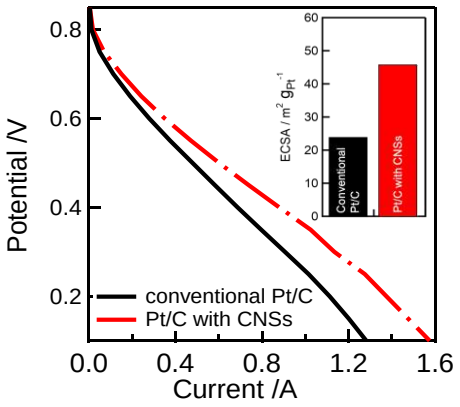

Figure 2. Polarization curves of MEAs with/without CNSs ; ECSA shown in inset.

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N-doped graphitic layer encapsulated AuCo nanoparticles as core–shell structured bifunctional electrocatalyst for Zn-air batteries

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Abstract

AuCo nanoparticles encapsulated with N-doped graphitic layer and embedded homogeneously in a carbon framework are synthesised via a pyrolysis method. The AuCo nanoparticles have FCC structure as confirmed via powder XRD. The nanoparticles are in a carbon matrix as observed in SEM. The core-shell structure of nanoparticles was confirmed in HAADF-STEM. Gold covering over cobalt, along with an alloy phase, was observed in HAADF-STEM and confirmed by P-XRD. The Raman spectroscopy and HR-XPS confirm the presence of nitrogen in the graphitic framework. This sample (NC@AuCo) was used as an electrocatalyst for the supercapacitor cum zinc-air battery. Incorporation of nitrogen in graphitic layers creates the neighbouring carbon atoms as active centres for electrocatalytic reactions [1]. The carbon framework is porous and has different types of defects, which enhance the surface area. The catalyst was used for oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) in 0.1 M KOH. The result showed that the Janus particles covering over Co using a one-step method embedded N-doped carbon catalysts improve the electrical behaviour and reduce the activation barrier; therefore, it reflects on the result as exhibiting low overpotential (@10 $mAcm^{-2}$), minimum activation energy, large ECSA and stability in aq. 0.1M KOH alkaline media, which is better than the catalyst RuO_2. Furthermore, our results provide an opportunity for a coherent depiction of the multifunctional, efficient, and durable electrocatalysts for a straightforward, low-cost, and scalable production of the supercapacitor cum zinc-air battery. This prototype device can function as both a charge storage device and an energy generation device. Hence, the significance of our device lies in its adaptability, allowing us to adjust it to function either as a battery or a supercapacitor, depending on the specific needs.

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Systematic study on operating conditions and interaction mechanisms for enhanced VRFB Stack performance

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Abstract

Vanadium redox flow batteries (VRFBs) have been widely recognized for their long cycle life, independent design of energy capacity, and high potential for large-scale applications[1,2]. However, enhancing stack performance and reducing operating costs remain key challenges for practical deployment. In this study, a systematic investigation was carried out to examine the effects of operating conditions on VRFB stack performance through multi-parameter interaction experiments. Two stack configurations were tested under various conditions involving four primary operating parameters. An orthogonal experimental design was adopted to comprehensively assess the influence of these variables. Key performance metrics, including voltage efficiency, coulombic efficiency, and energy efficiency, were measured for each condition to clarify the relationships between operational factors and performance indicators. Preliminary results demonstrate that flow field design and electrolyte flow rate have significant impacts on mass transport within the stack, thereby affecting voltage and overall energy efficiency. Interaction effect analysis further reveals complex nonlinear relationships among parameters, suggesting that single-variable optimization is insufficient to achieve overall system optimization.

Keywords: Vanadium redox flow batteries stack, Energy efficiency, Mass transfer, Multi-parameter

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From Lab to Production: Evaluating Coating Techniques for Catalyst Coated Membrane Fabrication for Scale-Up

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Abstract

As the demand for high-performance, cost-effective hydrogen fuel cells and water electrolyzers grows, scalable fabrication of catalyst-coated membranes (CCMs) has become a critical challenge and the fabrication method of CCMs plays a crucial role in determining the performance, reproducibility, and manufacturability of polymer electrolyte membrane fuel cells (PEMFCs) and PEM-electrolyzers. The coating method used significantly influences not only electrochemical output but also manufacturing viability. In this study, we compare three primary CCM fabrication methods decal transfer, spray coating, and slot-die coating based on their coating uniformity, practicality, material efficiency, choice of substrate, equipment maintenance and scale up viability. At laboratory scale, decal transfer is valued for its high control over uniformity but is limited by its multi-step processing, low throughput, operator dependency and significant material losses. Spray coating offers versatility and control at small scale but requires elaborate setup, frequent maintenance and suffers from high catalyst ink wastage. On the other hand, the slot die coating can be good alternative technique for the direct coating of catalyst on the membrane surface and also is suitable for the mass-manufacturing of CCMs. Slot-die coating demonstrates compatibility with roll-to-roll platforms, offering higher material utilization and speed, but introduces new challenges at scale such as the need for precise control of rheology, web tension, and drying parameters. A detailed comparison was made of coating time per CCM, ink consumption, adhesion to substrate, wettability and drying, scale up viability, ink rheology, post coating processing and reproducibility across the aforementioned three methods. Additionally, cost per CCM, process integration complexity, and the need for in line quality monitoring were also compared in this study. This work provides a comprehensive view of the trade-offs involved and establishes a practical framework for selecting coating technologies for scaling up to achieve manufacturing goals.

Keywords: Manufacturing Readiness Level, Catalyst Coating, CCMs, Roll-to-Roll, PEM Fuel Cell Scale up

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Work Function Centric Theory for Heterogeneous Electron Transfer on Graphene and Graphene/Metal Composites

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Abstract

A semi-microscopic theory is developed for the standard rate constant (k^0) of heterogeneous electron transfer (HET) and the potential of zero charge (PZC) at the basal and edge planes of graphene and graphene/metal composites. Our curvature-dependent theory for the electrochemical work function (EWF) enables us to account for complexities arising from graphene edges and their interaction with metals and dipolar solvents in solution at IHP. EWF is directly related to PZC and the interfacial electron affinity ratio (A_i). The activation barrier for HET is the product of A_i and the energy gap (Δ). Δ is defined as the difference between the WF (of graphene or graphene/metal composite) and the solvent reorganization-driven fluctuating energy levels of the frontier molecular orbital (FMO) of an electroactive molecule. The curvature-dependent theory reveals a doubling of electronic capacitance and a lowering in work function at the graphene edge by a factor of 2.3 compared to the basal plane. Theory predicts a giant amplification of k^0 at the graphene edge compared to the basal plane. Graphene composites show a $\approx 19 - 33\%$ reduction in the work function compared to the pristine metal. Surprisingly, graphene coating slows the kinetics for $[Ru(NH_3)_6]^{3+/2+}$, and enhances for $[Fe(CN)_6]^{3-/4-}$ in comparison to the substrate metal. The difference in kinetics is attributed to the higher and lower values of Δ compared to the pristine metal.

Keywords: Graphene, Graphene/Metal Composites, Electrochemical Work Function, Potential of Zero Charge, Outer Sphere Heterogeneous Electron Transfer

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Unraveling the Fundamental Understanding of Anionic Redox Chemistry in Transition Metal Oxide Cathode Materials through First-Principles Calculations

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Abstract

Although anionic redox chemistry has gained considerable interest in recent years for its potential in designing high-capacity battery materials, incorporating reversible anionic redox chemistry into cathode materials remains a challenge, primarily due to the release of gaseous molecular oxygen and resulting structural degradation upon cycling. In the present study, we utilized the machine learning (ML) models and first-principles computational methods (density functional theory, DFT) together to screen and elucidate the structural stability of series of layered transition metal (TM) cathodes ($Na_xM_{1-y}M'_yO_3$) by varying the concentration of TM (y = 0.0, 0.25, 0.5, 0.75). We systematically investigate the electronic structures and compute Na-intercalation potentials for a series of doped cathode materials at different deintercalation levels (x = 0.0, 0.25, 0.5, 0.75, 1.0). In this study, we proposed an empirical model by training a wide range of datasets to identify key descriptors (including changes in the occupancy of metal-*d* and oxygen-*p* orbitals, the number of holes generated in these states, and shifts in average net atomic charges) and trends that can support the comprehensive understanding of the fundamental mechanism of anionic redox chemistry. Our results demonstrate an application of ML-based techniques in conjunction with DFT findings to stabilize anionic redox in existing materials and design new Na-based cathode materials.

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Dimensional change study of Li metal anode during operation of Solid-state battery

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Abstract

With the increasing demand for high energy density and power density, better energy storage options like solid state batteries (SSBs) are emerging. In SSBs, the Li metal anode plays a crucial role in improving the energy density. However, the lithium metal anode undergoes plastic deformation during the charging and discharging operation of the battery due to its low yielding point, as shown in Figure 1. In the present study, a thin-film full cell solid state battery model is coupled with the plastic deformation model of the Li metal anode to study the dimensional change of the metal anode and the associated effects during operation of the battery. Earlier plastic deformation studies of Li metal anode were considered, but they were not explicit in terms of dimensional change, and these models only considered the interface of Li metal anode and solid electrolyte, not the full-scale battery model. In the present study, a full cell model is integrated with the plastic deformation model of the Li metal anode, considering transverse anisotropy, which is very prevalent in battery-grade lithium metal used inside the battery [1]. It is observed that at higher C-rates, the dimensional change of the lithium metal anode is more during charging, and it leads to relative stress reduction inside the battery. Thus, this model becomes useful in predicting the failure-prone zones inside the SSB while operating it.

Keywords: Solid-state battery, Li metal anode, plastic deformation

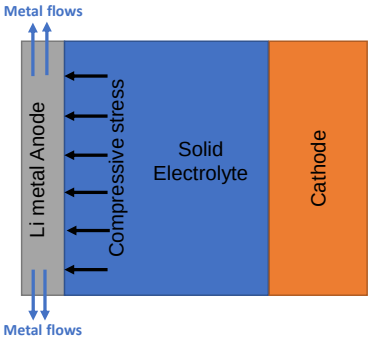

Figure 1 Schematics of Li metal anode deformation inside SSBs.

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Solvent co-intercalation in layered cathode active materials for sodium-ion batteries

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Abstract

Solvent co-intercalation, i.e. the combined intercalation of ions and solvent molecules into electrode materials, is an additional but much less explored lever for modifying the properties of electrodes in metal-ion batteries (metal= Li, Na, Mg, …). So far, the knowledge on solvent co-intercalation is relatively scarce and largely limited to graphite anodes, for which in Na-ion batteries, the co-intercalation of glyme molecules is found to be very fast and highly reversible over many cycles. The use of co-intercalation in metal-ion batteries, however, still lacks a scientific breakthrough with respect to cathode active materials (CAMs). In this talk, we show for a series of Na-layered CAMs by experimental methods and theory, under which conditions solvent co-intercalation occurs and how this process impacts the phase behavior, electrode breathing, redox potential, and cycle life compared to "Na^+-only" intercalation.[1] Co-intercalation is a complex process that can, for example, cause opposing fluxes, meaning that solvents intercalate into the CAMs while Na-ions simultaneously deintercalate. Co-intercalation leads to layered structures that can include different amounts of confined solvated ions, ions and unbound solvent molecules. It is an approach to designing structurally diverse, layered materials with potential applications for batteries and beyond.[2]

Keywords: Sodium-ion batteries, Solvent co-intercalation, Layered cathodes

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Upcycling of spent lithium-iron phosphate cathode material through the embedding of pitch carbon precursor

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Abstract

The rapid development of electric vehicles in recent years has significantly increased the demand for lithium-ion batteries. With a lifespan of 5–10 years, these batteries will generate substantial waste in the near future. Lithium-ion battery cathodes are primarily composed of materials such as lithium cobalt oxide, nickel manganese cobalt oxide, and lithium iron phosphate (LFP), which contain valuable transition metals like cobalt, nickel, manganese, and iron. With rising transition metal prices and the increasing volume of waste lithium-ion batteries, the recycling of these cathodes has become essential. Current recycling methods include pyrometallurgy, hydrometallurgy, and direct resynthesis. Both pyro and hydrometallurgy are energy-consuming and highly chemical-consuming processes. In contrast, the direct resynthesis approach offers a more energy-efficient alternative by employing a shorter process to regenerate cathode materials. LFP is a popular cathode material for lithium-ion batteries due to its affordability, non-toxicity, excellent cycle life, and thermal stability. Overextended cycling of the LFP cathode experiences significant capacity loss and structural degradation caused by forming Li-ion vacancy defects and Fe-Li antisite defects. Here, we used lithium sulfate and hydrazine hydrate to regenerate the spent lithium iron phosphate (SLFP) cathode to get regenerated lithium iron phosphate (RLFP). Further modification is done by pitch to improve the performance. The pitch-coated RLFP(PRLFP) gives a discharge capacity of 148mAh g^{-1}, and regenerated LFP shows a discharge capacity of 133 mAh g^{-1} at 0.1C, while spent lithium iron phosphate shows a discharge capacity of 40 mAh g^{-1} at 0.1C. The PRLFP shows a discharge capacity of 137.3 mAh g^{-1} at 1C with a capacity retention of 93 % over 1000 cycles, whereas RLFP gives a discharge capacity of 117.5 mAh g^{-1} at 1C with a capacity retention of 93% over 700 cycles. The PRLFP offers high discharge capacity and better capacity retention over the RLFP cathode.

Keywords: Recycling, direct regeneration, lithium iron phosphate cathode, surface coating, High capacity retention.

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Decoupling Mechanical and Ionic Properties via Molecular Engineering of Polymers for Anion Exchange Membrane Fuel Cell

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Abstract

The increasing demand for sustainable materials in energy conversion technologies has accelerated research on fuel cells for stationary, automotive, and portable power applications. The anion exchange membranes fuel cells (AEMFCs) can be operated at low temperatures and using non-precious metal-based catalysts. The high performance AEMs that show high thermo-mechanical and chemical stability and possess excellent hydroxide conductivity, are prerequisites to achieve high power output and durability of fuel cells. Molecular engineering of the polymers allows precise tuning of these properties and can result in membranes with the desired properties. This study deals with newer approaches in the design of polymer membranes through the introduction of specifically tailored cationic groups to promote hydroxide ion transport. Further, the goal is to achieve decoupling of the mechanical and ionic properties in the AEM, which has been a major challenge often limited to the improvement of one property at a time. The newly proposed functional polymer membrane can potentially result in higher power output and durability in AEMFCs through simultaneously enhanced ionic properties and thermo-chemo-mechanical stabilities of the AEMs.

Keywords: Fuel Cell, Anion Exchange Membrane, Molecular Engineering, Polymer Membrane, Ion Transport.

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Nickel-Coated Hollow Mn-PBAs as Durable Cathodes for High-Performance for Sustainable Sodium-Ion Battery

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Abstract

To meet the growing demand for sustainable, safe, and cost-effective energy storage, Prussian Blue Analogues (PBAs) have emerged as promising cathode materials for sodium-ion batteries (SIBs) due to their open-framework structure and the use of earth-abundant elements. Manganese-based PBAs offer high theoretical capacity and favorable multi-electron redox activity. However, challenges such as structural instability and rapid capacity fading hinder their practical deployment. In this study, we report the synthesis of nickel-coated hollow Mn-PBA cathodes via a self-template hydrothermal method to address these limitations. Field emission scanning electron microscopy (FESEM) confirmed the formation of uniform hollow cage structures, while the nickel coating effectively preserved the structural integrity during cycling. X-ray diffraction (XRD) and Fourier-transform infrared (FT-IR) spectroscopy verified the monoclinic phase and identified interstitial and absorbed water molecules. Thermogravimetric analysis (TGA) revealed enhanced thermal stability for the Ni-coated samples, with reduced weight loss. Electrochemical measurements demonstrated a high specific capacity of 160 mAh g^{-1} at a current density of 0.01 A g^{-1}. Notably, the material retained 81% of its initial capacity after 500 charge-discharge cycles, indicating excellent cycling stability. These results highlight the effectiveness of Ni-coating in enhancing the electrochemical and structural stability of Mn-PBAs. Overall, this work presents nickel-coated Mn-PBAs as promising cathode materials for advanced SIBs, offering a balanced combination of high energy density, long-term durability, environmental sustainability, and cost-efficiency.

Keywords: Prussian blue analogue, Sodium ion battery, Energy storage.

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Stabilisation of Metastable β-Bi_2O_3@Carbon Core-Shell Architecture and its Application in Na-Ion Battery

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Abstract

The ever-growing global energy demand amid resource scarcity requires innovative materials capable of addressing multiple technological challenges. Among these, metastable inorganic materials have emerged as promising candidates due to their superior chemical activity and enhanced properties compared to stable phases. However, synthesising and stabilising such metastable materials under mild and scalable conditions remains a significant challenge. This study introduces a novel synthesis strategy to stabilise the metastable β-Bi_2O_3 phase by developing a unique core–shell β-Bi_2O_3@C architecture. Bismuth oxide, with its suitable bandgap of 2.6–2.9 eV, high refractive index, and excellent photocatalytic and photoluminescence properties, is an attractive material for various applications. However, its β-phase is thermodynamically unstable at elevated temperatures. Here, an in-situ carbon coating plays a dual role: it stabilises the β-Bi_2O_3 phase and enhances its electrical conductivity. This scalable and straightforward synthesis approach overcomes the limitations of existing complex methods, enabling practical implementation. When tested as an anode material in sodium-ion batteries, the β-Bi_2O_3@C composite delivered a high initial specific capacity of approximately 500–600 mAh g^{-1} at 0.1 A g^{-1}, retaining around 33 % of its capacity over long cycling. The carbon shell effectively maintains structural integrity, ensures efficient electron transport, and mitigates the severe volume changes typically observed in anode materials.

Keywords: Metastable phase, Battery, Na-ion, Bi_2O_3, core-shell