NAZARBAYEV UNIVERSITY

Institute of Batteries

NAZARBAYEV UNIVERSITY
INSTITUTE OF NEW MATERIALS AND ENERGY TECHNOLOGIES

NATIONAL ACADEMY OF SCIENCES
UNDER THE PRESIDENT OF THE REPUBLIC OF KAZAKHSTAN

*Dedicated to the 80th Anniversary of the National Academy of Sciences of the Republic of Kazakhstan under the President of the Republic of Kazakhstan*

# NESS 2026

14th International Conference on

## NANOMATERIALS & ADVANCED ENERGY STORAGE SYSTEMS

# ABSTRACT BOOK



5–7 August, 2026

Astana, Kazakhstan

**Dear Colleagues!**

**We are delighted to welcome you to the 14th International Conference on Nanomaterials and Advanced Energy Storage Systems (INESS-2026), held in celebration of a significant milestone — the 80th Anniversary of the National Academy of Sciences of the Republic of Kazakhstan under the President of the Republic of Kazakhstan.**

**INESS-2026 provides a unique forum for leading researchers, scientists, and industry experts to present recent advancements, exchange innovative ideas, and explore opportunities for collaboration in the rapidly evolving fields of nanomaterials and energy storage systems.**

**We are confident that this conference will inspire meaningful discussions, foster new partnerships, and contribute to the global advancement of sustainable energy solutions.**

**Thank you for being part of INESS-2026. We wish you a productive and inspiring experience.**

**Sincerely,**

**On behalf of the Organizing Committee,**

**Prof. Zhumabay Bakenov,**

**General Director of Institute of New Materials**

**and Energy Technologies (INMET)**

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## KEYNOTE

# Polytypes and Stoichiometry of Layered $NaMnO_2$ & $Na_{2/3}MnO_2$

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We first demonstrated cobalt-free Na-ion batteries (NIB) based on layered oxides and hard carbon as disordered positive and negative electrodes [1] as sustainable and cost-effective alternatives to Li-ion batteries. We believe that layered oxide materials, particularly, hold great promise as positive electrodes for NIB. Enabling the $Mn^{3+/4+}$ redox couple in the layered structures is one of the key factors for achieving high energy density without using expensive metals, such as cobalt and nickel. However, the Jahn-Teller distortion of $Mn^{3+}$ ions complicates phase formation and electrochemical reactions.
An α-type (O'3-type) $NaMnO_2$ electrode suffers from rapid capacity fading well as multiple phase transitions during electrochemical cycling [2]. The impact of doping on structural stability was further discussed by comparing with the polytype, β-type $NaMnO_2$ having corrugated $MnO_2$ layers [3] which has the same crystal structure as zig-zag layered $LiMnO_2$ as previously reported [4]. In our recent papers, we discussed in greater detail the correlation between unique stacking defects and the electrochemistry of β-type $NaMnO_2$ doped with Cu [5] and Zn [6].
Other layered polytypes, namely P2-type [7] and P3-type [8] structures, can be found in te off-stoichiometric composition of $Na_{2/3}MnO_2$ containing Mn(III):Mn(IV) = 1:2. Through our understanding of crystallization process, we developed new synthetic routs enabling us to prepare P'2-type (a distorted P2 structure) and P2-type single-phase products. Accordingly, we precisely characterized both of P'2- and P2-type $Na_{2/3}MnO_2$. The P'2 phase has stoichiometric composition of $Na_{2/3}MnO_2$ with no Mn-site vacancies, leading to cooperative Jahn-Teller distortion and orthorhombic unit cell. In contrast, the P2 phase is formed via over-oxidation, resulting in Mn vacancies and a distortion-free hexagonal unit cell [7].
According to this understanding we extended our systematic study to P'2-type $Na_{2/3}[Mn,Me]O_2$ (Me = Mg, Ti, Co, Ni, Zn [9], Cu [9,10], and Sc [11,12]) materials. Electrochemical tests revealed superior cycle stability and rate capability for the Sc-substituted materials compared with the non-substituted ones [12]. To utilize such 1/3 Na-deficient $Na_{2/3}MnO_2$ materials, we proposed the use of $Na_2CO_3$ as a sacrificial electrode additive to balance the sodium content (i.e., state of charge) in full cells employing sodium-free negative electrode [13].

In this presentation, we will provide an overview of the latest development in layered oxides, $NaMeO_2$ (Me = 3d metals) for battery applications.

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# Mn-Rich Layered Cathode Materials for Lithium and Sodium Intercalation

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Mn-based P2-$Na_x[Li_yTM_{1-y}]O_2$ cathode materials are available to reach high capacity through the combination of cationic and anionic redox in Na cells.[1] The Na–O–Li configuration induces the delivery of additional capacity assisted by the oxidation of oxygen when lone-pair electrons are formed in the O 2*p* orbital, provided that at least one of the following conditions is satisfied: 1) lattice oxygen evolution[1] or 2) migration of the Li element to Na layers although the corresponding charge transfer is kinetically sluggish.[2] The reaction is not limited to compounds that have alkali ions in the TM layer but is also available with divalent ions; namely, the presence of Mg in the TM layer, P2-$Na_x[Mg_yMn_{1-y}]O_2$ (x = ~2/3, y = ~0.28).
The effect of the 4*d* Ru element in P2-$Na_{0.6}[Mg_{0.2}Ru_{0.2}Mn_{0.6}]O_2$ is investigated. Ru-free $Na_{0.6}[Mg_{0.2}Mn_{0.8}]O_2$ is activated with the $Mn^{3+}/Mn^{4+}$ redox, after which the charge is compensated by the sluggish oxidation of lattice oxygen ($O^{2-}$) to $O_2^{n-}$ triggered by $O_2$ evolution from the oxide lattice. These effects are generally unfavorable and result in poor long-term cycle stability induced by the irreversible migration of $Mg^{2+}$ from the transition metal (TM) to Na layers in the P2 structural framework. Benefiting from the covalent Ru bonded with O in the TM layers, the Mg migration reversibly progresses from the TM to sodium slabs without $O_2$ evolution in the structure. The associated reaction progresses via the active $Mn^{4+}/Mn^{3+}$ and $O^{2-}/(O_2)^{n-}$ reaction in addition to the $Ru^{5+}/Ru^{4+}/Ru^{3+}$ redox pairs, endorsing the capacity increase (~210 mAh $g^{-1}$), with ~72.1% retention for 300 cycles.

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# Microstructure-Driven Electro-Chemo-Mechanical Behavior and Degradation Pathways in Si-Al Alloy Anodes with Different Al Contents

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Silicon (Si) offers very high capacity for lithium-ion battery anodes, but severe volume-change-driven damage limits cycle life [1]. Although nanostructured Si can mitigate pulverization, its complex and costly processing hinders scalable use [2]. Here, we demonstrate a post-treatment-free approach in which water-atomized Si–Al-based alloy powders are directly used as anode active materials [3,4]. By tuning the Al content, three alloys with distinct rapidly solidified microstructures were produced, and their electro-chemo-mechanical degradation was examined using cross-sectional SEM, in situ electrochemical dilatometry, TEM-based phase analysis, and nanoindentation. With increasing Al content, the powders exhibit apparent refinement of Si-rich domains; however, cycling stability does not improve, indicating that refinement alone is insufficient for atomized Si alloy anodes. Instead, durability is governed by the stability and electrochemical reactivity of the metallic matrix [5]. The Si-rich alloy primarily shows degradation consistent with progressive SEI-related losses, whereas the Al-rich alloys undergo rapid capacity fade associated with lithiation of the Al-containing matrix (LiAl formation), which promotes deformation-driven damage, cracking, and electrical disconnection [6,7]. These results suggest a processing–composition trade-off for scalable Si–Al alloy anodes: Al can assist microstructure refinement during atomization, but excessive Al increases matrix participation and accelerates mechanically driven failure.

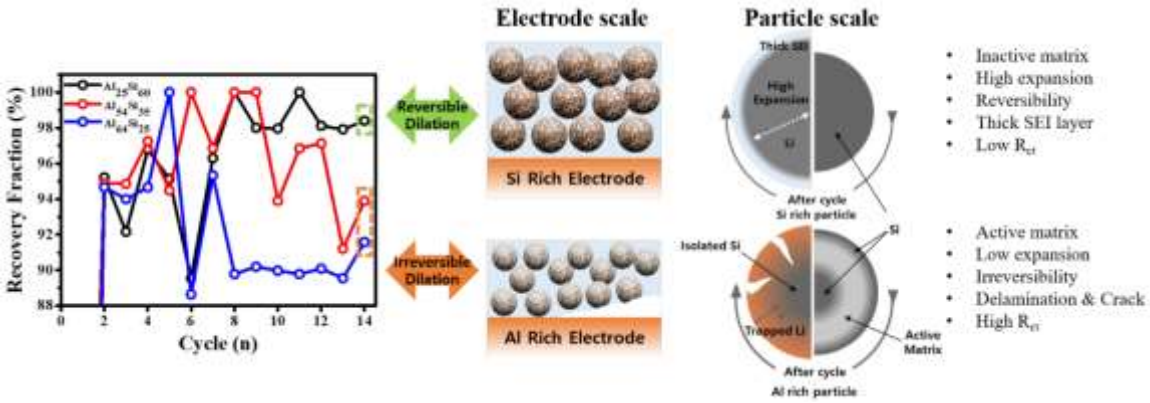



Figure 1. Schematic illustration of composition-dependent electro-chemo-mechanical degradation pathways in Si–Al alloy anodes.

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# Designing and Architecting Battery Electrode Materials Across Length Scales

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The design and operation of rechargeable batteries is predicated on orchestrating flows of mass, charge, and energy across multiple interfaces. Understanding such flows requires knowledge of atomistic and mesoscale diffusion pathways and the coupling of ion transport with electron conduction (**Fig. 1**). Using multiple polymorphs of $V_2O_5$ as model systems, I will discuss our efforts to develop an Ångstrom-level view of ion diffusion pathways.[1] Topochemical single-crystal-to-single-crystal transformations provide an atomistic perspective of how diffusion pathways are altered by modification of V—O connectivity, pre-intercalation, and high degrees of lithiation.[2] Recently devised multi-step synthetic schemes enable the positioning of Li-ions across four distinct interstitial sites of a $V_2O_5$ insertion host and allow for deterministic redirection of Li-ion flows through site-selective modification.

At higher length scales, scanning transmission X-ray microscopy and ptychography imaging provide a means of mapping the accumulative results of atomic scale inhomogeneities at mesoscale dimensions and further enable tracing of stress gradients across individual particles. I will discuss strategies for the mitigation of diffusion impediments and degradation mechanisms based on controlling the coupling of chemistry, geometry, and mechanics.[3] Some of these strategies include (a) utilization of Riemannian manifolds as a geometric design principle for electrode architectures; (b) atomistic design of polymorphs with well-defined diffusion pathways that provide frustrated coordination; and (c) site-selective modification as a means of tuning lattice incommensurability between lithiated and unlithiated phases.

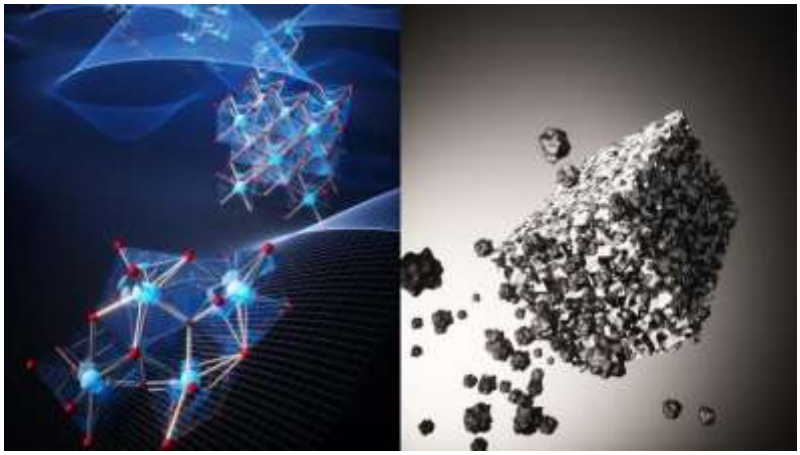


Figure 1. Design of insertion electrodes from atomistc to mesoscale structure

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# “Doping” in Ni-Rich NMC Cathode Materials

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Overcoming the technological barrier in specific energy of Li-ion battery cells of 350-400 Wh/kg calls for advanced cathode materials (CAMs), such as Ni-rich layered transition metal oxides providing electrochemical capacity up to ~240 mAh/g. NMC (LiNixMnyCozO2, x+y+z = 1) CAMs are still the subject of intense research aimed at increasing mass and volumetric energy density, cycle life, and performance at elevated charge/discharge rates. Almost all elements of the Periodic Table were used to dope and/or create protective coatings for NMCs except for highly toxic, radioactive and chemically inert ones [1]. Multiple effects are ascribed to these additives, including improving structural and mechanical stability, suppression of phase transitions and layer gliding, preventing unwanted (electro)chemical reactions through surface passivation and optimizing the particle size and morphology. The improvements in electrochemical performance are most often reported when these minor additives are introduced in rather small quantities (typically less than 1 at.%) that makes their unambiguous location extremely difficult, hence their structural and chemical influence remain elusive.

In this talk five chemically distinct dopants – sulphur, boron, magnesium, tin, and tantalum – will be compared allowing for embracing broad landscape ranging from anionic to cationic additives, from the cations with moderate formal charge to highly charged cations, from solvable to immiscible species in the NMC structure, and from structural doping to surface coating [2-5]. Combination of diffraction, imaging and spectroscopic techniques will be used to determine the spatial location of the additives and their entrance at certain crystallographic position of the layered oxide structure (Fig. 1). The connection will be drawn between crystallographic and chemical ways of action and improvement in the electrochemical performance for the discussed additives.

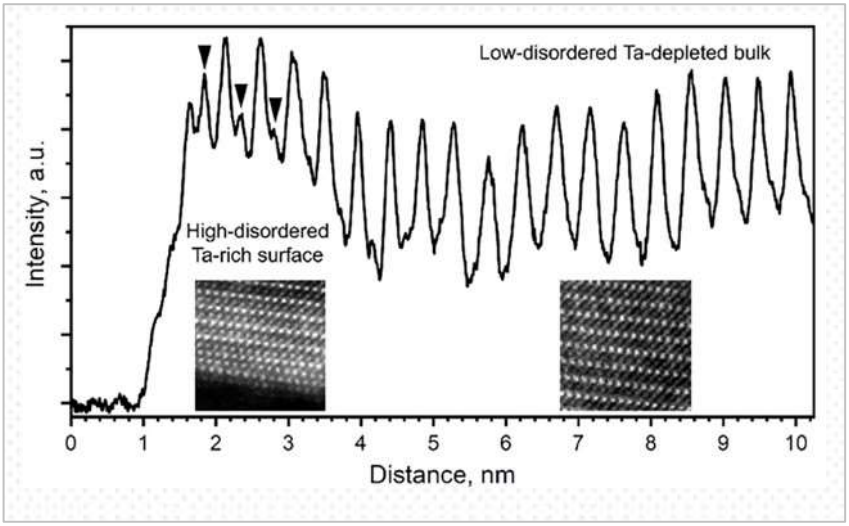



Figure 1. HAADF-intensity profile and enlarged HAADF-STEM images of surface and bulk areas of the ta-doped Ni-rich NMC.

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# Development and Application of Surface Enhanced IR Absorption Spectroscopy in Researches of Energy Electrocatalysis

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Platinum-group metals (PGMs) as a representative class of electrocatalysts play a vital role in contemporary energy conversion and storage, including but not limited to fuel cells, metal-air batteries, and precise electrosynthesis. Metalloid B doping into the interstices of a PGM lattice is an alternative tuning knob and has attracted growing interest in effectively upgrading the reactivity, selectivity, and durability of surface PGM sites toward a multitude of electrocatalytic reactions, since the report on Pd–B-catalyzed formic acid electro-oxidation in 2009 [1]. In this talk, I will briefly overview the advances of B-doped PGMs for different electrocatalytic application scenarios with an emphasis on the development and application of Pd-B/C catalyst for direct formic fuel cells [2] and Pt-B/C catalyst for hydrogen oxygen fuel cells [3], showing how binding strengths of key intermediates can be properly tuned with the B-doping level on reactive surfaces. Insights from advanced structural characterizations, operando spectroelectrochemistry, and theoretical simulations on the B-doping effect are provided, together with our viewpoints on the future research and development of efficient B-doped PGMs in electrocatalysis.

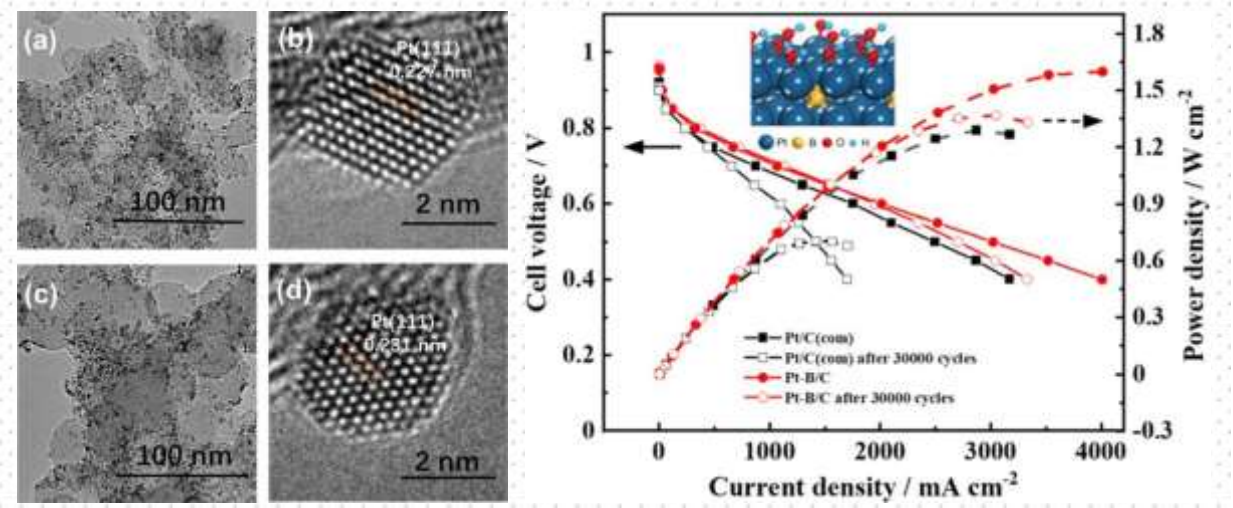
Figure. (Left panel) (a, b) TEM and high-resolution STEM images of Pt/C(com); (c, d) TEM and high-resolution STEM images of Pt–B/C. (Right panel ) Performances of the fuel cells using Pt/C and Pt-B/C as the ORR catalysts, respectively, under otherwise same conditions.

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# From Quantum Hall Physics to Quantum Sensing: Low-Field Spin-Polarised Transport in Compressively Strained Germanium On Silicon

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The ability to engineer highly spin-polarised electronic states at technologically accessible magnetic fields is of growing interest for both fundamental quantum science and emerging sensing technologies. Since the discovery of the quantum Hall effect,[1] fully spin-polarised quantum Hall states in semiconductor two-dimensional systems have generally required magnetic fields of several tesla, where orbital quantisation dominates over Zeeman splitting.[2] Accessing the opposite regime, in which spin physics governs the lowest Landau level at low magnetic fields, demands an exceptional combination of ultra-low disorder, low carrier density, and enhanced effective spin splitting.

In this invited talk, I will present recent experimental advances demonstrating fully spin-polarised quantum transport at remarkably low sub-tesla magnetic fields in an ultra-high-mobility two-dimensional hole gas realised in compressively strained germanium on silicon (cs-GoS), a silicon-compatible quantum material platform based on epitaxial SiGe heterostructures engineered on standard silicon wafers. This advanced platform combines exceptionally low disorder, strong spin–orbit coupling, enhanced hole g*-factor, low effective mass, and excellent electrostatic tunability,[3-5], enabling access to a previously unexplored regime in which Zeeman splitting dominates orbital quantisation over a broad low-field parameter space.[6]

Magnetotransport measurements reveal robust Hall quantisation accompanied by vanishing longitudinal resistance at magnetic fields as low as ~0.25–0.3 T, establishing one of the lowest-field fully spin-polarised quantum Hall states reported in a semiconductor platform. Landau fan analysis confirms pronounced spin-resolved behaviour and an anomalously stable spin-polarised ground state persisting over an extended magnetic field range and remaining observable at elevated temperatures. Beyond the fundamental significance of this unconventional quantum transport regime, the demonstrated low-field spin-polarised response opens intriguing prospects for advanced magnetic sensing. Ultra-clean quantum transport systems exhibit exceptionally sharp electrical responses to small magnetic perturbations, making them inherently attractive for precision cryogenic magnetometry and local magnetic field detection. The unique combination of low-field operation, strong spin sensitivity, ultra-high transport quality, and silicon compatibility offered by cs-GoS suggests a promising route towards integrated quantum magnetic sensors compatible with superconducting circuits, spintronic architectures, and future semiconductor-based quantum technologies. More broadly, this work illustrates how advances in quantum Hall physics can inform
the development of practical sensing platforms based on scalable semiconductor materials.

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# A Robust Li-Ion Permeable Interphase for Ni-Rich NCM Cathodes In Poly(ethylene oxide)-Based All-Solid-State Li-IonBatteries

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Poly(ethylene oxide) (PEO)-based solid polymer electrolytes (SPEs) are widely used for all-solid-statelithium-ion batteries (ASSLIBs) because they offer high processibility, good thermal stability and improvedsafety compared to traditional organic electrolytes. However, they encounter challenges of poor interfacial stability and significant degradation of the cathode structure when used with the high-voltage Ni-rich NCMcathodes. This presentation introduces lithium sulfonated poly(1,4-phenylene ether-ether-sulfone)(SPEESLi) as a robust artificial cathode-electrolyte interphase (A-CEI) for $LiNi_{0.83}Co_{0.12}Mn_{0.05}O_2$(NCM83) cathodes to address those challenges. It is demonstrated that the SPEESLi A-CEI is capable ofeffectively enhancing the interfacial stability, reducing side reactions, and suppressing impedance growth,leading to substantially enhanced cycle stability. Meanwhile, as revealed by high-resolution microscopicanalysis, its high mechanical strength minimizes cathode microcracks, limits volume changes, andreduces rock-salt layer thickness, preserving cathode integrity. Synchrotron X-ray absorption analysisconfirms suppressed Ni reduction, further demonstrating the efficacy of SPEESLi in enhancing interfacialand structural stability, enabling improved performance of the Ni-rich NCM in the PEO-based ASSLIBs.

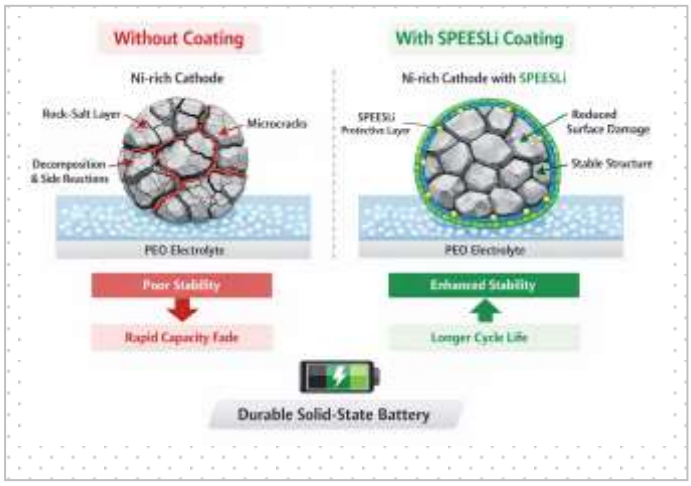



Figure 1. Schematics showing effects of SPEESLi interphase

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# Designing Functional Positive Electrode Materials through Defect Engineering

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Ni-rich layered oxides such as $LiNiO_2$ are attractive positive electrodes, but suffer from capacity degradation at high voltages due to Ni migration. Recent studies show that non-stoichiometry and antisite defects play a critical role, and defect engineering enables highly reversible pure Ni-based layered materials without metal substitution.[2] In parallel, Co-/Ni-free Mn-based electrodes are important for cost-effective electric vehicles.[2–5] While typically synthesized by energy-intensive milling, nanostructured $LiMnO_2$ with high energy density (~800 W h $kg^{-1}$) has recently been obtained through conventional calcination, demonstrating scalability. For safety, solid electrolytes are promising, but electrode volume changes complicate interface stability. Dimensionally invariable cation-disordered rocksalt oxides address this issue, achieving excellent reversibility with solid electrolytes.[6, 7]
Overall, defect-engineered and nanostructured lithium insertion materials are central to the development of safe, high-energy, and practical Li-ion batteries.
**Keywords**: Insertion material, structural defect, high capacity, phase transtiion, electrolyte

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# Modern Chemical Silicon Carbon Materials are Amazing

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Silicon carbon composites are supplementing graphite in the negative electrode of Li-ion batteries due to their large specific capacity of about 1800 mAh/g. But have you stopped to wonder how chemical silicon carbon particles can expand and contract about a factor of 2.5 in volume thousands of times during charge and discharge without cracking? This question has kept Dalhousie University researchers awake at night for several years. The materials have Si nanoparticles embedded in the nanopores of hard carbon, so this behaviour is difficult to understand. We will share our experiments and thoughts as we attempt to answer this question.

## INVITED SPEAKERS

# Non-Linear Voltammetry (NLV): a multi-task battery technology for enhanced performances

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For the last ten years we developed a new method for battery management based on Non-Linear Voltammetry. Using artificial intelligence methods NLV enables the following battery management tasks:
Ultra-fast and safe battery charging (down to 6 min for 0-100% SOC charge)

- Accurate assessment of:
  - State of charge (SOC)
  - State of health (SOH)
  - State of safety (SOS)
- Quality control (stress test)
- >2x lifespan extension
- Early detection of internal short-circuit

Moreover, we will present some new approaches to assess battery performances according to charge and discharge power (3D Ragone plots as illustrated in Fig.1) [1]

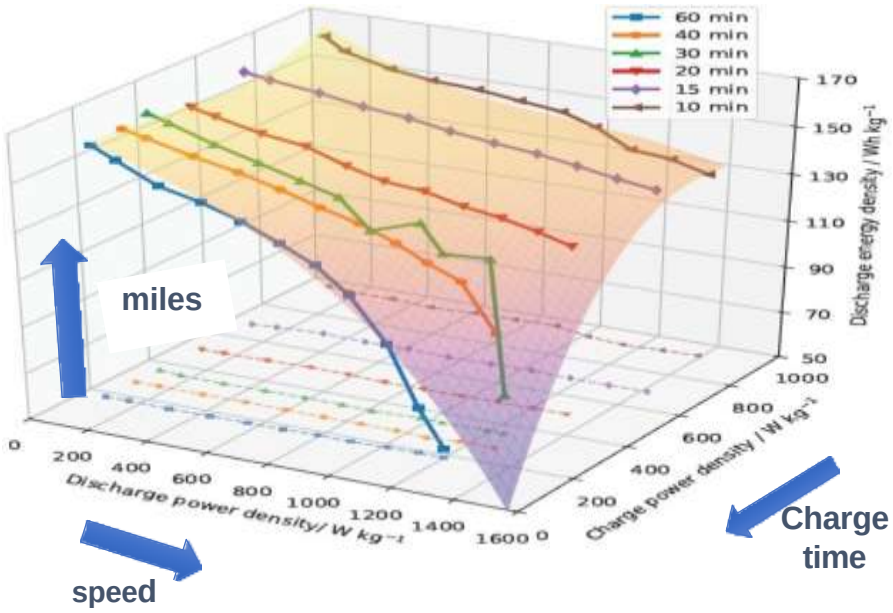



Figure 1. 3D Ragone plot of Samsung 30T cell

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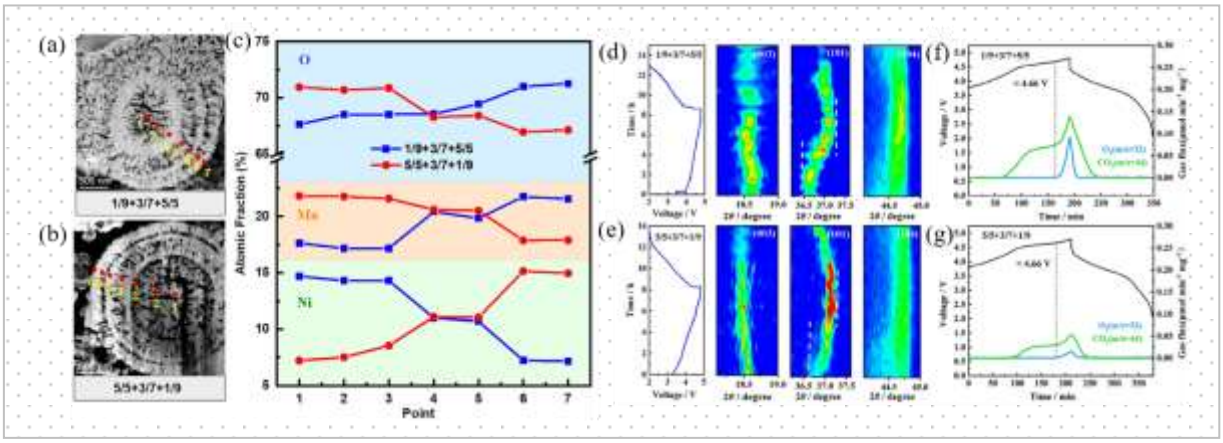
# Study on Structural Design and Performance Tuning of Cobalt-Free Lithium-Rich Manganese-Based Cathode Materials

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Cobalt-free lithium-rich layered manganese-based oxides (LLMOs) are expected to become the next generation cathode materials for lithium-ion batteries due to its high capacity and low cost. In this study, a series of cobalt-free high-nickel lithium-rich layered cathode materials $Li_{1.5-3x}Al_xMn_{0.55}Ni_{0.45}O_{2.5}$ (LLMO-Al x, x =0, 0.025, 0.075 and 0.1) with excellent electrochemical performance were synthesized through a simple calcination process of LLMO precursor with nano-alumina particles and non-stoichiometric amounts of lithium salts. The cross-sectional SEM measurement of as-prepared samples shows that a unique micro-porous structure is formed in Al-doped LLMOs and maintained even after 200 cycles of charge-discharge process at 1C rate, whereas the original LLMO with compact structure breaks into particles at the same cyclability test condition. As a result, the optimized LLMO-Al 0.075 cathode material has a discharge capacity of 353.8 mAh g at 0.1C, a capacity retention of more than 92.9% after 200 cycles at 1C.[1]

Secondly, we address these challenges by incorporating sulfur into $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$ (LNMO, a Co-free LRM cathode material) via a precisely controlled high-temperature solid-state reaction. Comprehensive characterizations and theoretical analyses demonstrate that sulfur replaces lattice oxygen, stabilizing the oxygen environment and modulating the electronic structure of transition metals (TM) through the formation of TM-O-S/TM-S bonds. This mechanism effectively suppresses TM migration and irreversible oxygen loss. The results show that the initial discharge capacity of optimized LNMOS-0.08 (S doping ratio is 0.08%) sample is 261.8 mAh $g^{-1}$, and the initial Coulomb efficiency is 81.35%. After 300 cycles at 1C, it retains 80.01% of its capacity with minimal voltage decay. This work provides a simple and effective strategy to enhance the electrochemical performance and structural stability of cobalt-free LRM cathodes.[2]

Finally, the novel cobalt-free lithium-richmanganese-based oxide cathode with Ni/Mn concentration gradient,“5/5+3/7+1/9” (n/m, $nLi_2MnO_3{\cdot}mLiMn_{0.5}Ni_{0.5}O_2$,core+ transition layer +shell), is successfully synthesized. Since the oxygen release from the “5/5”core is restricted by the stable “1/9” shell and is difficult to be removed fromthe oxide cathode, the regulated “5/5+3/7+1/9” cathode exhibits a reversibleanionic redox reaction and suppressed structural transition compared withthe homogeneous “5/5” oxide cathode. Moreover, the transitional 3/7 regionrelieves the concentration difference and the lattice strain caused by theheterogeneous electrochemistry of the 1/9 shell and 5/5 core. The structuralcharacterization elucidates that the concentration gradient regulation still exists even after long-term cycling, which interprets the durability andreliability of the regulated strategy. As a result, the “5/5+3/7+1/9” cathode delivers high Coulombic efficiency during cycling, stabilized cycling performance, and enhanced rate capacity.[3]




Figures 1 EDS elemental mapping analysis of a) 1/9+3/7+5/5 and b) 5/5+3/7+1/9 oxides illustrating 7 points locations. c) Elemental spot-scan analysis of O, Mn, Ni elements by taking 7 points from the center to the edge of 1/9+3/7+5/5 and 5/5+3/7+1/9 oxides. 2D contour plots of in situ XRD for d) 1/9+3/7+5/5 and e) 5/5+3/7+1/9 cathodes (0.2 C/2.0-4.8 V). Initial voltage profiles and gas evolution curves of $CO_2$ and $O_2$ for f) 1/9+3/7+5/5 and g) 5/5+3/7+1/9 samples (0.2 C/2.0-4.8 V)

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# Molecular Mass Growth Processes in Extreme Environments –from Polycyclic Aromatic Hydrocarbons via Nanobowls to Buckyballs

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Research on the gas-phase formation of polycyclic aromatic hydrocarbons (PAHs), nanobowls, and fullerene-type "buckyballs" provides a fundamental foundation for advancing next-generation energy materials and computational design approaches. These processes reveal how complex carbon nanostructures emerge from molecular precursors, offering insight into scalable synthesis routes for functional carbon materials used in batteries, catalysis, and photovoltaics. By understanding and controlling PAH growth pathways and curvature evolution, it becomes possible to tailor electronic, structural, and surface properties critical for energy system performance. At the same time, the inherent complexity of these reaction networks makes them well-suited for integration with artificial intelligence and computational materials engineering, where machine learning and atomistic simulations can accelerate mechanism discovery, optimize synthesis conditions, and enable inverse design of targeted nanostructures. Together, this research bridges fundamental chemical physics with applied energy technologies, positioning gas-phase carbon formation as a key platform for both high-performance material development and data-driven innovation.

This talk offers the latest developments in our knowledge on the mechanisms and pathways to PAHs via radical–radical reactions (RRR) probed in crossed molecular beams and a chemical microreactor at temperatures as high as 1,500 K. [1-10] Product preservation in a molecular beam coupled with synchrotron vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry and photoelectron photoion coincidence spectroscopy enables isomer-selective detection of PAHs of up to three rings by their photoionization efficiency curves, which were fit with a linear combination of reference curves for identification. Experiments were combined with computational fluid dynamics modeling of the physico-chemical processes in the microreactor, as well as high-level electronic structure calculations to reveal the reaction pathways of each system. Six distinct reaction mechanisms were discovered in this work: Propargyl Addition – Benz-Annulation (PABA), Methyl Addition – Ring Expansion (MARE), CycloPentadienyl Addition – Naphthylization (CPAN), Fulvene-allenyl Addition – Cyclization – Aromatization (FACA), Benzyl Addition – Aromatization (BAA), and Phenyl Addition – Pentacyclization (PAP). By systematically varying the number of carbon atoms in the radical reactants, molecular mass growth processes involving reactions between radicals with odd numbers of carbon atoms access aromatics carrying one, two, or three six-membered rings, whereas reactions between even- and odd-carbon-numbered radicals produce aromatics combining five- and six-membered rings. Our investigations reveal unconventional cycloadditions on excited state triplet surfaces, additions of radicals to low spin density carbon-centered radicals, spiroaromatic and fulvene-type intermediates, and highly strained bicyclic reaction intermediates, challenging current perceptions of PAH molecular mass growth processes. These versatile concepts can be expanded to molecular mass growth processes forming more complex aromatics by introducing a "periodic system" of PAHs that organizes aromatic structures according to transferable radical–radical motifs thus establishing a predictive framework that unifies PAH molecular growth from laboratory microreactors to extreme environments.

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# An Investigation of Prelithiated Effects of $Sio_x$: the Effects Lithiated Organic Coverages on the Interaction of Surface Si-O-Si Bond

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Silicon oxide ($SiO_x$) is a high-capacity anode material for lithium-ion batteries. $SiO_x$ offers lower irreversible capacity loss, improved cycling stability, and reduced volume expansion, which facilitate practical electrode design and manufacturing. Nevertheless, $SiO_x$ faces challenges such as the formation of inactive lithium silicates, the need for conductive carbon composites, and a relatively high lithiation potential plateau. Prelithiation has proven particularly effective, as it mitigates irreversible reactions associated with solid electrolyte interphase (SEI) formation and lithium intercalation. In this study, two lithiated organic coatings (LiOCs) were developed and applied onto the $SiO_x$ surface. The LiOCs introduce additional $Li^+$ species and functional groups containing O and N atoms, which strongly interact with the surface Si-O-Si bonds of $SiO_x$. These interactions induce asymmetric stretching and promote the formation of extended Si clusters prior to electrochemical cycling. The LiOCs effectively suppress the formation of lithium silicates ($Li_xSiO_y$) while promoting $Li_2O$ generation. Consequently, the LiOCs@$SiO_x$ anode exhibits significantly improved cycle retention, attributed to the minimized formation of small Si clusters and enhanced interfacial $Li^+$ transport. $Li_2O$ offers superior $Li^+$ diffusivity compared to $Li_xSiO_y$. Combininng with mechanical press effect from metallic Li during conventional prelithiation, the LiOC-modified $SiO_x$ anode demonstrates twin synergistic effects with Ni-rich cathodes.

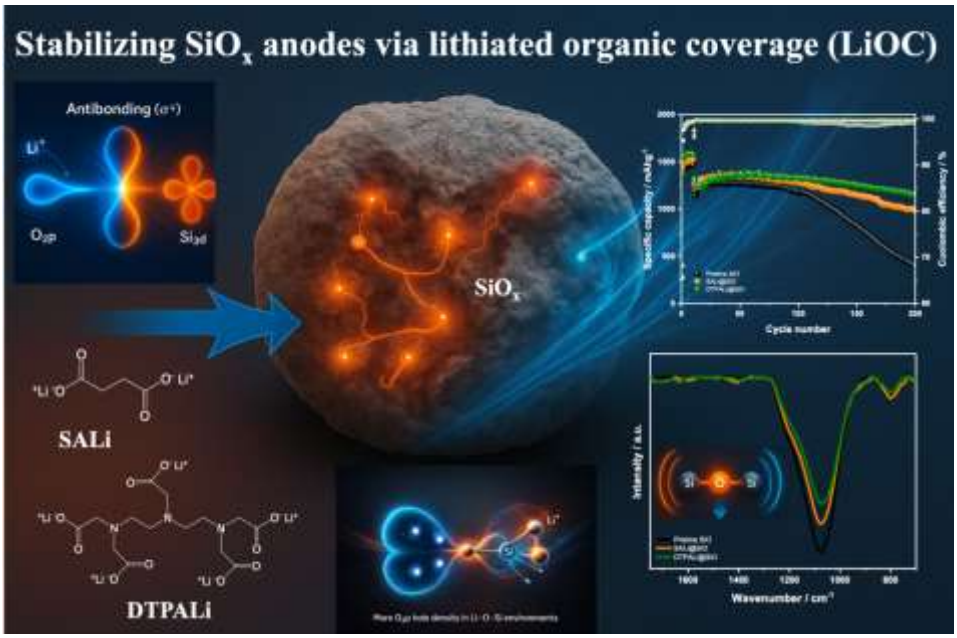



Fig.1. The illustration of LiOC effect to $SiO_x$ anode material.

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# A Novel Multi-Channel Online Electrochemical Mass Spectrometer for Battery Gas Analysis Applied to Electrolyte Additive Screening

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At Dalhousie University we built a novel multi-channel Online Electrochemical Mass Spectrometry (OEMS) system that can sample gases from up to six battery cells with a single quadrupole mass analyzer. We will explain how this system helps us to understand the reaction mechanisms of new additives.

OEMS is an operando gas analysis method that continuously samples the evolved/consumed gases in battery cells.[1] In our efforts to develop high energy density Li-ion cells, we screen novel additives with this method to understand how they improve high-voltage operation. The type of gases and gas concentration in the cell headspace are used to draw conclusions about the reaction mechanisms.

Figure 1 shows the multi-channel Online Electrochemical Mass Spectrometer at Dalhousie University. It features two vacuum chambers connected with a central gas line to six battery cells in individually controlled temperature boxes. The right vacuum chamber contains the mass spectrometer for sampling gases from the battery cells, while the left vacuum chamber is empty and merely serves for purging the central gas line. The multi-OEMS system samples each cell once per hour using an automated switching sequence of computer-controlled valves optimized to remove residual gases from the central gas line connecting the six cells without affecting the vacuum chamber containing the quadrupole mass analyzer.

Using this new multi-OEMS system we will try to uncover how novel electrolyte additives improve the passivation of the negative electrode and how they affect gas generation at high voltage.

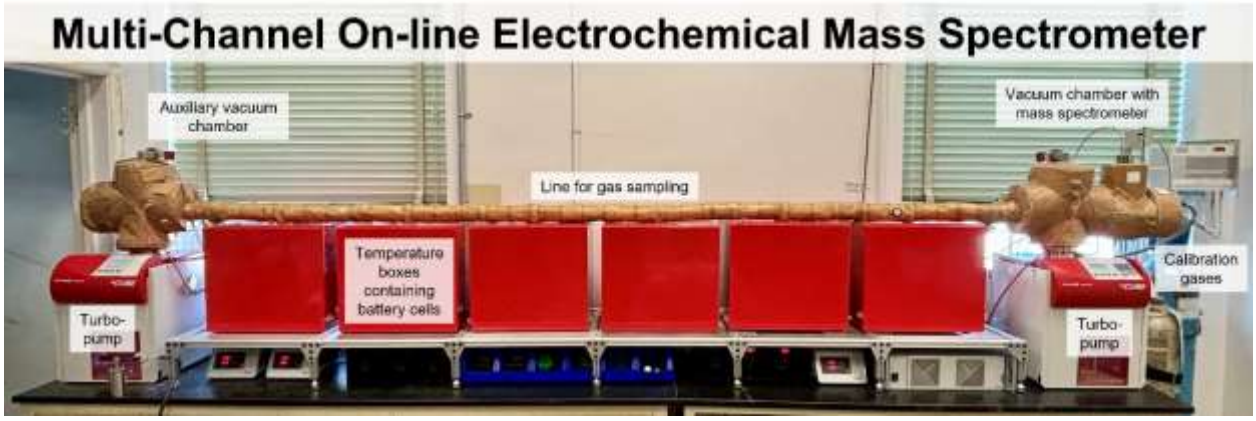



Figure 1. Muti-channel OEMS for quantification of gases in battery cells during cycling.

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# Stabilizing Prussian Blue Analogue Cathodes through Cation-Selective Intercalation for Long-Cycle Sodium-Ion Batteries

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Sodium-ion batteries (SIBs) are an attractive solution for next-generation energy storage, offering cost and power advantages over Li-ion batteries.[1] Prussian blue analogues (PBAs, $A_xM_1[M_2(CN)_6]$) have attracted considerable interest as SIB cathodes owing to their cyanide-linked open framework allowing fast $Na^+$ transport. Among them, $Na_xMn[Fe(CN)_6]$ (NaMnHCF) offers a high theoretical capacity but suffers from severe capacity fade caused by large lattice strain upon $Na^+$ insertion/extraction.[2] By contrast, $K^+$ insertion into the $K_xMn[Fe(CN)_6]$ (KMnHCF) framework induces a markedly smaller volume change than $Na^+$ insertion,[3] and PBAs intrinsically prefer $K^+$ over $Na^+$.[3] Here, we demonstrate that the long-cycle stability of PBA cathodes is governed primarily by which cation, $K^+$ or $Na^+$, is preferentially (de)inserted into the host, by directly comparing KMnHCF and NaMnHCF cycled in Na–K hybrid electrolytes.

Single-phase KMnHCF and NaMnHCF were prepared by a precipitation method as previously reported by our group.[4] Na–K hybrid half-cells were assembled with a Na metal counter electrode and 1 mol $L^{-1}$ $NaPF_6$ in EC:PC, to which $KPF_6$ was added to vary the K/Na ratio from 0 to 10 mol%. Figure 1a shows the initial charge–discharge curves at 0.1 C: both hosts deliver a similar reversible capacity of ~140 mAh $g^{-1}$, but with markedly different voltage profiles reflecting their distinct (de)insertion chemistries. The contrast becomes much more striking upon repeated cycling (Figure 1c). KMnHCF retains 96% of its initial capacity after 80 cycles in the K-free Na electrolyte (K-0), and an essentially identical 96% retention is reached with 10 mol% added $KPF_6$ (K-10). NaMnHCF in the same K-0 electrolyte fades to only 48% over the same window. This significant improvement in cycle life of KMnHCF pinpoints cation-selective $K^+$ (de)insertion within the host as the dominant factor governing the long-cycle stability of PBA cathodes.

To probe the origin of this selectivity, d*Q*/d*V* analysis of the discharge profiles of KMnHCF was performed as a function of the K/Na ratio (Figure 1b). With increasing $K^+$ content from K-1 to K-10, the peak attributed to $K^+$ insertion progressively grows while the $Na^+$ response is suppressed, consistent with the thermodynamic preference of PBAs for $K^+$ (de)insertion when $K^+$ is available.[2] Under high-rate discharge, however, the $Na^+$ plateau partially reappears, suggesting that fast operation kinetically forces $Na^+$ insertion. Nevertheless, *operando* synchrotron X-ray diffraction reveals no clear phase separation, indicating that this minor $Na^+$ insertion does not trigger structural transformation of the KMnHCF framework, which is consistent with the observed long-cycle stability in K-0 electrolyte. The detailed (de)intercalation mechanism and a demonstration of the Na–K hybrid full cell will be presented.

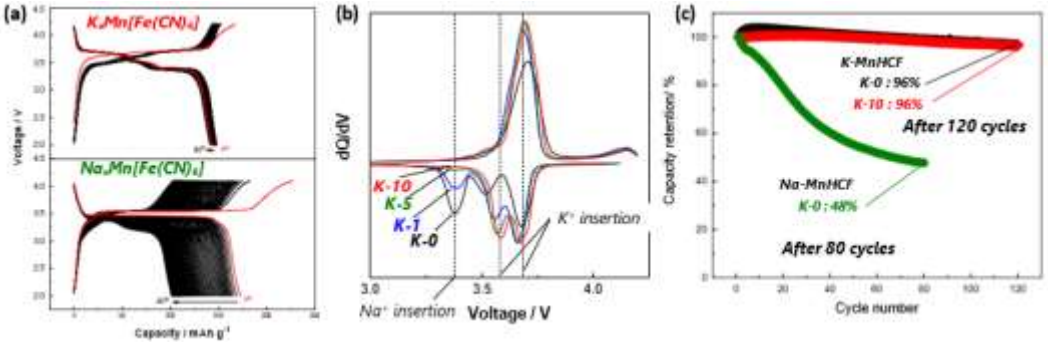



Figure 1. (a) Initial charge–discharge curves of $K_xMn[Fe(CN)_6]$ (KMnHCF, top) and $Na_xMn[Fe(CN)_6]$ (NaMnHCF, bottom) at 0.1 C in K-0 electrolyte. (b) d*Q*/d*V* plots of the (dis)charge profiles of KMnHCF in K-1, K-5, and K-10 electrolytes. (c) Cycle performance of KMnHCF in both K-0 and K-10 electrolytes, and NaMnHCF in K-0.

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# Anode Supported Solid Oxide Fuel Cells with Enhanced Mechanical Strength and Thermal Cycle Stability

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Ensuring long-term stable and continuous operation is a major challenge for the commercial application of solid oxide fuel cells (SOFCs). In this study, we report a method that effectively improves the mechanical strength and durability of NiO-YSZ anode-supported SOFCs without compromising their electrochemical performance. Finger-like porous NiO-YSZ anode green tapes were prepared by phase-inversion tape casting and sintered at 1400 °C for 5 hours. The as-prepared NiO-YSZ support exhibited a mechanical strength of only 17.80 MPa. To enhance its mechanical strength, the green tapes were infiltrated with paraffin wax, subjected to warm isostatic pressing (3000 psi, 80 °C), and then sintered at 1400 °C for 5 hours. The resulting support showed a substantially higher mechanical strength of 29.17 MPa. As shown in Figure 1, a cell incorporating the anode with improved mechanical strength demonstrated much better durability. At 700 °C in humidified hydrogen (3 vol.% $H_2O$), the cell delivered a current density of 0.776 A $cm^{-2}$ at a constant voltage of 0.7 V. After 10 thermal cycles between 700 and 400 °C at a heating/cooling rate of 10 °C $min^{-1}$, the current density decreased slightly to 0.753 A $cm^{-2}$, a reduction of 3%. In contrast, a cell with the lower strength anode showed a significant drop in current density from 0.833 to 0.628 A $cm^{-2}$, a decrease of 25%.

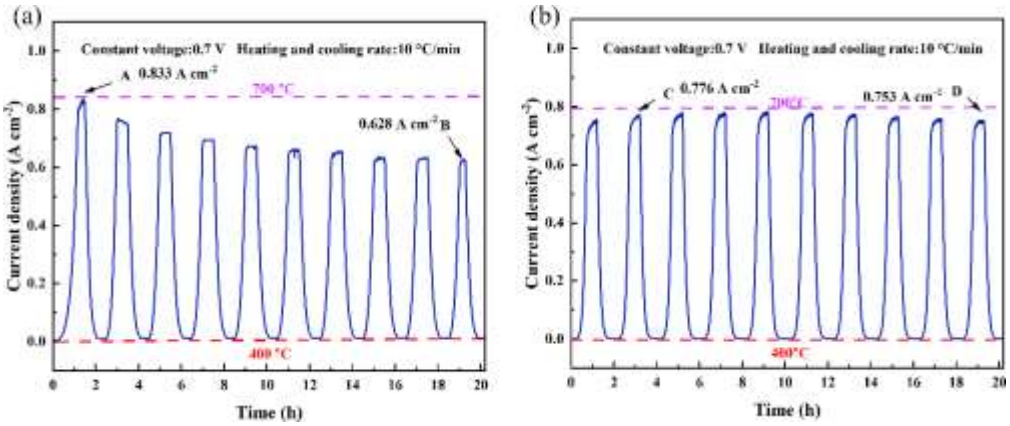



Figure 1. Effect of thermal cycling on the current density of SOFCs supported on NiO-YSZ anodes with (a) lower mechanical strength and (b) improved mechanical strength..

# Operando Studies on $Li^+$ Inventory Loss Mechanisms in High-Energy-Density NMC Cells

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The comprehensive understanding of interface formation and evolution remains one of the most important challenges for rapid battery innovation, as these interfaces play a pivotal role on both performance and safety [1]. The gas evolution signature of interfacial processes can be highly informative, and operando gas analysis techniques have become an essential tool for accelerating battery innovation [2-6]. Electrochemical mass spectrometry (EMS) can provide quantitative information of individual processes occurring in the cell, as well as their interconnectivity (e.g., cathode-anode crosstalk and anode slippage) with high sensitivity and resolution, as it can be seen in the figure [1].
Here we present online electrochemical mass spectrometry (OEMS) studies of systems with both high-nickel cathode materials and high-voltage anode materials that show the nature, onset, extent and interconnectivity of parasitic reactions leading to cell aging using very short test protocols. Our results indicate the need for better understanding these processes in order to accurately target solutions such as electrolyte formulations, coatings, etc., to accelerate materials innovation in batteries.

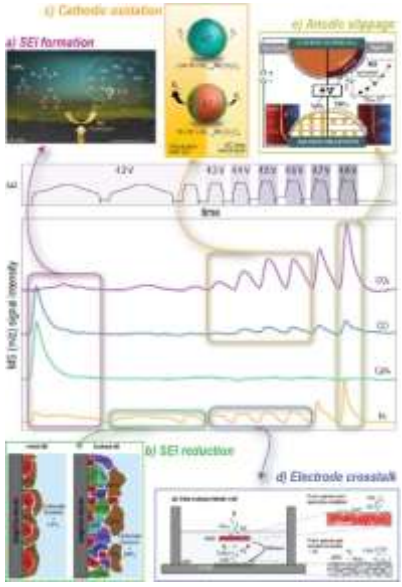



Figure 2. Operando gas analysis data (OEMS) showing voltage profile (top) alongside typical gas evolution profiles (for $H_2$, $C_2H_4$, CO and $CO_2$) of electrochemical processes contributing to the formation/evolution of interfaces in lithium-ion batteries.

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# Sustainable Production of Nanostructured Activated Carbon from Coconut Shell Waste for Water Treatment

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The increasing generation of agricultural bio-waste and the growing demand for sustainable water treatment technologies have encouraged the development of low-cost and eco-friendly adsorbent materials. This study focuses on the production of nanoparticle-based activated carbon from coconut shells for water purification applications. Activated carbon was synthesized through chemical activation using phosphoric acid ($H_3PO_4$), while silver nanoparticles (AgNPs) were prepared via a green synthesis method using neem (Azadirachta indica) leaf extract. The synthesized AgNPs were subsequently immobilized onto the activated carbon surface through a wet-impregnation technique to enhance adsorption efficiency, antimicrobial activity, and surface morphology. The prepared AgNPs–AC composite was characterized using Fourier Transform Infrared Spectroscopy (FTIR), Ultra-Violet Visible Spectroscopy (UV–Vis), Scanning Electron Microscopy (SEM), and CHNS elemental analysis. Results confirmed the successful synthesis and deposition of silver nanoparticles onto the activated carbon surface. Proximate analysis revealed a high fixed carbon content of 74.89% and low moisture content of 3.16%, indicating good adsorptive properties. Performance evaluation using synthetic wastewater demonstrated significant reductions in turbidity, conductivity, salt concentration, and color intensity with increasing contact time and agitation speed. The composite also showed enhanced adsorption capacity and improved antibacterial potential due to the presence of AgNPs. This research highlights the potential of utilizing coconut shell bio-waste for the development of sustainable and cost-effective nanocomposite adsorbents. The produced AgNPs–AC material offers promising applications in wastewater treatment, dye removal, and antimicrobial purification processes while supporting waste-to-wealth and environmentally sustainable approaches.

**Keywords:** Coconut shell waste, Activated carbon, Silver nanoparticles, Neem extract, Nanocomposite adsorbent, Wastewater treatment, Antimicrobial activity, Bio-waste utilization.

# "Single" Electrode Electrochemiluminescence

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Electrochemiluminescence (ECL) is luminescence as a result of electrochemical reactions. Traditional ECL devices have at least two electrodes, including anode and cathode [1-3]. Bipolar ECL devices have two driving electrodes and at least one bipolar electrode. For multiplex ECL experiments, electrode array is necessary in both traditional ECL devices and bipolar ECL devices. However, it is difficult and costly to make electrode array with some materials. It is desiring to develop simpler ECL systems.

We present here our recent research progress in "single" electrode ECL systems, such as wireless ECL system, single electrode ECL based on resistance-induced potential difference (Figure 1), and self-powered ECL system as well as their applications (e.g. ECL multiplex analysis and corrosion imaging) [4-10].

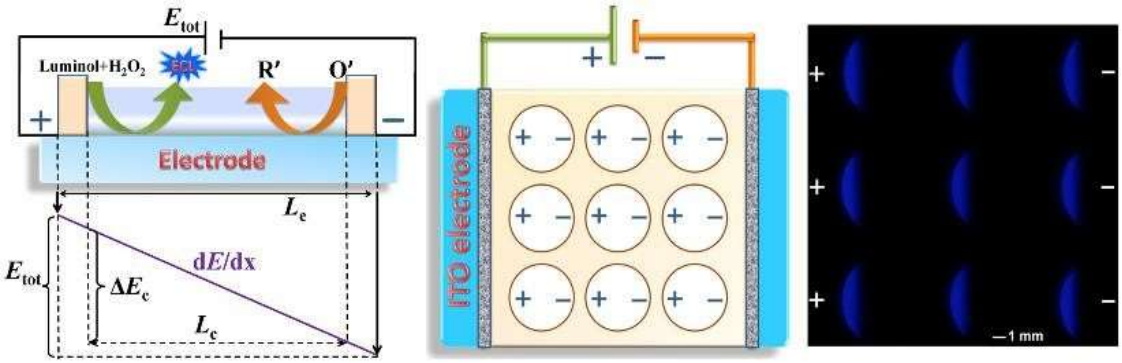



Figure 1. ECL mechanism, schematic diagram and image of single electrode ECL based on resistance-induced potential difference.

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# Thermal Management to Enhance Proton Exchange Membrane Fuel Cell Efficiency

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A Proton Exchange Membrane Fuel Cell System (PEMFCS) consists of fuel cell stack and a balance of plant (BOP). The former converts chemical energy into electricity and the latter supplies reactants and ensures expected reaction boundary conditions. Because PEMFC systems operate in highly dynamic environments (like heavy-duty vehicles), the BOP components consume a portion of the generated power (for example, to drive the air compressor and coolant pumps). Optimizing the BOP—through better component integration and advanced control algorithms—is a primary focus of improving total system efficiency, reducing cost, and extending stack lifetime.

PEMFCs could become a major energy solution for decarbonising vehicle transportation. Their advantages are, that they operate at relatively low temperatures, they are highly reliable and they have a quick startup response. They also have a high-power density and shorter refueling times compared to conventional electric battery systems. However, to increase their current efficiency remains a challenge so hindering large-scale commercial applications. Targets for the increase in efficiency are set at 68% by 2030 and 72% as the ultimate target by the American DOE.

In this presentation how to increase PEMFC efficiency will be discussed. Using advanced thermal management is one way to increase efficiency. Thermal management falls into two main categories, namely, develop more efficient cooling methods to keep within a suitable temperature range, and, secondly, recycle what would be otherwise wasted heat from the PEMFs so enhancing overall efficiency. About 30 ~ 50% of hydrogen chemical energy is converted into heat during the electro-chemical reaction process and a thermal management system is vital to guarantee the fuel cell is working properly especially under high current density conditions. There are various methods of cooling including, air cooling, liquid cooling and phase change.

For efficiency improvement by efficient cooling, the target of a stack thermal management system is to control the working temperature in a range with minimum temperature deviation and to minimize parasitic loss. Among all the cooling methods available, the liquid-cooling method is widely adopted in commercial PEMFCs. A typical liquid-cooling system used in PEMFC vehicles comprises a radiator, a reservoir, a cooling pump, an electric radiator fan and a bypass valve or electric three-way valve. There is also the method of phase-change cooling, with the advantage of no need for a cooling pump. This has disadvantages however, e.g., cost, space and weight. For the optimum control of the PEMFC temperature, the optimal operating temperature is largely dictated by the mitigation of electrode "flooding", PEM hydration and material degradation. Under low-temperature conditions, water vapor condenses into liquid water, which can accumulate within the porous structure and impede the diffusion of reactants to the catalytic sites, thereby increasing the transport resistance and leading to the concentration polarization of the electrodes. Under high operation temperature, though the fuel cell reversible voltage will decrease theoretically, the measured FC efficiency increases due to the enhanced electrode kinetics for the electrochemical reaction, increased membrane proton conductivity, and improved mass transfer of the reactants. There are various approaches to achieve a proper working temperature of PEMFCs by a cooling system integrated with the controller, including Linear Quadratic Integral (LQI) controllers, adaptive Linear Quadratic Regulator (LQR) controllers, fuzzy logic controllers optimized by genetic algorithms, and fuzzy PID control strategies.

Also needed is a reduction of parasitic power by optimal control. Different cooling system control strategies are varied according to the working load level. For low current density output, a pump working with state feedback control and a fan working under PI control show the lowest parasitic power. For high-load conditions, constant speed control performs better. An excellent temperature controller integrated into TMS has been recognised to satisfy these attributes as follows: optimal tracking of the set-point temperature, minimising parasitic losses and simplifying algorithm implements by a favourable hardware platform. Waste heat recovery also improves efficiency where waste heat from fuel cells can be reclaimed directly through heat utilization and indirectly through thermal cycles and thermoelectric conversion.

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# Radiation Defects and Functional Optical Materials for Extreme Radiation Environments

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The development of fusion energy systems, advanced nuclear reactors, high-energy particle accelerators, and space technologies requires functional optical materials capable of maintaining their performance under extreme irradiation conditions. Radiation-induced point defects govern the optical, luminescent, dielectric, and mechanical properties of these materials and therefore determine their operational lifetime. Understanding the formation, evolution, and thermal stability of radiation defects remains one of the central challenges of modern materials science.

This invited lecture presents an overview of recent progress in the physics of radiation defects in insulating and optical materials, with emphasis on oxides, fluorides, perovskites, diamond, and scintillation crystals. The discussion covers the current understanding of primary defect formation processes under neutron, electron, proton, gamma-ray, and heavy-ion irradiation, as well as the mechanisms responsible for defect aggregation, recovery, and long-term radiation damage accumulation.

Recent advances in optical spectroscopy, synchrotron-based vacuum ultraviolet techniques, and first-principles modelling have significantly improved our ability to identify radiation-induced defects and quantify their migration parameters. These developments provide new insight into the relationship between microscopic defect processes and macroscopic functional properties, including optical transparency, luminescence efficiency, and radiation hardness.

The lecture will highlight how modern experimental and theoretical approaches enable predictive modelling of radiation damage and long-term material stability under reactor-relevant conditions. The presentation will also discuss major open questions in radiation defect physics and future directions toward the development of radiation-tolerant functional materials for sustainable energy technologies.

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# Present and Future: Turkish Accelerator and Radiation Laboratory

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The Turkish Accelerator and Radiation Laboratory (TARLA) is a user facility based on a superconducting linear accelerator designed to reach 40 MeV and 1.6 mA. TARLA will be equipped with two beamlines: one for bremsstrahlung, and the other for a free-electron laser.
Currently, the first accelerating section, providing 20 MeV acceleration, is completed, while the second, for 40 MeV, is under construction. At present, the utilization of the operational 20 MeV section for activation and other radiation physics experiments during a pause in the 40 MeV section's construction has begun. By activating samples and using the fast sample transfer system measurements of bremsstrahlung and decay properties of nuclei can be made. These measurements aim at measurements of half-lifes of a few short lived nuclei as demonstrator of the accelerator and sample transfer system capabilities. The aim of this research was to measure the energy transitions and half-lives of these isotopes as a test of the detector and transfer system capabilities. Following transfer the irradiated samples will be counted using two pairs of CLOVER and single-crystal HPGe detectors with BGO active Compton suppression. Both the use of CLOVER detectors and well as active Compton suppression with BGO is a first for Turkiye and mastering the know-how for its utilization is needed. The first part of this presentation will be devoted to the presentation of first set of results aiming a characterizing and testing capabilities of all TARLA component from accelerator to the detectors.
As the next step the construction of two beamlines is planed. Out of these two bremsstrahlung beamline is expected to be available first and start to serve Nuclear resonance fluorescence experiments as soon as available. Complementing the standard high-flux bremsstrahlung option we plan to develop and implement a polarized bremsstrahlung capability at TARLA. Such capability would expand our experimental potential. The conceptual design and technical considerations for generating and controlling photon polarization within the existing beamline infrastructure will be outlined. The current status of the accelerator, project plans and beam application schedule will also be presented. This presentation will detail the TARLA future plans.

**Keywords:** superconducting linac, bremsstrahlung, activation, gamma-ray spectroscopy

# Structure-Guided Understanding of Self-Trapped Hole Delocalization in Binary and Complex Halides

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Self-trapped holes (STHs), commonly known as Vk centers in halide crystals, represent one of the most important manifestations of small-polaron formation in ionic solids. Since their discovery in alkali halides, these defects have served as model systems for understanding charge localization, migration, and recombination processes in wide-band-gap materials. Renewed interest in $V_k$ centers has emerged with the rapid development of complex halide scintillators, storage phosphors, and halide perovskites, where radiation-induced hole states strongly influence energy-transfer and luminescence mechanisms.

In this invited lecture, we present a comprehensive overview of thermal delocalization processes of self-trapped holes in binary and complex halides. Experimental results obtained by optical spectroscopy, electron paramagnetic resonance, and thermally stimulated luminescence are analyzed together with literature data covering alkali halides, alkaline-earth fluorides, fluoroperovskites, iodide scintillators, storage phosphors, and related compounds.

A central result is the identification of a systematic relationship between the thermal stability of $V_k$ centers and crystal structure. Across a broad range of materials, the onset temperature of hole delocalization exhibits a strong correlation with the nearest halogen–halogen separation, providing a simple structural descriptor for self-trapped-hole stability. This trend is shown to hold not only for classical alkali halides but also for fluorite-type crystals, fluoroperovskites, rutile-type halides, layered iodides, and several recently investigated materials, including $ScF_3$.

The proposed structure–property framework offers a unified interpretation of previously scattered experimental observations and enables prediction of $V_k$-center stability and migration characteristics in unexplored halide compounds. These findings contribute to a deeper understanding of carrier transport in ionic solids and provide practical guidelines for the design of advanced scintillation and radiation-resistant materials.

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# Digital Twin-Guided Microstructure Design of Battery Electrodes and Separators

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The performance and durability of rechargeable batteries are governed not only by the intrinsic properties of active materials, electrolytes, and separators, but also by their complex microstructures formed during processing and operation. In high-energy-density battery systems, such as thick electrodes, highly calendered electrodes, dry-processed electrodes, and solid-state battery architectures, local heterogeneity in pore networks, conductive pathways, interfacial contact, and mechanical deformation becomes a decisive factor controlling ion/electron transport, reaction uniformity, rate capability, and degradation behavior. Therefore, a quantitative framework that connects material properties, processing conditions, microstructure evolution, and electrochemical performance is essential for rational battery design.

In this invited talk, I will present our recent efforts to develop digital twin-guided microstructure design strategies for battery electrodes and separators. By combining advanced structural characterization with three-dimensional, microstructure-resolved simulations, digital twin models allow direct quantification of key descriptors such as porosity, tortuosity, pore connectivity, particle coordination, carbon–binder domain distribution, interfacial contact area, and effective ionic/electronic conductivity. These descriptors are correlated with electrochemical polarization, local reaction heterogeneity, power capability, and mechanical stability, providing mechanistic insights that are difficult to obtain from conventional cell-level measurements alone.

Representative examples will include virtual calendering of composite electrodes, microstructure optimization of dry-processed high-energy cathodes, stochastic digital twin modeling of porous separators, and microstructure-resolved analysis of solid-state battery components. These studies demonstrate how digital twins can identify transport bottlenecks, predict process–structure–property relationships, and guide the design of electrode and separator architectures with improved energy density, rate performance, and durability.

Overall, digital twin battery modeling provides a predictive and physically grounded platform for accelerating the development of next-generation rechargeable batteries. By bridging materials innovation, processing science, and microstructure-level simulation, this approach offers a versatile design strategy for advanced lithium-ion and all-solid-state battery systems.

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# Beyond the Cathode: Engineering Next-Generation Circularity for Graphite and Solid-State Batteries

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As the global electric vehicle (EV) fleet expands, the influx of end-of-life lithium-ion batteries (EoL-LIBs) presents both an unprecedented waste management crisis and a critical supply chain opportunity. Historically, industrial recycling has been optimized almost exclusively for the extraction of high-value cathode transition metals (e.g., cobalt and nickel) via pyrometallurgical smelting and hydrometallurgical leaching. This cathode-centric approach routinely sacrifices graphite, which constitutes up to 15% of the cell's cost and 10% of its total mass, while remaining structurally incapable of safely processing next-generation energy storage technologies. This presentation outlines a comprehensive engineering blueprint to move beyond the cathode, focusing on graphite reclamation and the systemic architectural shifts required for All-Solid-State Batteries (ASSBs). First, we address the imperative of anode circularity. Relying on simple physical separation (e.g., froth flotation) for graphite recovery yields heavily contaminated concentrates (roughly 82% purity) that induce catastrophic lithium plating if reused. We evaluate three advanced regeneration pathways: direct solvent washing, hybrid chemical-thermal treatments utilizing optimized sulfuric acid leaching, and ultra-high-heat regraphitization. We demonstrate that thermal curing at 3000 °C effectively fuses fractured microcrystalline boundaries and eliminates lattice distortions, restoring the graphitization degree to match virgin synthetic materials. Second, we confront the fundamental architectural transition brought by ASSBs. The replacement of porous polymer separators and liquid electrolytes with dense, co-sintered solid electrolytes (SEs) fundamentally breaks current mechanical shredding infrastructures. We categorize the unique failure modes of ASSBs into three vectors: the explosive reactivity of metallic lithium anodes, the extreme hardness of oxide ceramics (e.g., LLZO) that destroy mechanical shredders, and the lethal generation of hydrogen sulfide ($H_2S$) gas from sulfide-based SEs upon moisture exposure.

To solve this, we propose a transition to a data-driven, polymorphic recycling infrastructure, conceptualized as the Multi-Stream Gigafactory Topology (Figure 1). Attempting to process diverse solid-state and liquid chemistries through a single industrial shredder results in irreversible cross-contamination and severe safety risks. Instead, the proposed topology utilizes a "diverge-then-converge" architecture. At the frontend, a Digital Gatekeeper utilizes Battery Passports and RFID/QR scanners to instantly identify cell chemistry, triggering automated gates that divert packs into specialized demanufacturing tracks. Traditional liquid cells enter a standard shredding line, while sticky polymer matrices are routed to a wet dissolution line for solvent depolymerization. Crucially, sulfide-based ASSBs are directed to an anhydrous inert line, utilizing dry crushing under an argon atmosphere to completely prevent toxic $H_2S$ gas release. As depicted in the schematic, these divergent frontends safely isolate the raw active materials before funneling them into a single, unified hydrometallurgical backend. This shared convergence minimizes capital expenditure while allowing for the chemical "upcycling" of obsolete feedstocks into modern, high-nickel precursor salts. Ultimately, achieving true circularity requires treating the entire cell as a recoverable asset. By integrating anode regraphitization with smart, multi-stream solid-state processing, the recycling industry can safely adapt to the evolving battery landscape while safeguarding critical mineral supply chains.

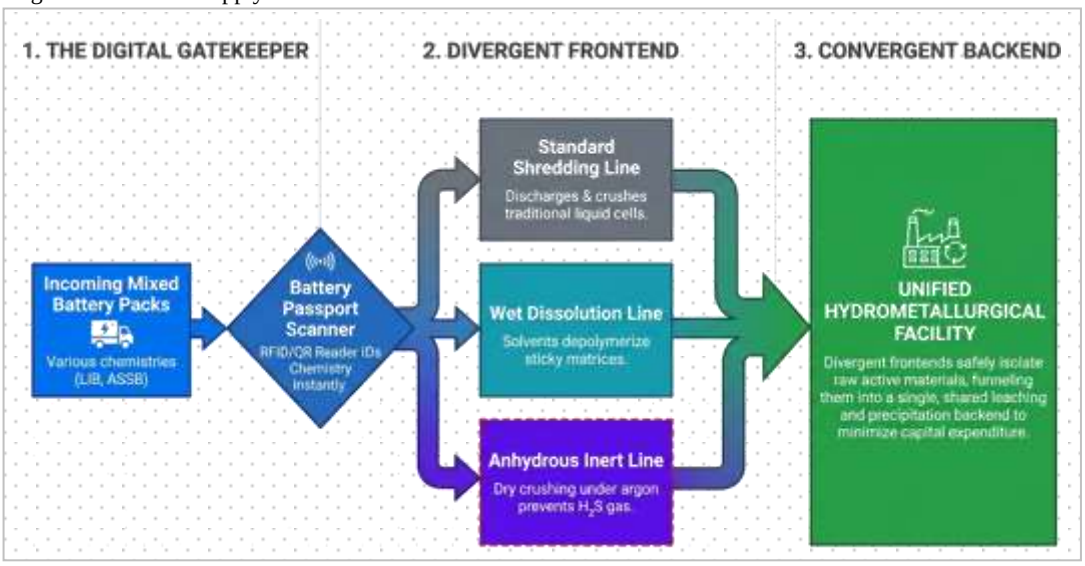



Figure 1. Schematic of the "Diverge-then-Converge" multi-stream Gigafactory topology. (1) The Digital Gatekeeper utilizes battery passports for instantaneous chemistry identification and sorting. (2) The Divergent Frontend routes incoming packs to specialized processing tracks, Standard Shredding, Wet Dissolution, or an Anhydrous Inert Line, to safely mitigate chemistry-specific hazards. (3) The Convergent Backend funnels the isolated raw active materials into a single unified hydrometallurgical facility, minimizing overall capital expenditure.

# Beyond Materials: Scalable Thick Electrode Engineering for Cell-Level Energy Density

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A major roadblock to achieving practical cell-level energy density lies not only in discovering new active materials, but in engineering scalable electrode architectures that can sustain transport, mechanical integrity, and redox uniformity at extreme mass loadings. Thick electrodes increase the active-material fraction in full cells, yet conventional slurry-cast and dry-processed electrodes suffer from drying-induced heterogeneity, conductive-carbon/binder migration, particle aggregation, cracking, cracking, delamination, tortuous transport pathways, and through-thickness redox heterogeneity. In this talk, I present a process-integrated framework for scalable thick-electrode engineering, where slurry and powder chemistry are deliberately designed to control electrode architecture during manufacturing. Electrostatic slurry engineering uses charged binder networks to generate osmotic pressure, enhance particle diffusion, and suppress drying-induced segregation. Capillary-bridged slurry engineering introduces a trace immiscible solvent that forms interparticle liquid bridges, stabilizing percolated particle networks and enabling uniform cathodes with areal capacities approaching 27 mAh $cm^{-2}$. In parallel, amphiphilic binder design for dry electrodes resolves conductive-additive agglomeration and poor powder flowability, overcoming key limitations of PTFE-based processing. These results show that high-energy batteries require more than better materials: they require manufacturable electrode architectures that preserve transport, mechanics, and redox uniformity from slurry or powder to full-cell operation.

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# Sodium Metal Batteries: Positive, Negative, and Counter Electrodes

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Sodium secondary batteries have gained attention due to the abundant sodium resources and cost-effectiveness in constructing large-scale energy storage systems, which are increasingly crucial for renewable energy resources.[1,2] Sodium metal has shown impressive potential as a negative electrode material for high energy density sodium metal batteries on the grounds of its high specific capacity (1166 mAh $g^{-1}$ based on the weight in the charged state) and low potential (–2.71 V vs. SHE).[3] In this work, recent progress of sodium metal batteries in our group will be presented from the viewpoints of positive, negative, and counter electrodes.

Heterosite $FePO_4$ prepared by chemical desodiation of $LiFePO_4$ by $O_2$ serves as an efficient positive electrode in charged-state sodium metal batteries.[4] The use of thermally stable ionic liquid electrolytes [5] further bring out the potential of this positive electrode, providing the distinct plateau potentials during charge and discharge processes.

While high sodium metal plating-stripping efficiency has been reported in ether-based electrolytes, we usually use sodium metal counter electrodes with different electrolytes in half-cell tests. Our detailed investigation revealed that polarization of Na metal electrode significantly varies depending on the electrolytes, and thus the half-cell tests using the sodium metal counter electrode are not trustable enough to assess the target electrode. Instead, we propose the NASICON-type electrode materials as a counter electrode as they give flat potential profile with small polarization.[6].

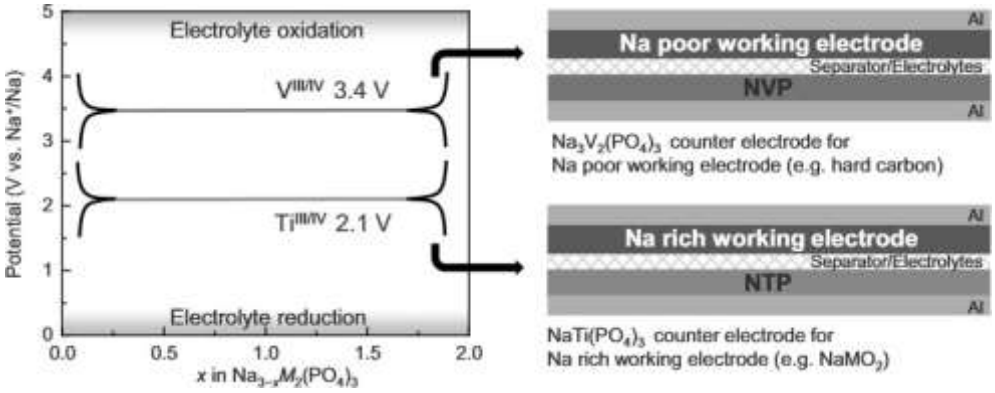



Figure 1. Concept of half-cell tests with NASICON counter electrodes.[6]

**Acknowledgements**

We thank Profs. Ko and Yamada of University of Tokyo for the discussion on the Na metal counter electrode. This study was supported by the Japan Science and Technology Agency (JST, GteX Grant number JPMJGX23S4).

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# Sustainable Nanomaterials from Combustion and Biomass Valorization

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Carbon-based nanomaterials continue to play a central role in advanced engineering systems due to their tunable surface chemistry, hierarchical porosity, chemical stability, and scalability of synthesis. This plenary presentation highlights original research conducted at the Institute of Combustion Problems (Kazakhstan), demonstrating an integrated materials-engineering platform that combines combustion-driven nanocarbon formation with circular waste valorization strategies for sustainable functional materials.

A key research direction focuses on biomass conversion into activated porous carbon sorbents for chemical protection and environmental remediation. Activated carbon derived from walnut shell exhibits a highly developed micro–mesoporous architecture, confirmed by low-temperature nitrogen adsorption and high specific surface area values. Controlled surface functionalization via Cu and Co ion impregnation significantly improves adsorption performance and breakthrough time toward both inorganic and organic toxic vapors. This approach demonstrates a scalable route for transforming agricultural waste into high-performance CBRN protective materials.

In parallel, sustainable fiber-based composites were developed for eco-friendly packaging applications. Grass-derived cellulose blended with recycled paper and mineral fillers was engineered to enhance mechanical integrity. While additive-free formulations showed weak inter-fiber bonding and limited strength, the incorporation of 2 wt.% functional additives (rosin glue, polyacrylamide, aluminum sulfate) substantially improved structural cohesion. The optimized composition (40% cellulose / 40% recycled cardboard / 20% wollastonite) achieved 91 double folds and a bursting strength of 903 kPa, demonstrating the feasibility of high-performance bio-based packaging materials derived from local renewable resources.

Another direction involves the synthesis of nanostructured hydroxyapatite (HAp) from eggshell waste via aqueous precipitation. The resulting HAp reached >95% purity, while thermal treatment at 1100 °C enhanced crystallinity and reduced particle size to ~200 nm. Electrospun polymer/HAp nanofibrous films were fabricated as biodegradable scaffolds for tissue engineering and controlled drug delivery. Importantly, HAp incorporation did not alter antibiotic release kinetics, confirming structural compatibility within polymer matrices.

Fundamental combustion studies were conducted to elucidate soot formation mechanisms in hydrocarbon-rich flames. The results reveal strong pressure dependence of soot evolution: low pressure suppresses collision-driven coagulation, while atmospheric pressure promotes nucleation, aggregation, and growth into carbon black-type clusters. A mechanistic pathway is proposed in which PAH and PCAH species serve as molecular precursors governing soot inception and nanocarbon growth.

Overall, the presented work demonstrates a multidisciplinary engineering strategy that bridges combustion science, nanomaterials design, and circular waste valorization. The developed materials – porous carbons, bio-based composites, and nano-hydroxyapatite systems – illustrate scalable pathways toward sustainable, high-performance solutions for environmental protection, packaging technologies, and biomedical applications.

# Defect Engineering Strategy of Non-Noble Metals for Enhancing Oxygen Evolution Reaction Performance

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**Abstract:**To address the intrinsic drawbacks of layered double hydroxides (LDHs) in terms of activity, stability, and electrical conductivity for the oxygen evolution reaction (OER), we propose an electrochemical-assisted strategy to quantitatively engineer defects in NiFeCo-LDH. By leveraging a coordination reaction between $Fe^{3+}$ and $SCN^-$ under an applied potential, we achieve selective and controllable iron extraction, which induces the formation of both oxygen and metal vacancies in a targeted manner. The as-prepared catalyst shows a higher Ni oxidation state and significantly improved OER activity. The optimal sample (with Fe extraction for 60 s) exhibits a low overpotential of 254 mV at 100 mA/cm$^2$ and a Tafel slope of 48 mV/dec, while maintaining more than 90% of its initial activity after 400 h. In-situ Raman spectroscopy indicates that Fe extraction facilitates the phase transformation from Ni(II)-O/OH to Ni(III)-OOH and triggers the lattice oxygen mechanism (LOM), thereby boosting the reaction kinetics. Furthermore, the catalyst performs well under simulated industrial conditions and in seawater electrolytes, underscoring its promise for practical large-scale water electrolysis.

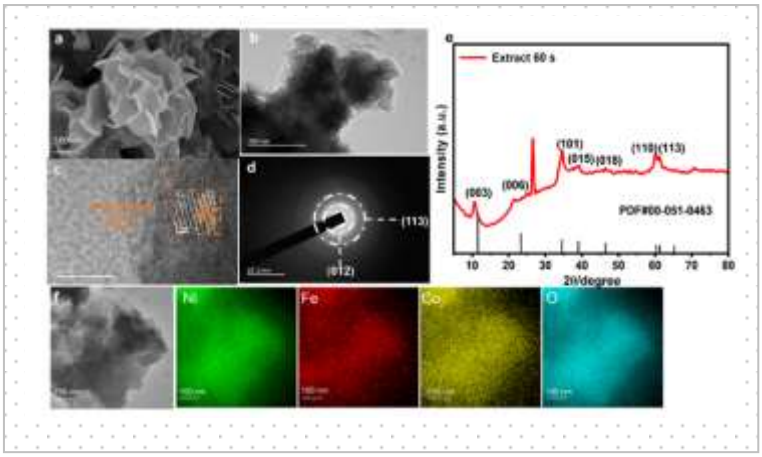



Figure 1. (a)SEM of Fe-extracted NiFeCo-LDH. (b, c)TEM of Fe-extracted NiFeCo-LDH. (d) SAED of Fe-extracted NiFeCo-LDH. (e) XRD of Fe-extracted NiFeCo-LDH (f) .mapping of Fe-extracted NiFeCo-LDH.

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# Electrochemiluminescence immunoarray sensor Coupled with Machine Learning for Diagnosis of Acute Myocardial Infarction

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Acute myocardial infarction (AMI) is a cardiovascular diseases characterized by myocardial necrosis resulting from acute and persistent obstruction of a coronary artery. AMI accounts for one third of overall cardiovascular diseases deaths, exceeding the mortality of any single tumor. It shows an increasing trend year by year[1-2]. Cardiac troponin T is the gold standard for diagnosis of AMI, but has insufficient specificity at early times[3-4]. Here we report a new three-biomarker joint strategy for early and accurate diagnosis of AMI via an electrochemiluminescence (ECL) immunoarray coupled with robust machine learning. Three biomarkers, including cardiac troponin I, heart type fatty acid binding protein, and copeptin, could be simultaneously detected by the ECL immunoarray, which combined an ECL immuno-gold nanoassembly with a simple, multiplexed, single-electrode detection platform. The determination of >200 clinical serum samples was carried out. A three-biomarker joint assessment model was established via quadratic discriminants analysis to completely discriminate AMI from non-AMI patients across a broad patient population all admitted to the hospital with chest pain, achieving 100% specificity and sensitivity, including those within three hours of symptom onset. The model is independent of patient age, biological sex, and blood collection time, and outperforms traditional cardiac troponin testing, particularly at early time points. The proposed three-biomarker joint strategy provides an efficient tool for early and accurate diagnosis of AMI, hopefully reducing AMI mortality as well as saving limited medical resources[5].

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# ITP-RED: Reverse Electrodialysis as an Inverse Thermodynamic Probe – Thermodynamic Identifiability Limits and Activity-Coefficient Inference in Hypersaline Brines

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Electrochemical voltages encode ionic activities rather than concentrations, yet conventional forward modeling struggles to resolve individual activity coefficients when both electrolyte and membrane phases exhibit strong non-ideality. We demonstrate that open-circuit voltage measurements inherently constrain only an effective non-ideality factor ($\Gamma$) that integrates bulk-solution, membrane, and interfacial contributions, establishing a fundamental structural identifiability limit arising from the logarithmic form of the electrochemical potential.

Building on this theoretical foundation, we introduce Inverse Thermodynamic Probing by Reverse Electrodialysis (ITP-RED), a novel inverse electrochemical framework that treats reverse electrodialysis (RED) stacks as thermodynamic transducers. Deviations of the RED open-circuit voltage from the ideal Nernst baseline ($\Delta E_\gamma$) directly map onto the ratio of mean ionic activity coefficients between concentrated and dilute streams. By reframing RED observables as constraints on a reduced thermodynamic descriptor vector (effective divalent fraction $\phi_{div}$ and interaction-scaling parameter $\lambda_{int}$) within a Pitzer-consistent excess-Gibbs-energy formulation, stable inverse inference is achieved without full multi-ion speciation.

A proof-of-concept application of ITP-RED to hypersaline Aral Sea brine ($I \approx 5.13$ mol kg$^{-1}$) demonstrates that RED-derived electrochemical constraints accurately reproduce the observed activity-coefficient contrast with high numerical stability under realistic voltage uncertainty (±1–2 mV). Despite large seasonal variations in composition and total salt load, the effective NaCl-equivalent thermodynamic activity of such brines remains narrowly constrained between 1.00–1.11 mol kg$^{-1}$, substantially lower than concentration-only estimates would suggest.

These results establish ITP-RED as a practical electrochemical probe for non-ideal electrolyte thermodynamics. The approach opens a pathway for real-time, activity-based sensing and diagnostics in hypersaline brine management, desalination concentrate valorization, and geochemical monitoring of complex multi-ionic.

# Effects of Electronic Spin Excitations in Electrochemical Reactions on Transition-Metal-Based Catalysts

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Electronic state of a catalyst directly affects its activity. This is well known and widely exploited in photocatalysis. In thermal heterogeneous catalysis one typically considers only the ground-state Born-Oppenheimer potential-energy surface (PES). In many cases this is a good approximation, because thermal energy is usually much lower than the energy of any electronically exited state. However, this is only true if the chemical reaction on the ground-state PES is not inhibited by symmetry constraints. One of such constraints, the spin conservation, is in fact ubiquitous. In many practically important heterogeneous catalytic systems, the coupling between electronic states of different multiplicity (spin-orbit coupling) is weak. As a result, the total multiplicity of reactants and the catalyst is preserved throughout the reaction. This can have a strong effect on catalytic activity, since the reaction proceeds on an excited-state PES instead of the ground-state one. However, in theoretical electrochemistry the effects of spin are rarely properly considered [1], mainly due to the difficulty of taking them into account using the standard computational tools.

In this work, we present a comprehensive investigation of the spin-resolved oxygen evolution reaction (OER) mechanism on Ni oxyhydroxide surfaces. OER is the kinetically hindered half-reaction of the overall water electrolysis, which can be used to produce “green” hydrogen (with zero carbon footprint), if the electricity required for this process is obtained from renewable sources, such as solar radiation. Ni (oxy)hydroxides are the active phase of Ni-based non-noble-metal catalysts. We study the influence of the spin conservation rule on the OER pathway for a nickel oxyhydroxide surface, modeled using DFT with the HSE06 hybrid functional. We construct carefully converged embedded cluster models that allow for an accurate atomic relaxation of the active site region in different spin states, and incorporate solvation effects via an implicit solvation model to systematically examine how the spin multiplicity of the active site evolves throughout the OER cycle. Based on the obtained reaction barriers, we model kinetics of OER using kinetic Monte Carlo approach. We find that taking into account spin excitations of Ni near the active site during the reaction significantly reduces the OER overpotential calculated by DFT, bringing it close to experimental value. However, the low-overpotential pathway can only be reached due to coupling between different spin states.

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# Scale-up and Data-driven Materials Development of FFJ REBCO Coated Conductors for Future Energy Applications

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High temperature superconducting (HTS) materials are expected to play a central role in future technologies, including health care, transportation, electric energy transmission, and energy generation including compact fusion power systems. In particular, second-generation high-temperature superconducting tapes (2G-HTS) based on REBCO compounds represent an emerging platform for carrying very high electrical current with zero electrical resistance under cryogenic conditions. Their practical development involves fundamental materials-science challenges due to multicomponent oxide chemistry, defect engineering, texture control, oxygen stoichiometry, scalable thin-film processing, and reliable structure–property optimization.

Faraday Factory Japan (FFJ) has been developing a reel-to-reel manufacturing platform (see Figure 1) for 15 years and in 2025 reached an annual production capacity of 3,000 km/year of standard YBCO-based Hermes tape [1-3]. This scale of production has generated large datasets covering processing parameters, conductor real structure, and functional properties under different operating conditions. This accumulated knowledge is a basis for faster materials development and statistically meaningful evaluation of structure–process–property relationships for development of new conductors more efficiently than by isolated trial-and-error experiments. In this approach we are developing automated processing of production datasets for faster process control and accelerated optimization of conductors for fusion magnets, power cables, and aircraft motor technologies.

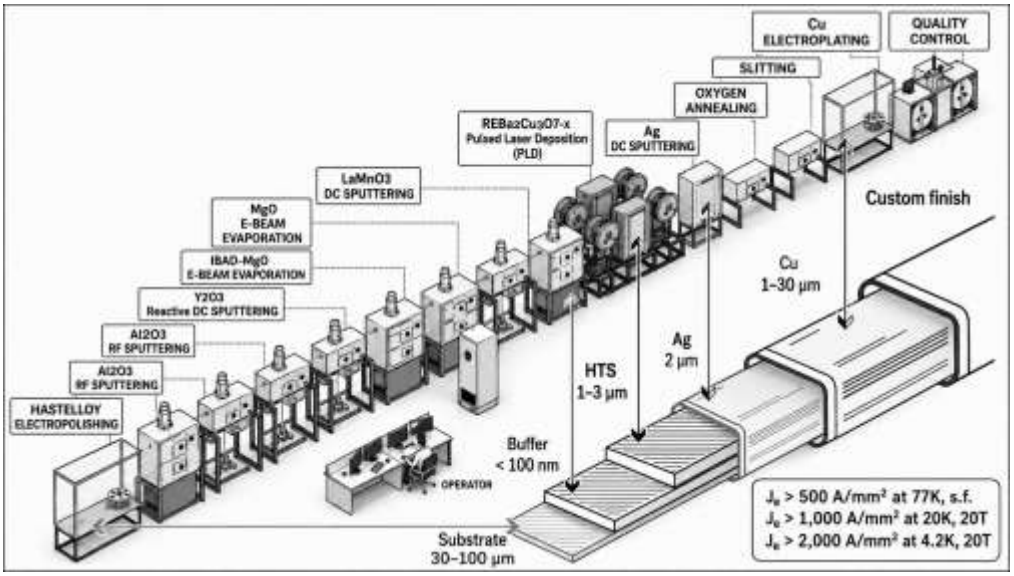



Figure 1. IBAD and Pulsed Laser Deposition based banufacturing of 2G-HTS tapes at FFJ .

In this presentation, we will summarize FFJ's current manufacturing profile and application-driven R&D strategy. For high-magnetic-field applications such as compact fusion magnets, we report the status of Mirai conductors with Ic(20 K, 20 T) ≈ 300 A/4 mm, corresponding to Je > 1,200 A/mm² under these conditions. For cable-oriented conductors, we describe progress on REBCO-based Electra tapes achieving Ic(77 K, self-field) ≈ 1,200 A/12 mm, or approximately 350 A/4 mm. In addition, we discuss recent work on filamentized conductors produced by laser scribing, with 10–15 filaments per 4 mm tape, aimed at reducing AC losses in alternating-current applications. We will also discuss selected R&D results related to buffer-layer engineering and REBCO film growth. To understand connection between processing conditions with functional performance, we applied advanced characterization methods including Cu-K and O-K XANES and Raman spectroscopy. These techniques help link local electronic structure, oxygen content, and lattice/defect states with in-field transport properties.

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# Why Good Technologies Fail to Commercialize: Structural Barriers Between Materials Innovation and Industrial Deployment

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Across the battery materials commercialization projects I have been directly involved in — spanning different regions and stages of maturity — one pattern recurs: technologies strong at the lab scale often stall at commercialization. The cause is rarely scientific immaturity; it is that the provider has not understood what the receiving cell manufacturer truly needs. Priorities vary by market, and lab-scale performance does not guarantee the speed, yield, and reproducibility mass production requires. These real concerns are rarely voiced in a single conversation — they emerge only through sustained dialogue and iterative verification. Having watched this repeatedly, I no longer see it as bad luck. It is structural.

This is not irrelevant to regions now building their position in the value chain. Whether the technology comes from outside or from domestic research, growing it into a business always raises the same question: can the organization understand what the receiving side truly needs?

The foundation for that is the habit of asking "why" — why a specification exists, why a process behaves as it does. Only an organization that digests these questions across functions can later, as a provider itself, understand the receiving side deeply and deliver value that is genuinely explainable. This habit is indispensable for anyone aiming at high-value, differentiated products.

At the same time, asking "why" alone does not turn a technology into a product. Value emerges only when combined with the ability to read where value concentrates and shifts across the chain — keeping a mental map of the world.

I close with a hope for regions building their place in this value chain: treat your technological foundation, wherever it comes from, not as a finished answer but as a starting point for asking your own "why." That is what determines whether what is built here endures at high value.

# Promising Energy and Therapeutic Perspectives of Green Nano-technology: Recent Advances and Challenges

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World population are struggling with numerous problems related to environmental issues such as pollution, availability of food, as well as the demand and supply of energy. The pollution caused due to the inappropriate management of natural resources is raising grave concerns towards environment safety and sustainability. Certain scientific fields including chemistry and nanotechnology play a fundamental role in the sustainability of environment by promoting green technologies. Recent advances in new and less toxic or nonhazardous materials for industries have been assisting in generating and promoting sources for renewable energy, which is crucial for environmental protection. Considering the demand of energy for all industries and the developmental processes, it is very much necessary to promote the production and consumption of sustainable / green energy. For achieving a green economy, it is necessary to find new ways of producing green energy by using nanosystems and nanoparticles. This entry will focus on the evaluation of the green nanochemistry for sustainable development and will highlight recent advances in the green technology by using nanotechnology-based systems and materials.

# Multi-Objective Energy Management Strategies for Fuel Cell Vehicles Integrating Driving Condition Recognition

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Under the comprehensive promotion of carbon neutrality strategies, the transportation sector is facing an urgent demand for deep low-carbon transformation. Proton exchange membrane fuel cell vehicles (FCVs), characterized by zero emissions and high energy efficiency, have emerged as a promising solution for sustainable transportation[1]. Due to the slow dynamic response and inability of fuel cells to recover braking energy, FCVs generally adopt a hybrid architecture combining fuel cells and batteries. The energy management strategy (EMS), which determines power allocation among multiple energy sources, plays a crucial role in vehicle performance, economy, and durability. However, existing EMSs still suffer from insufficient adaptability to complex driving conditions, inadequate integration of driving condition recognition with energy control, and difficulties in achieving coordinated optimization of multiple objectives [2].

To address these issues, this study proposes multi-objective energy management strategies for fuel cell vehicles integrating driving condition recognition. First, an indirect hybrid powertrain architecture consisting of a fuel cell and a power battery was established. Key system parameters were matched based on longitudinal vehicle dynamics, and a vehicle simulation model considering electrochemical characteristics, degradation mechanisms, and thermal behaviors of power sources was developed in MATLAB/Simulink. Subsequently, a driving cycle database covering multiple standard driving cycles was constructed. Principal component analysis (PCA) and K-means++ clustering were employed to classify driving conditions into four categories: urban congestion, urban free-flow, suburban, and highway conditions. A CNN-LSTM-based driving condition recognition model was then developed, achieving an identification accuracy of 95.31%.

Furthermore, a driving-condition-based multi-objective optimization EMS was proposed using the Non-dominated Sorting Genetic Algorithm III (NSGA-III) to optimize fuzzy controller parameters with objectives of minimizing equivalent hydrogen consumption and component degradation. Compared with the conventional fuzzy strategy, the proposed strategy reduced SOC-corrected equivalent hydrogen consumption by 8.99%, fuel cell degradation by 2.02%, and battery degradation by 22.24%. To further improve adaptability, a Twin Delayed Deep Deterministic Policy Gradient (TD3)-based deep reinforcement learning EMS incorporating driving condition information was developed. Results demonstrate that the proposed strategy achieves superior overall performance by effectively balancing economic efficiency, durability, and thermal safety.

Keywords: Fuel cell vehicle; Energy management strategy; Driving condition recognition; Multi-objective optimization; Deep reinforcement learning

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## ORAL PRESENTATIONS

# Surface Engineering of Current Collector for Stable High-Mass-Loading Cathodes in Aqueous Zn-$LiFePO_4$ Batteries

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High mass-loading cathodes are critical for the practical realization of large-format aqueous Zn/Li-ion batteries; however, weak adhesion between $LiFePO_4$ (LFP) electrodes and metallic current collectors[1] often causes cathode delamination, mechanical instability, and rapid performance degradation (**Figure 1a**). In this work, we address this challenge through surface engineering[2] of titanium (Ti) current collectors for aqueous Zn-LFP pouch cells.

Two scalable modification strategies were employed (**Figure 1b**): (i) magnetron sputtering of a thin chromium (Cr) interlayer to form a chemically stable passivating interface, and (ii) acid etching of Ti using 37% HCl at 80 °C to increase surface roughness and enhance mechanical interlocking with the electrode layer. Both modifications substantially improved slurry adhesion and enabled fabrication of stable high-loading LFP cathodes with areal mass loadings of ~10–12 mg $cm^{-2}$ without observable delamination.

Electrochemical evaluation further revealed enhanced cycling stability and reduced polarization in chloride-based electrolytes compared with sulfate-based systems. Acid-etched Ti collectors promoted faster charge-transfer kinetics, delivering an initial discharge capacity of 150.2 mAh $g^{-1}$ with 83.0% capacity retention and 99.1% Coulombic efficiency at 0.1 C. Meanwhile, Cr-coated Ti collectors provided effective surface passivation and stable interfacial chemistry, resulting in improved structural integrity, 83.6% capacity retention, and reliable rate capability up to 0.25 C. Overall, this study demonstrates that rational surface engineering of Ti current collectors represents a practical and scalable strategy for developing mechanically robust, high-loading aqueous Zn-LFP batteries.

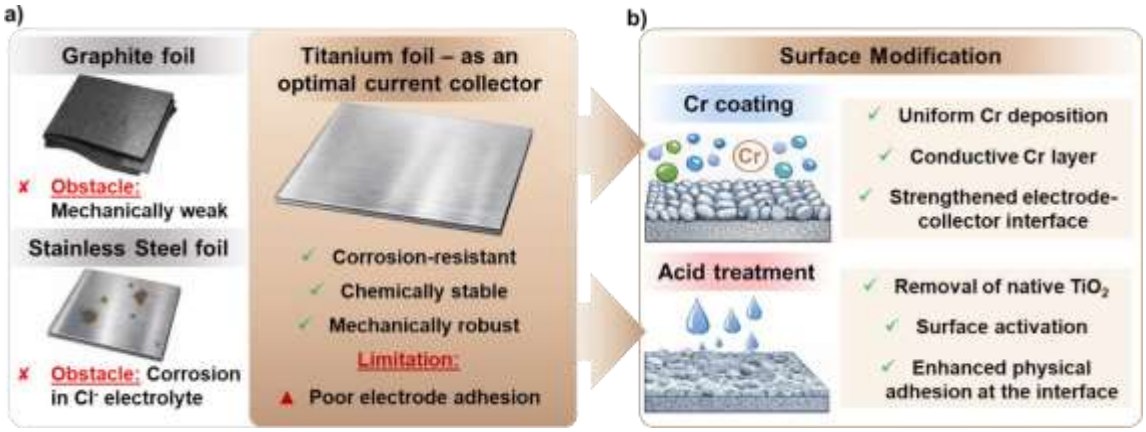



Figure 1. (a) Schematic comparison of candidate current collectors and (b) surface modification strategies for AZLIBs.

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# Recovery of Battery-Grade Nickel Sulfate from Chrysotile-Asbestos Waste

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This study investigated the recovery of nickel and cobalt concentrates from chrysotile-asbestos production waste using magnetic separation, followed by sulfuric acid leaching and transfer of valuable components into solution. A review of scientific literature and patent studies was conducted on methods for separating nickel and cobalt from mineral raw materials in Kazakhstan and abroad. Based on the analysis, the optimal magnetic separation process for chrysotile-asbestos waste was identified.

Wet magnetic separation was performed depending on slurry density to divide the material into magnetic and non-magnetic fractions.

A neodymium magnet of N35 grade with a magnetic induction of 1170–1220 mT was used as the magnetic separator. Prior to separation, the initial sample was crushed to a particle size of less than 0.1 mm. The resulting material was then subjected to wet magnetic separation. After separation, the obtained products were dried at 105 °C and analyzed using X-ray fluorescence analysis. A material balance was calculated for the distribution of nickel, cobalt, and iron between magnetic and non-magnetic fractions. Nickel recovery into the magnetic fraction of the “PShS” product was 70.27%, cobalt 10.85%, and iron 71.76%.

To study the size-dependent distribution of components, the initial sample was fractionated into different size classes: -1+0.5 mm, -0.5+0.25 mm, and -0.25 mm. All fractions were subjected to chemical and X-ray phase analyses. The mineralogical composition of the asbestos waste was investigated. The main mineral phase was serpentine – $3MgO \cdot 2SiO_2 \cdot 2H_2O$. The sample consisted of serpentinite containing crystalline and amorphous silica. Minor components (up to 5–6%) included oxides such as hematite and magnetite. It was found that nickel and cobalt contents in different size fractions did not differ significantly, indicating that all particle sizes are suitable for processing.

It was established that chrysotile-asbestos waste in loose form is effectively amenable to magnetic separation with relatively high recovery of nickel and cobalt into the magnetic fraction. Nickel content increased from 0.2% to 0.74%, and cobalt from 0.045% to 0.182%. The non-magnetic fraction was depleted in nickel and can be considered a magnesium-rich product. Therefore, only the magnetic fraction was subjected to leaching.

Sulfuric acid leaching of the magnetic fraction was optimized. The optimal conditions were: temperature 85 °C, leaching time 1.5 hours, solid-to-liquid ratio 1:3, and sulfuric acid concentration 250 g/L. Under these conditions, nickel extraction reached 74%, with a concentration of 1.4–1.5 g/L in the pregnant solution, suitable for sorption recovery.

Ion-exchange resins were studied for nickel sorption. Resin ISC-475 showed the highest performance, with a static exchange capacity of 60 kg/t and a dynamic exchange capacity of up to 70 kg/t. Nickel desorption using sulfuric acid solution achieved 99.4% recovery, producing a desorbate with a nickel concentration of 10.5 g/L.

Nickel precipitation was carried out using an ammonia solution under controlled pH (7.0–9.0), followed by filtration and drying. The final product contained 20.40% Ni with low impurity levels, corresponding to technical-grade nickel sulfate.

# Understanding Mn Dissolution from $LiMn_{0.8}Fe_{0.2}PO_4$ Cathode Through Optimization of Synthesis and Process Parameters

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$LiMn_xFe_{1-x}PO_4$ ($x \geq 0.5$) is an attractive positive electrode material due to its higher achievable energy density than $LiFePO_4$, enabled by the high-voltage $Mn^{2+/3+}$ redox couple at ~ 4.1 V vs $Li^+/Li$ [1]. However, $LiMnFePO_4$ with high Mn content suffers from transition metal (TM) dissolution, which is particularly severe at elevated temperatures [2]. In this study, $LiMn_{0.8}Fe_{0.2}PO_4$ (LMFP82) was selected to investigate the TM dissolution process using the micro X-ray fluorescence (μXRF) technique to quantify the TM deposited on the graphite negative electrode after high-temperature full-coin cell cycling. Two types of in-house LMFP82 materials, synthesized using surfactant and non-surfactant-based methods, were used to examine the impact of synthesis methods and carbon source on TM dissolution. Additionally, LMFP82 was coated with varying amounts of carbon in an attempt to suppress the TM dissolution. A series of LMFP materials with different Fe to Mn ratios was also synthesized to evaluate the effect of composition on the amount and rate of Mn deposition on the negative electrode. This work includes thorough physico-chemical and electrochemical characterization to reveal the relationship between carbon coating, chemical composition and the resulting electrochemical performance and TM dissolution data, thereby providing critical insights for the rational design of LMFP positive electrode materials.

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# Comprehensive Processing of Lead Cakes as a Source of Strategic Metals for Energy Systems, Superalloys, and Future Technologies

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The rapid development of high-tech industries has led to a steadily increasing demand for strategic and critical metals. Among these, rhenium, osmium, and lead play a crucial role in the production of aerospace and power-generation superalloys, energy storage systems, petrochemical catalysts, electronic components, precision instruments, and other advanced technological applications. According to international forecasts, the consumption of critical metals is expected to grow significantly over the coming decades due to the expansion of renewable energy, energy storage technologies, digital industries, and the aerospace sector.

Rhenium is one of the rarest elements in the Earth's crust and is considered an indispensable component of high-temperature nickel-based superalloys used in gas turbine blades and aircraft engines. The addition of rhenium significantly improves creep resistance, high-temperature strength, and long-term durability of structural materials operating under extreme conditions. Osmium, a member of the platinum group metals, possesses exceptional density, corrosion resistance, and wear resistance, making it valuable for electronics, specialized alloys, and precision engineering applications. Despite the emergence of new battery technologies, lead remains an essential component of lead-acid batteries widely used in transportation, energy infrastructure, and telecommunications systems.

Alongside the increasing demand for these metals, the utilization of technogenic waste as a secondary resource has become increasingly important. Large quantities of lead-bearing cakes, sludges, and other non-ferrous metallurgical wastes are accumulated in tailings storage facilities and waste dumps, representing both an environmental challenge and a potential source of valuable metals. Modern trends in the mining and metallurgical industry are focused on the transition toward a circular economy, emphasizing maximum resource utilization and the reintegration of valuable metals into industrial production cycles.

Lead cakes represent one of the most promising types of technogenic raw materials due to their high concentrations of lead and associated rare metals. The investigated material contains approximately 50 wt.% lead and up to 1000 g/t rhenium. Such concentrations make these wastes attractive not only from an environmental perspective but also as a strategic source of critical metals for advanced industrial applications.

In this study, a comprehensive processing technology for lead cakes was developed to enable the sequential recovery of osmium, rhenium, and lead. The first stage involves low-temperature roasting to remove organic matter and prepare the material for subsequent treatment. This is followed by oxidative roasting, during which osmium is transferred into the gas phase with an efficiency of up to 90%. Simultaneously, arsenic, mercury, and other volatile impurities are removed. The resulting gas stream undergoes selective purification for osmium recovery, followed by environmentally safe treatment of the remaining off-gases.

After osmium separation, the calcine is subjected to reduction smelting at approximately 1100°C. During smelting, lead is transferred into the metallic phase, producing crude lead containing up to 98% Pb, while rhenium is concentrated in the slag phase. Lead recovery exceeds 90%, whereas the transfer of rhenium into the slag reaches approximately 95%.

The resulting rhenium-bearing slag is subsequently processed using hydrometallurgical methods. The technological route includes water leaching, sorption recovery of rhenium from solution, and desorption to obtain ammonium perrhenate ($NH_4ReO_4$) as the final marketable product. The overall rhenium recovery reaches 95%, demonstrating the high efficiency of the developed process.

A key advantage of the proposed technology is its integrated approach to metal recovery. Unlike conventional technologies focused primarily on a single valuable component, the developed process enables the production of several marketable products simultaneously, including metallic lead, osmium concentrate, and ammonium perrhenate. This significantly improves the economic efficiency of processing while ensuring more complete utilization of mineral resources.

An additional benefit of the technology is the reduction of environmental impacts through the minimization of technogenic waste accumulation and the prevention of toxic element release into the environment. The recovery of osmium, arsenic, and mercury at the early stages of processing contributes to reduced emissions and compliance with modern environmental regulations.

Implementation of the proposed technology could contribute to the establishment of a domestic resource base for critical metals in Kazakhstan. The recovered lead, rhenium, and osmium may be utilized in the production of energy storage systems and batteries, aerospace and power-generation superalloys, catalysts, electronic components, specialized equipment, and advanced materials for future technologies. In the context of the growing global demand for critical metals, such technologies can provide additional competitive advantages for the national mining and metallurgical sector and enhance the country's technological independence.

In conclusion, the developed technology for comprehensive processing of lead cakes represents an efficient solution combining high recovery rates of valuable metals, environmental sustainability, and significant industrial potential. Further development of this approach will contribute to expanding the resource base of rare metals, promoting the utilization of technogenic raw materials, and supporting the sustainable development of Kazakhstan's mining and metallurgical industry.

# Nickel and Titania Co-Decorated Carbon Nanofibers: a Novel Scaffold for High-Loading Lithium Polysulfide Catholytes

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Lithium-Sulfur (Li-S) batteries offer high energy density and affordability, but their commercial application is limited by the poor kinetics of intermediate lithium polysulfides (LiPSs)[1-2]. To address these obstacles, this study presents a free-standing current collector composed of carbon nanofibers decorated with nickel and titanium dioxide nanoparticles Ni(1.0%)/TiO2@CNF with a high sulfur loading of 2 mg*cm$^{-2}$. As shown in **fig. 1d**, the Ni(1.0%)/TiO2@CNF electrode delivers a high initial specific capacity of over 1150 mAh*g$^{-1}$ at a 0.5C rate, demonstrating robust capacity retention and stability over 200 cycles, which is further supported by the voltage profiles in **fig. 1c** that exhibit stable and well-defined discharge plateaus. Cyclic Voltammetry (CV) at varying scan rates in **fig. 1f** and over initial cycles in **fig. 1c** confirms rapid, highly reversible LiPS conversion. Furthermore, SEM and TEM analyses in **fig. 1a** and 1**b** reveal that the Ni and $TiO_2$ nanoparticles are uniformly distributed across the conductive CNF network, providing abundant catalytic active sites. These results highlight that the synergistic effect of metal and metal oxide nanoparticles effectively accelerates sluggish electrochemical kinetics, making Ni(1.0%)/TiO2@CNF a highly promising composite for high-performance Li-S batteries.

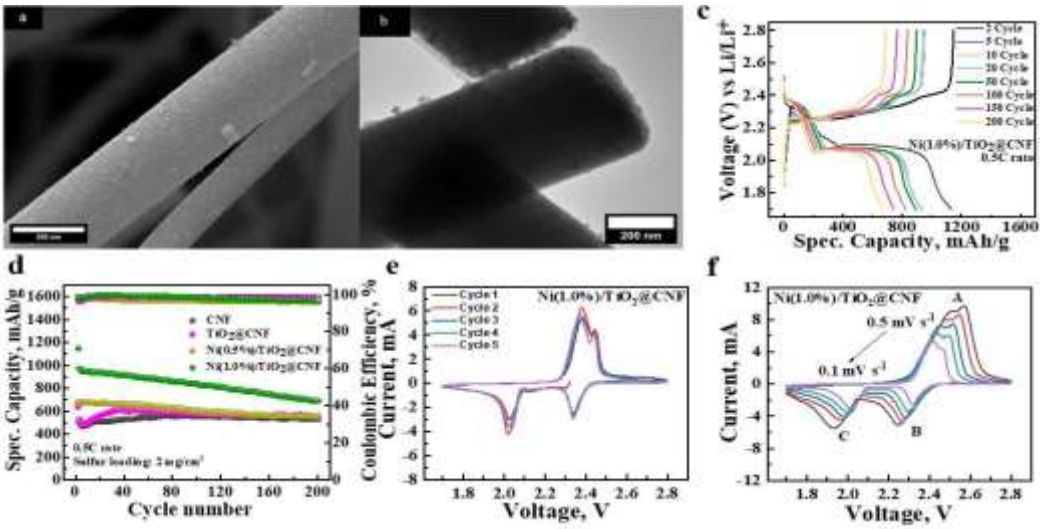



Figure 1. Morphological characterization of Ni(1.0%)/TiO2@CNF: (a) SEM image; (b) TEM; electrochemical performance: (e) voltage profile; (d) 0.5C rate long-term cyclability; (e) cyclic voltammetry; (f) cyclic voltammetry at different scan rates

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# Investigation of the Structure and Mechanical Properties of ZrCN Coating Deposited on 65G Steel by the HVOF Method

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In modern engineering practice, particularly within mechanical and automotive industries, enhancing the durability of steel components against wear, corrosion, and elevated temperatures remains a significant scientific and technological challenge. Among various surface engineering solutions, ceramic coatings such as ZrCN (zirconium carbon nitride) have attracted considerable attention due to their superior hardness, chemical stability, and resistance to abrasive degradation. However, achieving strong adhesion and a stable diffusion layer between ZrCN coatings and 65G steel substrates still requires detailed investigation [1]. The performance of ZrCN coatings is strongly governed by their microstructural features, phase composition, and interfacial characteristics. In particular, coating uniformity, thickness distribution, residual thermal stresses, and internal pressure gradients play a decisive role in determining mechanical stability. Accordingly, optimization of deposition parameters is essential to improve coating reliability and functional performance. This study focuses on the fabrication and characterization of ZrCN coatings deposited on 65G spring steel using the High Velocity Oxy-Fuel (HVOF) spraying technique. Experiments were performed using a Termika-3 installation in accordance with GOST 14959–2016 standards. Prior to deposition, the substrate surface was mechanically prepared and grit-blasted to enhance coating adhesion. ZrCN powder with a particle size of 25–40 μm was thermally accelerated and deposited onto the substrate under controlled process conditions, with gas pressure varying between 2.6 and 2.8 bar. The phase composition of the coatings was examined using X-ray diffraction analysis with Cu-Kα radiation. Microhardness measurements were carried out using the Vickers method under an HV0.5 load, while adhesion strength was evaluated according to GOST R ISO 4624–2016 using a hydraulic pull-off tester. Preliminary findings indicate that HVOF-deposited ZrCN coatings exhibit a dense microstructure, enhanced adhesion to the 65G steel substrate, and improved wear resistance. Furthermore, variations in spraying parameters, particularly gas pressure, significantly influence the formation of the diffusion layer and the resulting mechanical properties of the coating. Overall, the results contribute to a deeper understanding of the relationship between processing conditions, microstructure, and mechanical performance of ZrCN coatings, and provide a foundation for optimizing HVOF spraying parameters for advanced industrial applications.

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# Clue to Fast Chargeable Hard Carbons for Sodium-Ion Battery Anode Clarifing via Combination of Diluted-Electrode Method and Synthesis

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Although hard carbons (HCs) are commonly used as negative electrode material for commercial sodium-ion batteries[1], the improvement of input rate-capability has remained challenging due to rate-limiting attributed to not only the active material property but also the composite electrode structure, i.e., ion depletion/saturation in the electrode.[2] To address this issue, we have been using the *diluted-electrode method*,[2] which allows us to identify the accurate rate-performance of insertion materials without concentration overvoltage in composite electrode.[3,4] Here, we studied the fast sodiation of HCs through diluted electrode method, rate-capability test, and chronoamperometry to find the rate-limiting factor attributes to HC structure, and propose a synthetic perspect towards high-power HCs, maintaining good capacity and operation potential.

HC, aluminum oxide, and sodium polyacrylate were used as active material, diluent, and binder, respectively. The powders were mixed at a volumetric ratio of $x$ : (95−$x$) : 5, with total volume of 0.1 cm$^3$, and 0.8 mg of single-walled carbon nanotube was added as a conductive additive. The loading of HC in the electrode was proportional to HC concentration. Galvanostatic charge-discharge and chronoamperometry were carried out to evaluate the electrochemical properties. We compared fast sodiation abilities of commercial and lignin-derived HCs[1] in diluted electrodes.

Figure 1a shows a SEM-EDS mapping image of a diluted electrode with 5 vol.% HC electrode. All HC particles are isolated from each other in $Al_2O_3$ powders. Although the HC concentration in the electrode is only 5 vol.%, galvanostatic charge-discharge curves had identical voltage slope and plateau, which are respectively attributed to sodium storage at interlayer and pore in HCs with good reversibility (Figure 1b). Its rate-capability was comparable to diluted-graphite electrode in Li-cell.[4] Through chronoamperometric analysis, we found that the nucleation of pseudo-metallic cluster occuring at plateau region can be the rate-limiting of full sodiation. Furthermore, the rate-capability accompanying Na-cluster formation was accelerated by size decrease of closed pore in HCs, which was partially adjustable via pre-heating at < 300°C during carbonization (Figure 1c). This finding contributes to the development of high-rate sodium-ion batteries

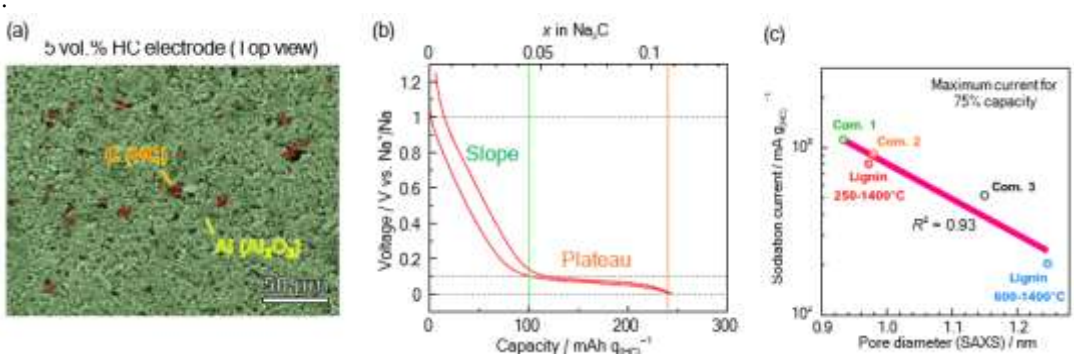



**Figure 1**. (a) SEM-EDS mapping image and (b) galvanostatic charge-discharge curves for sodiation of a diluted electrode with 5 vol.% of a commercial HC. (c) Correlation between sodiation rate-capability of diluted electrode and closed-pore diameter in various HCs including our homemade.

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# Magnetron Sputtering of $YBa_2Cu_3O_{7-x}$ Thin Films on Biaxially Textured Flexible Substrates (under industrial conditions) in Reel-to-Reel Deposition System

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Industrial production of second-generation high-temperature superconducting tapes (2G-HTS) commonly employs pulsed laser deposition (PLD), chemical vapor deposition (CVD), reactive co-evaporation (RCE) or solution-based process (MOD) for the fabrication of superconducting $REBa_2Cu_3O_{7-x}$ (REBCO) layer [1]. While PLD is the "gold standard" for high-quality REBCO epitaxial growth [2], magnetron sputtering offers a potentially more scalable alternative for industrial applications. In this work, we deposited YBCO thin films onto the biaxially textured flexible substrates using direct current (DC) and radio-frequency (RF) magnetron sputtering. We used industrial multilayer buffer substrate tapes of the following architecture $Al_2O_3$ / $Y_2O_3$ / IBAD-MgO / epitaxial MgO /LMO (IBAD = ion-beam-assisted deposition). It has both out-of-plane and in-plane orientation and serves as a texture template for $YBa_2Cu_3O_{7-x}$ (YBCO) sputter deposition with optimized process parameters. X-ray diffraction (XRD) confirmed the formation of required YBCO phase and strong c-axis texture with in-plane alignment. Common issues in YBCO magnetron sputtering include maintaining correct stoichiometry due to selective sputtering and oxygen depletion, negative ion bombardment causing re-sputtering and plasma instability are discussed. Prospect of increasing nanoparticles formation likelihood for pining centers densification in YBCO thin films by utilization deposition techniques with a higher ionization degree like cathodic arc (CA) ablation and high-power impulse magnetron sputtering (HiPIMS) is also discussed.

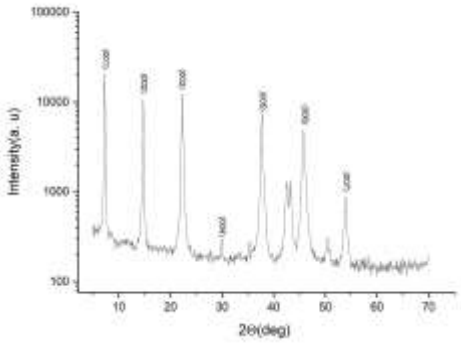



Fig.1 XRD patterns of the YBCO layer.

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# Nanomaterial-Enhanced Trombe Walls for Improved Thermal Energy Storage in Passive Solar Buildings

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Trombe walls are among the most widely used passive solar heating systems in building design, relying on solar radiation, thermal mass, and delayed heat transfer to reduce heating demand and improve indoor thermal comfort. Despite their simplicity and reliability, conventional Trombe wall systems often face limitations related to low thermal storage density, slow heat transfer rates, and significant heat losses during night-time operation. Recent developments in nanomaterials offer new opportunities to address these limitations by enhancing heat storage capacity, improving solar absorption, and reducing thermal losses. This paper examines recent progress in the application of nanomaterials to Trombe wall systems, with particular emphasis on improving thermal energy storage performance.

One of the most promising approaches involves the integration of nano-enhanced phase change materials (PCMs) into the thermal storage layer of Trombe walls. Conventional PCMs can significantly increase storage capacity through latent heat storage; however, their low thermal conductivity often limits charging and discharging efficiency. The incorporation of nanoparticles such as graphene nanoplatelets, carbon nanotubes, or metal oxides has been shown to increase thermal conductivity and improve heat transfer within the PCM matrix [1]. In addition, nano-encapsulation techniques provide improved material stability and prevent leakage during repeated melting and solidification cycles, making these materials suitable for long-term building applications [2].

Another important advancement is the use of nanostructured selective absorber coatings on the exterior surface of the Trombe wall. These coatings are engineered at the nanoscale to achieve high solar absorptance while minimizing infrared emittance. As a result, a greater fraction of incident solar radiation can be converted into stored thermal energy while reducing radiative heat losses during evening and night-time periods. Experimental studies have demonstrated that such coatings can significantly improve the thermal efficiency of passive solar wall systems compared with conventional dark surface treatments [3].

In addition to improvements in heat absorption and storage, nanotechnology also enables the development of advanced insulation materials that reduce unwanted heat transfer. Materials such as silica aerogels and nanoporous insulation panels exhibit extremely low thermal conductivity while maintaining sufficient solar transmittance when used in glazing systems. When integrated into Trombe wall assemblies, these materials help maintain higher internal temperatures and enhance the overall effectiveness of passive solar heating [4].

Recent numerical simulations and experimental investigations suggest that combining nano-enhanced PCMs, selective nanocoatings, and nano-insulation materials can significantly improve the overall thermal performance of Trombe wall systems. Integrated systems have been reported to achieve seasonal heating energy savings of approximately 25–35% compared with conventional Trombe wall configurations [5]. Although challenges remain regarding cost, scalability, and long-term durability, ongoing research indicates that nanomaterial integration could play a key role in advancing high-performance passive solar building envelopes.

Integrating nanomaterials into passive solar systems significantly boosts thermal storage and efficiency. This enhancement directly reduces building energy consumption. Continued modeling will be essential to optimize these advanced designs for sustainable architecture.

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# Electrochemiluminescence of Luminol for Heavy Metal Ions Detection

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Precise, reproducible and cost-effective *in-situ* detection of heavy metal ions in water solutions is a challenge for modern technology [1]. Existing methods for heavy metal ion concentration measurement include atomic absorption spectroscopy, X-ray fluorimetry and cyclic voltammetry, which are highly precise, but require expensive equipment and days to be complete. On the other hand, express tests, based on dyes and carbon dots, are fast and affordable, but lack reproducibility of measurements [2,3]. Electrochemiluminescence (ECL) methods offer more precision and reproducibility than express tests and can be used for *in-situ* monitoring unlike laboratory methods, but they either use complicated toxic ruthenium or iridium complexes as electrochemiluminophores, or suffer from insufficient signal intensity and low precision[4]. In this work a novel ECL-based approach of metal ion detection with environmentally friendly electrochemiluminophore and several responses was developed. The electrolyte solution was composed of carbon buffer with pH = 10 and 500 μM luminol. The electrochemical cell consisted of graphite anode and quartz disc with 30 nm Ti semi-transparent thin film, which was used as cathode. Ti film was deposited on quartz, using physical vapor deposition technique (Kurt J. Lesker, USA). Two electrodes were pressed together mechanically. A silicon gasket 1 mm thick with laser-engraved channels was placed between them. A handmade syringe pump was used, to infuse the electrolyte into the cell with the speed of 1 mL/min. The pulsed voltage of 1.5 V with pulse duration of 2.5 s and pause between the pulses of 12.5 s was used to excite the electrochemiluminescence of electrolyte solution with added $Co(NO_3)_2$ salt of different concentrations. The signal was recorded with a photomultiplier tube (Hamamatsu, Japan) (Figure 1.)

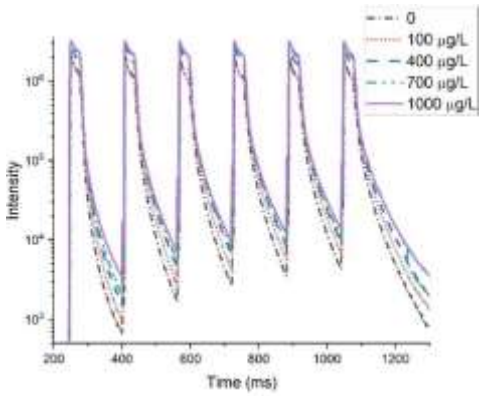



Figure 1. Electrochemiluminescence kinetics for different $Co^{2+}$ ion concentrations

The concentration of heavy metals varies from 100 μg/L to 1000 μg/L as these are concentrations that may harm the living beings [5].

The difference between concentrations may be distinguished not only through the ECL peak intensity, but also through the ECL decay speed and remaining chemiluminescence intensity evolution after each pulse. As a consequence, the pulsed ECL measurement technique makes the obtained results more precise and reproducible through additional responses, while not requiring extra equipment or reagents. The results of this work may be used in wastewater systems for *in-situ* heavy metal ion concentration monitoring at battery and electronics production plants. Also, this technology can be utilized in generic environmental monitoring and healthcare applications.

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# Development of Gel Polymer Electrolytes Based on Graphene Oxide-Doped Track-Etched Membranes for All-Solid-State Supercapacitors

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Developing functional solid-state gel polymer electrolytes (GPEs) with high ionic conductivity and excellent mechanical integrity is essential for flexible next-generation energy storage systems [1]. Track-etched membranes (TeMs) serve as an ideal mechanically robust platform with highly uniform, continuous cylindrical nanochannels. However, their native polymeric matrices exhibit low ionic conductivity, requiring tailored chemical functionalization of the pore walls. In this study, we present a comprehensive comparative evaluation of functional GPE architectures based on polyethylene terephthalate (PET) and polycarbonate (PC) track-etched host matrices modified via UV-initiated controlled radical polymerization.

The functional hybrid matrices were fabricated using two distinct synthetic approaches. For the PET-based systems, a poly(acrylic acid) (PAA) track-etched framework was combined with electrospun composite nanofibers made from poly(vinylidene fluoride-hexafluoropropylene) (PVDF-HFP), an ionic liquid ($EMIMBF_4$), and varying concentrations of graphene oxide (GO) as a functional top coating. For the PC-based platforms, GO nanosheets were introduced directly into the polycarbonate composite precursor films prior to ion-beam irradiation and subsequent chemical track-etching. To introduce intensive and uniform ionic conductive pathways along the nanochannel interiors without initiating pore blockage, reversible addition–fragmentation chain-transfer (RAFT) graft polymerization of acrylic acid was successfully optimized for both systems. Successful surface functionalization, progressive nanochannel constriction, and homogeneous filler dispersion were verified by FTIR, XPS, SEM-EDX, and nitrogen adsorption-desorption analyses.

Electrochemical characterizations, including cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS), revealed a pronounced non-linear dependence of transport behavior on GO filler loading. A moderate GO concentration of 0.5 wt% was identified as the absolute optimum for balancing continuous interconnected pathway formation and preventing adverse filler agglomeration or channel obstruction. For the single-sided PVDF-HFP_GO@PET-g-PAA configuration, the total room-temperature ionic conductivity reached $14.83\times10^{-3}$ mS $cm^{-1}$, which further enhanced to $39.08\times10^{-3}$ mS $cm^{-1}$ when deploying a symmetric double-sided electrospun configuration. In parallel, the self-supported, completely layout-flexible PC_GO-g-PAA (0.5 wt% GO) electrolyte matrix exhibited a high specific capacitance of 60 mF $g^{-1}$ at 5 mV $s^{-1}$, combined with exceptional cycling stability characterized by negligible performance loss and a Coulombic efficiency remaining near ~100% over 1500 intensive cycles. The synergetic interaction between confined RAFT grafting networks and carefully adjusted carbonaceous nanofillers highlights the massive potential of multi-component track-etched membrane designs as durable, leakage-resistant electrolytes for supercapacitors.

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# Tribromide-Assisted Low-Dimensional/3d Heterojunction for Efficient and Stable Wide-Bandgap Perovskite Solar Cells

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Wide-bandgap perovskites (WBG, 1.68eV) are highly important for perovskite/silicon tandem solar cells for efficient utilization of the solar spectrum, enabling efficiency beyond the single junction limit. However, their performance remains constrained by a substantial open-circuit voltage (V OC ) deficit, typically due to trap-assisted non-radiative recombination, segregation of halide ions and interfacial recombination. Here, we introduce tribromide-assited strategy to constract a low-dimensional/3D heterojunction on mixed-halide WBG perovskite thin films using benzyl trimethylammonium tribromide (BTMABr 3 ). The optimal treatment suppressed the non-radiative recombination rate, improved energy-level alignment, enhanced carrier lifetime and mitigated bromide deficiency across both the surface and bulk of the perovskite. In addition,

BTMABr 3 promoted formation of a low-dimensional perovskite layer through reaction with uncoordinated PbI 2 , while metallic lead (Pb 0 ) formation was also suppressed. These effects reduced trap densities and block pathways for halide-ion migration, therefore suppressing segregation. The results are further supported by hyperspectral PL, TRPL, XRD, XPS, and ToF-SIMS analyses.

As a result, the optimized 1.68eV WBG perovskite solar cells achieve a champion efficiency of 22.4% with V OC -1.27V , and FF-84.2%. More importantly, the treatment enhanced the photo and thermal stability of devices (85, 1 Sun, open-circuit). This work establishes an effective route to mitigating V OC losses in WBG perovskites.

# Numerical Simulation of the Thermal State of an Electroslag Remelting Mold During the Processing of Solid Radioactive Waste

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The decommissioning of research and power nuclear facilities, as well as the remediation of contaminated areas, is inevitably accompanied by the generation of radioactive waste (RW) requiring regulated handling and subsequent isolation. Despite the application of technologies aimed at minimizing the volume of generated waste, significant amounts of both liquid radioactive waste (LRW) and solid radioactive waste (SRW) are produced during these activities. A substantial portion of the accumulated SRW consists of metallic products and structural components made of metals and alloys [1, 2].

The processing and decontamination of metallic radioactive waste is one of the pressing challenges in the field of nuclear energy utilization. One of the promising methods for treating metallic radioactive waste is electroslag remelting (ESR). The process is based on the ohmic heating of a slag pool by an electric current passing between a consumable electrode and the formed ingot.

In this work, CFD modeling of the thermophysical state of an electroslag remelting mold is carried out. A three-dimensional geometric model and computational mesh were developed, and an unsteady simulation of the thermophysical state of the mold (Fig. 1) was performed, followed by comparison with parameters obtained in previous experiments.

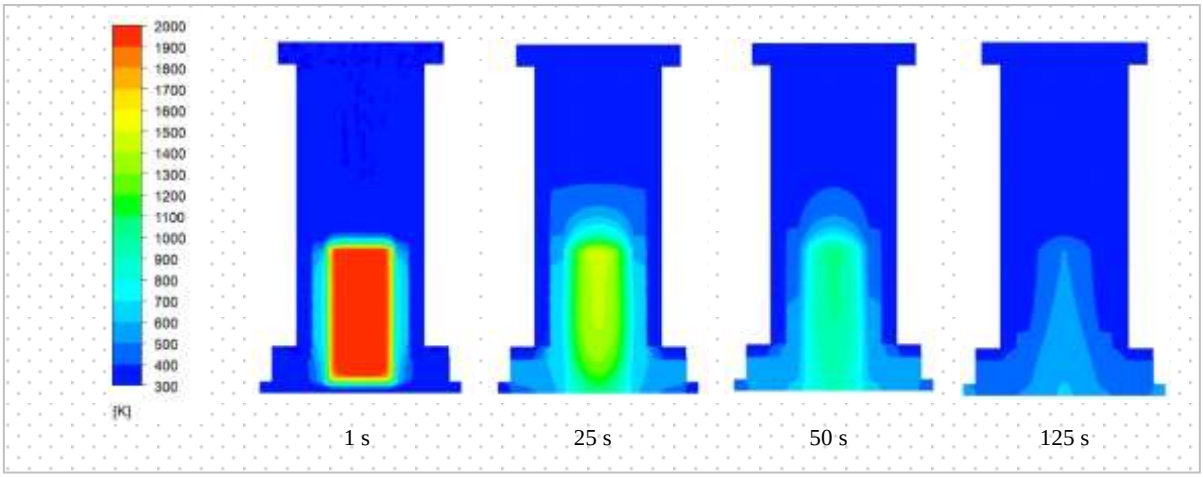



Figure 1. Temperature distribution in the central longitudinal section of the ESR mold.

The simulation results demonstrate the validity of the imposed boundary conditions and heat transfer parameters, and also confirm the dominant role of radial heat removal in forming a stable shape of the molten pool and ensuring controlled solidification of the melt. The proposed CFD modeling approach using ANSYS FLUENT has demonstrated its reliability. The work was carried out within the framework of the program-targeted funding project BR24993118, «Research on substantiating the selection and implementation of a technology for the processing of solid radioactive waste».

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# First-Principles Study of Y-Doped FeCrAl Alloys: Linking Mechanical Properties with $H_2$ and $O_2$ Surface Interactions

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FeCrAl alloys are considered promising candidates for accident-tolerant fuel cladding due to their excellent oxidation resistance and high-temperature stability; however, their performance is strongly influenced by alloying elements such as yttrium (Y). In this study, a comprehensive first-principles investigation based on density functional theory (DFT) is conducted to evaluate the effect of Y incorporation on the mechanical properties, electronic structure, and surface reactivity of FeCrAl alloys. The results show that Y doping induces lattice expansion and modifies the electronic structure through hybridization of Y-d states with Fe and Cr orbitals. Elastic analysis reveals that although both alloys satisfy mechanical stability criteria, Y addition leads to a reduction in bulk modulus, shear modulus, and hardness, accompanied by increased ductility. Electron localization function (ELF) analysis indicates the formation of localized bonding regions around Y, resulting in heterogeneous bonding and reduced mechanical strength. Surface calculations demonstrate that Y significantly lowers the (110) surface energy, enhancing thermodynamic stability. Adsorption studies reveal weak molecular adsorption of $H_2$ on both surfaces, while $O_2$ undergoes strong dissociative adsorption with substantial charge transfer. Notably, Y doping enhances oxygen adsorption strength and promotes dissociation by increasing electron donation to antibonding orbitals. These findings provide new insights into the role of reactive elements in tuning both bulk and surface properties of FeCrAl alloys, contributing to the design of advanced materials for nuclear energy applications

# Elucidating the Mechanisms and Optimizing Electrode Chemistry for Advanced Sodium Ion Batteries (SIBs)

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The global transition to renewable energy and the electrification of key sectors require energy storage technologies that are efficient, sustainable, and economically viable. While lithium-ion batteries dominate the present market, their long-term scalability is hampered by finite lithium deposits, growing prices, and unequal regional distribution. Sodium-ion batteries (SIBs) have emerged as a possible alternative, benefiting from sodium's natural availability, affordability, and chemical similarity with lithium. However, their practical application is hindered by persisting problems in electrode materials, such as structural instability, capacity fading with extended cycling and low initial coulombic efficiency (ICE). This dissertation tackles these difficulties through four interrelated studies: cathode synthesis, development, anode optimization, and full-cell integration. We produced sodium-deficient layered oxides ($Na_xMnO_2$, x = 0.6, 0.7 and 0.8) with a custom-built ultrasonic spray pyrolysis (USP) technique. Meticulously changing precursor stoichiometry, carrier gas flow, and temperature gradients, phase-pure cathodes with controllable morphology and crystallinity were synthesized, providing stable cycling and strong rate capability. Second, a robust Ni-substituted layered oxide, $Na_{0.67}Mn_{0.67}Ni_{0.33}O_2$, was produced using improved solid-state methods. A comparison of dry and wet-milled precursors highlighted the intricate interaction of phase purity, microstructure, and electrochemical reversibility, with the dry-milled sample displaying improved long-term stability and capacity retention. Third, bio-waste-derived hard carbon was produced from walnut shells using a designed two-step thermal process that included pre-oxidation and high-temperature carbonization. This method resulted in a disordered carbon with enlarged interlayer spacing and hierarchical porosity, attaining a reversible capacity of more than 300 mAh $g^{-1}$ and an ICE over 80%. This represents a substantial improvement for sustainable anodes. Finally, full-cell configurations that combine the optimized hard carbon anode with Ni doped cathodes were successfully demonstrated. The designed electrodes demonstrated high compatibility and practical potential. This study increases the knowledge of structure–property–performance correlations in sodium-ion battery electrodes and presents scalable synthesis methodologies for both cathodes and anodes. The main contributions of this work are: (i) fabrication of an inexpensive USP framework for $Na_xMnO_2$ cathodes; (ii) optimization of Ni-substituted $Na_{0.67}Mn_{0.67}Ni_{0.33}O_2$ with improved reversibility; (iii) customized pre-treatment method for hard carbon derived from bio-waste with ICE > 80%; and (iv) demonstration of synergistic full-cell performance. Our findings lay the groundwork for the rational design of next-generation sodium-ion batteries that are sustainable, scalable, and industrially feasible.

# Nanostructured Electrode Materials for High-Performance Hydrogen Storage in Subsurface Energy Systems

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The global transition toward low-carbon energy systems has intensified research into hydrogen as a clean energy carrier, particularly in the context of geological and subsurface storage applications relevant to the upstream petroleum industry. Underground hydrogen storage (UHS) in depleted hydrocarbon reservoirs and salt caverns represents a strategic pathway for seasonal energy balancing; however, its deployment is contingent upon advances in materials science governing adsorption kinetics, storage capacity, and thermodynamic stability. The present study investigates nanostructured electrode materials-specifically metal-organic frameworks (MOFs) functionalized with transition metal catalysts-as candidate systems for reversible hydrogen uptake in conditions representative of subsurface petroleum formations.

Experimental specimens were synthesized via solvothermal routes and characterized using X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET) surface area analysis, and transmission electron microscopy (TEM). Hydrogen uptake measurements were conducted on a Sievert-type volumetric apparatus (PCTPro-2000, Setaram Instrumentation) at pressures ranging from 0.1 to 15 MPa and temperatures of 77 K and 298 K, conditions chosen to bracket operational extremes encountered in deep reservoir environments. Electrochemical impedance spectroscopy (EIS) was employed to elucidate charge-transfer resistance at the electrode–electrolyte interface within proton-exchange membrane (PEM) configurations simulating downhole electrochemical conversion pathways.

Computational screening of candidate MOF topologies was performed using RASPA 2.0 molecular simulation software, with force-field parameters derived from the Universal Force Field (UFF). Grand Canonical Monte Carlo (GCMC) simulations at reservoir-representative pressures identified Ni-MIL-77 and Zr-UiO-66-$NH_2$ as top-performing architectures, yielding gravimetric uptake values of 4.8 and 5.3 wt% $H_2$ at 77 K, 1 bar, respectively. Experimental validation corroborated computational predictions within a 6% margin, confirming the predictive fidelity of the adopted forcefield parameterization. The integrated modelling and experimental workflow demonstrates that GCMC-based pre-screening can reduce empirical synthesis iterations by an estimated 40%, offering significant economic and temporal advantages in materials development pipelines for petroleum-adjacent energy applications.

The findings establish a quantitative framework linking nanopore geometry, metal node coordination chemistry, and macroscopic hydrogen storage performance, with direct implications for the design of solid-state storage systems deployable within Kazakhstan's expanding underground hydrogen infrastructure. Future work will address the long-term cyclability of functionalised MOF electrodes under cyclic pressure variations mimicking reservoir injection–withdrawal regimes, and will incorporate reservoir-scale simulation using CMG GEM compositional simulator to assess storage efficiency at field scale.

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# An Intergrowth of anti-NASICON and NASICON Frameworks in "Empty" $M_{0.5}Nb_{1.5}(PO_4)_3$ (M = Al, Cr, Sc) Phosphates with the $Nb^{+5}/Nb^{+4}/Nb^{+3}$ Multi-Electron Redox Activity

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The rapid implementation of metal-ion batteries in emerging sectors, such as electric vehicles and energy storage systems has sparked a demand for novel electrode materials that provide enhanced energy density, safety, and cycle life. For this purpose, the $A_xB_2(PO_4)_3$ phosphates are particularly attractive due to their robust covalent framework, maintaining improved rate performance, thermal and cycling stability. Recently the NASICON-type niobium phosphate $Nb_2(PO_4)_3$ with x=0 was introduced as possible 3e anode material for sodium-ion batteries [1]. However, its synthetic route through high-temperature annealing (T=1200°C) in evacuated ampoules seems to be the energy-intensive and hardly scalable procedure. From this point of view, the air-sintered $M_{0.5}Nb_{1.5}(PO_4)_3$ (M = Al, Cr, Sc) phosphates may be considered as advantageous high-capacity anode materials due to the $Nb^{+5}/Nb^{+4}/Nb^{+3}$ redox activity with the additional $Cr^{+3}/Cr^{+2}$ transfer in case of M=Cr.

The $M_{0.5}Nb_{1.5}(PO_4)_3$ (M=Al, Cr, Sc) samples were synthesized via a facile Pechini-type technique starting from aqueous solutions of $NH_4[NbO(C_2O_4)_2]$, $M(NO_3)_3$, and $NH_4H_2PO_4$, followed by two-step annealing in air at 850-950°C. Careful inspection of the XRPD patterns of $Al_{0.5}Nb_{1.5}(PO_4)_3$ (**ANP**), $Cr_{0.5}Nb_{1.5}(PO_4)_3$ (**CNP**), and $Sc_{0.5}Nb_{1.5}(PO_4)_3$ (**SNP**) revealed all of them were biphasic containing the NASICON (S.G. *R-3c*, *Z*=6) and anti-NASICON (S.G. *Pbcn*, *Z*=4) polymorphs with the latter predominating. This finding was confirmed by TEM study which unambigously disclosed a coherent intergrowth of these two frameworks in the samples.

Crystal structure refinement converged to low R-factors and proved that for each polymorph unit cell volume increase in the **ANP**-**CNP**-**SNP** series correlates well with the $r(M^{3+})$ growth. It is noteworthy and for all M the *V*/Z ratio of the NASICON-type phase exceeds that of the anti-NASICON one by about 3.2−3.5%. For all structures, no Nb/M ordering was observed. Both of the polymorphs are built up from the same $(Nb,M)_2(PO_4)_3$ "lantern" fragments and differ only by the way of their stacking, thus fascilitating the NASICON/anti-NASICON intergrowth. DFT calculations revealed the striking resemblance in energy between the NASICON and anti-NASICON polymorphs for all $M_{0.5}Nb_{1.5}(PO_4)_3$ (M = Al, Cr, Sc) phosphates with the formation energy difference between these two structures of only about 0.58 kJ/mol.

Electrochemical testing of the carbon-coated $M_{0.5}Nb_{1.5}(PO_4)_3$/C (M=Al, Cr, Sc) materials in the Na-half cells unveiled in case of **ANP** a poor reversibility of intercalation processes and fast degradation, while **CNP** and **SNP** at a C/10 rate deliver a reversible uptake of approximately 2.3 $Na^+$ (within the 1.2−3.0 V *vs.* $Na^+/Na$) and 2.5 $Na^+$ (within the 0.8−3.0 V *vs.* $Na^+/Na$) per formula unit, respectively. *Ex-situ* XANES spectra of **CNP** supported the $Nb^{+5}/Nb^{+4}/Nb^{+3}$ and the $Cr^{+3}/Cr^{+2}$ redox transfers on sodiation. However, even for **CNP** and **SNP** the electrochemical activity faded rapidly.

To understand the reasons behind electrochemical activity degradation and assess the diffusion barriers for $Na^+$ ions in the obtained niobium phosphates, BVSE calculations were performed. To highlight the NASICON/anti-NASICON border impact, we chose the "$InTi(PO_4)_3$" framework of the $Li_2InTi(PO_4)_3$ phosphate [2] as the basic model due to the alternating of the NASICON and anti-NASICON slabs in its crystal structure and the *V*/Z ratio closest to that of **SNP**. Indeed, the highest barrier for $Na^+$ migration was found precisely at the NASICON/anti-NASICON boundary being 2.5 times higher than the barrier for 3D diffusion inside the NASICON and anti-NASICON blocks separately. This hindered ion migration between the anti-NASICON and NASICON domains traps alkali metal ions at their boundaries and causes a capacity decline upon cycling [3]. The close resemblance in the formation energy for both polymorphs makes it challenging to obtain pure single-phase samples of $M^{III}Nb_{1.5}(PO_4)_3$, and only introduction of $Li^+$ or $Na^+$ ions into the phosphate composition can selectively stabilize the anti-NASICON or NASICON frameworks, respectively.

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# Composite Polymer Electrolytes Incorporating LATP Nanoparticles for Enhanced Interfacial Stability in All-Solid-State Lithium Batteries

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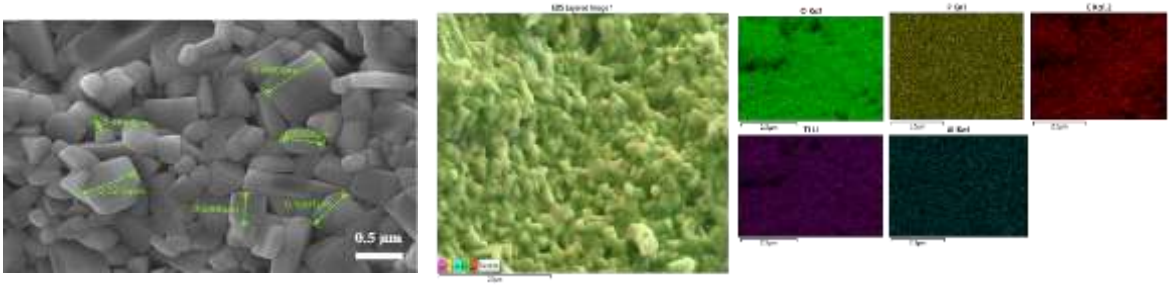
All-solid-state lithium batteries (ASSLBs) are considered a promising next-generation energy storage technology due to their superior safety, high energy density, and long cycle life compared to conventional lithium-ion batteries that use flammable liquid electrolytes. Among solid-state electrolytes, NASICON-type LATP ($Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$) has attracted significant attention owing to its high ionic conductivity, wide electrochemical window, and good air stability. However, its practical application is hindered by poor interfacial compatibility with lithium metal, which leads to $Ti^{4+}$ reduction, the formation of mixed-conducting interfaces, increased interfacial resistance, and lithium dendrite growth [1][2].

In this work, a composite solid polymer electrolyte strategy is proposed to address these limitations by incorporating LATP nanoparticles into a polymer matrix, with the aim of improving interfacial stability and suppressing lithium dendrite formation. The solid polymer electrolyte film was fabricated using acrylated poly(tetrahydrofuran) (aPTHF) as the host polymer, LiTFSI as the lithium salt, and a dual crosslinker system consisting of PEGDA and ETPTA, with propylene carbonate (PC) serving as a plasticizer. LATP nanoparticles were synthesized via a modified sol–gel method adapted from Kirianova [3]. The synthesis involved stoichiometric mixing of $Ti(C_4H_9O)_4$, $LiNO_3$, $Al(NO_3)_3{\cdot}9H_2O$, and $NH_4H_2PO_4$ in nitric acid, followed by gel formation through acrylamide-based polymerization, self-combustion at 150 °C, and subsequent calcination at 800 °C.

Structural and morphological characterization revealed nanoscale LATP particles (180–560 nm) with a cubic-like morphology and homogeneous elemental distribution (Figure 1). XRD analysis confirmed the formation of phase-pure NASICON-type LATP. The synthesized LATP was further utilized as a functional filler in composite polymer electrolytes prepared via an in situ UV polymerization approach to enhance interfacial contact and reduce impedance.

Ongoing studies focus on the electrochemical evaluation of the developed composite electrolyte in cells employing lithium iron phosphate cathodes, targeting improved interfacial stability and cycling performance for safe and high-energy ASSLB systems.

Figure 1.SEM/EDS images of synthesized LATP particles.




**Acknowledgments**

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# PIM-Based Electrolytes with Intrinsic Microporosity for Next-Generation Energy Storage

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Aqueous electrolytes have attracted significant attention for energy storage applications due to their intrinsic safety, low cost, and environmental compatibility. However, their practical implementation remains constrained by challenges such as limited electrochemical stability windows, parasitic side reactions, and uncontrolled interfacial processes. In this context, solid-state and gel polymer electrolytes have emerged as promising alternatives, offering enhanced stability, suppressed solvent-related degradation, and improved interfacial control while maintaining sufficient ionic transport [1,2].

Polymers of intrinsic microporosity (PIMs) represent a distinctive class of materials defined by rigid, contorted macromolecular backbones that prevent efficient chain packing, resulting in permanent, interconnected free volume at the sub-nanometer scale [3]. This intrinsic microporosity enables selective and continuous transport pathways while preserving mechanical integrity [4]. Furthermore, the chemical versatility of PIMs allows the incorporation of functional groups, such as carboxylic or other polar moieties, which can interact strongly with ionic species and facilitate ion coordination. These features position PIMs at the intersection of porous materials and functional polymers, offering a tunable platform where pore architecture, surface chemistry, and transport properties can be precisely engineered [5].

Building on these attributes, a conceptual framework is introduced in which PIM structures are functionalized with ionic liquid (IL) moieties to create hybrid ion-conducting networks [6]. The incorporation of polar functional groups facilitates strong interactions with ionic species, while the presence of ionic liquid domains promotes ion dissociation and dynamic coordination. This synergistic interplay between confined free volume and adaptable ionic environments allows precise tuning of physicochemical properties, bridging the gap between solid-state stability and liquid-like ion mobility.

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# Nano-Engineered Superhydrophobic Materials and Surfaces: Durable Solutions for Waterproofing, Self-Cleaning, and Environmental Remediation

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The growing demand for durable, self-cleaning, and water-repellent materials has accelerated research into nano-engineered superhydrophobic surfaces for construction, textiles, agriculture, and environmental remediation. This talk presents several advanced coatings and functional materials designed to improve water resistance, mechanical durability, and environmental stability.

Among the developed systems are ZnO–stearic acid–silane coatings for concrete and silica-based coatings for road surfaces, both exhibiting water contact angles above 150° and strong resistance to abrasion and weathering. Hydrophobic modification of textile fibers, including tweed, felt, and polyester, demonstrates applications in modern garments and traditional Kazakh yurts. Additional developments include waterproof concrete using hydrophobic sand blends, self-cleaning $SiO_2$/TMCS films, and functional nanomaterials such as reduced graphene oxide and nanodiamonds.

The talk also highlights sustainable hydrophobic coked sand produced from pyrolyzed oil-sand waste for gravity-driven oil/water separation. The carbon-coated quartz material showed durable hydrophobicity, achieving ~96% separation efficiency over 30 cycles without fluorinated additives. Finally, stearic acid-coated sand for moisture retention in arid soils is discussed. Overall, these studies demonstrate scalable and environmentally friendly approaches for designing multifunctional water-repellent surfaces with broad industrial and societal relevance.

# Enhanced Oil Recovery and $CO_2$ Storage Using Polymer Enhanced $CO_2$ Foam: Foam Strength and Mobility Control

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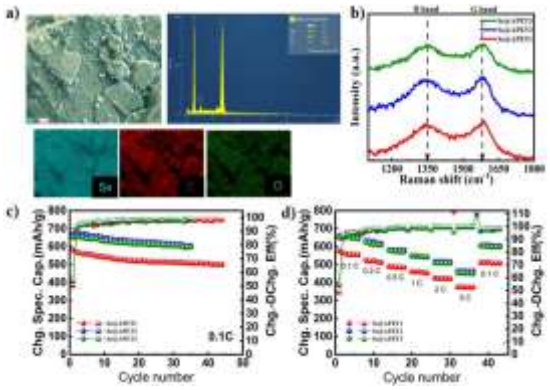
Geological $CO_2$ storage and enhanced oil recovery (EOR) are essential to addressing the global energy needs and preventing climate change. This research examines the polymer-enhanced $CO_2$ foam (PEF) as a superior technique in EOR and $CO_2$ sequestration. Traditional $CO_2$ foams are limited by their quick instability and inability to be controlled in mobility during severe reservoir conditions, which are often also high temperature (80 °C) and high salinity (approaching 15,000 mg/L). This research paper analyzes the performance of polymer-enhanced $CO_2$ foam (PEF) in improving the mobility control and oil recovery under simulated reservoir conditions. The PEF system was developed with 0.1 wt% anion-based Alpha Olefin Sulfonate (AOS) surfactant and 0.5 wt% hydrolyzed polyacrylamide (HPAM) in 4.0 wt% NaCl brine. Core flooding experiments were conducted at 10 bar and 60 C with a foam quality of 70% on four sister core samples with porosities ranging from 17.68 to 20.10% and gas permeabilities ranging from 1.25 to 1.60 mD. Experimental analysis revealed that the recovery factor with traditional $CO_2$ foam was 58.0 percent at an injection rate of 3 $ft^3$/day (the highest differential pressure was 10.39 psi) and 64.5 percent at 6 $ft^3$/day (13.00 psi). Conversely, the polymer-enhanced foam recovered 68.3 and 69.8% at 3 $ft^3$/day and 6 $ft^3$/day with 10.04 psi and 17.15 psi differential pressures, respectively. These results show the possibility of PEF to enhance the sweep efficiency and stability in EOR operations, as well as a contributing factor in the successful sequestration of $CO_2$.

# Upcycled PET-Derived Porous Carbon as a High-Capacity Anode for Low-Temperature Sodium–Selenium Batteries

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Waste PET plastic is building up faster than we can manage it, and global plastic production is expected to nearly double by 2100 [1]. In this work, we turned used PET bottles into a porous activated carbon material and tested it as an anode host for sodium–selenium (Na–Se) batteries. The whole synthesis was done in a single step. KOH was used to break down the PET, while at the same time the carbon was activated and carbonized during heating no separate processing stages were needed. By changing the KOH to PET ratio, we were able to control the porosity and degree of structural disorder in the final carbon. This was confirmed by Raman spectroscopy, where the D/G band ratio shifted across the three prepared materials (APET1, APET2, APET3). Selenium was then loaded into the carbon pores by melt-diffusion, which is known to promote uniform Se distribution and limit polyselenide dissolution [2,3]. SEM and EDS mapping showed that Se was spread evenly through the carbon host, which we believe contributed to the stable electrochemical performance. The best electrode, Se@APET2,
delivered an initial capacity of 674 mAh $g^{-1}$ at 0.1 C and kept 614 mAh $g^{-1}$ after 35 cycles (~91%), with Coulombic efficiency staying above 98%. At higher rates, capacity retentions were 94.9%, 88.2%, 82.7%, 78.3%, and 70.3% at 0.2, 0.5, 1, 2, and 5 C, and recovered to 606 mAh
$g^{-1}$ when returned to 0.1 C. Over 150 cycles at 0.5 C, the capacity went from 614 to 512 mAh $g^{-1}$, which means 83.4% retention and CE above 99%. These results show that waste PET can be a useful and affordable starting material for making carbon hosts in sodium-based batteries.




**Acknowledgement**
This research was funded by the Research Targeted Programs" BR24992766 "Development of methods and technologies for environmentally friendly "green" processing of polymer waste for energy storage" from the Ministry of Science and Higher Education of the Republic of Kazakhstan.

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# Role of Alkaline Metals in Promotion of Hydrogen Evolution in Electrocatalytic Water Decomposition

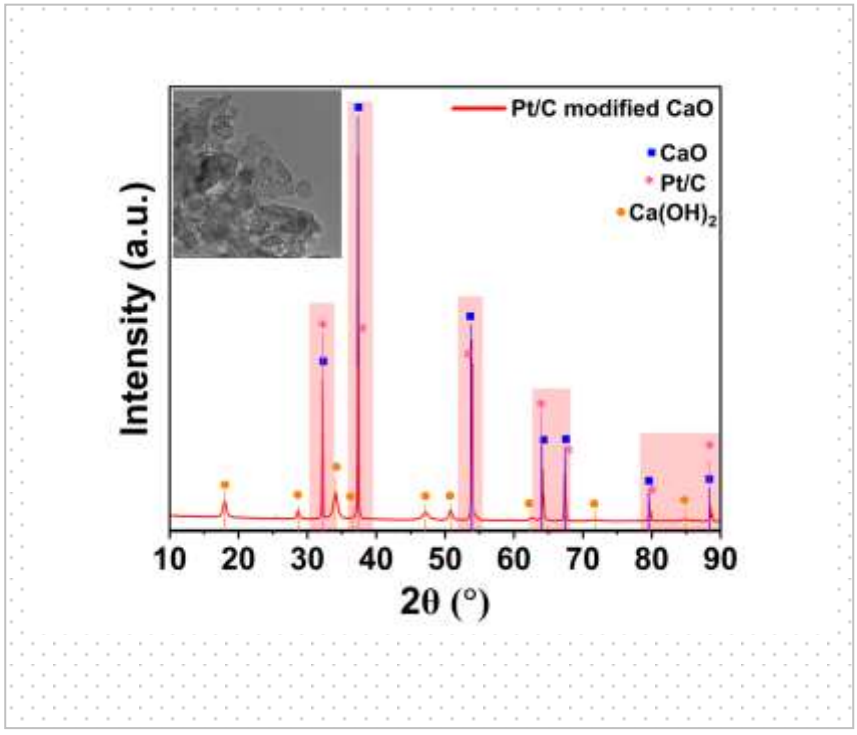
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Możesz to przepisać w bardziej oryginalnej formie, jednocześnie mocniej akcentując główny wniosek dotyczący CaO:> The development of efficient and economically viable electrocatalysts for the hydrogen evolution reaction (HER) remains challenging due to the high platinum loadings typically required to achieve satisfactory activity. In this work, a series of alkaline-earth metal oxides (MgO, CaO, SrO, and BaO) were systematically investigated as catalyst supports modified with trace amounts of commercial Pt/C. Among all examined oxides, CaO exhibited the most pronounced promotional effect, delivering the largest reduction in HER overpotential, the lowest Tafel slope, and the fastest charge-transfer kinetics (see XRD pattern of the samples and TEM image in the inset of Figure 1). The superior performance of the Pt/C–CaO composite is attributed to a strong metal–support interaction, whereby defect-rich CaO facilitates electron transport toward Pt active sites, enhances charge delocalization, and effectively suppresses Pt nanoparticle agglomeration. In contrast, the remaining alkaline-earth oxides provided only moderate improvements. These findings demonstrate that catalytic activity is governed not merely by the presence of platinum, but primarily by the nature and strength of the Pt–oxide interaction. The exceptional behavior of CaO highlights its unique ability to maximize Pt utilization while maintaining catalyst stability, making it the most effective support among all alkaline-earth oxides investigated in this study.




**Figures 1**.XRD pattern of the samples CaO with Pt and TEM image in the inset.

**Acknowledgement**
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# Plasma-Catalytic Conversion of Methane in Microwave Discharge

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Hydrogen today plays a key role among the promising energy sources of the future and is regarded as a crucial instrument in the fight against climate change. Various countries are actively developing approaches to its production aimed at overcoming existing technical, economic, and environmental barriers. In 2024, Kazakhstan approved an order of the Minister of Energy defining the Concept for the Development of Hydrogen Energy until 2030 [1]. The central idea of this concept is to advance hydrogen energy in Kazakhstan with the goal of reducing carbon emissions and stimulating economic growth.
Water, coal, oil, biomass, and natural gas are traditionally used as feedstocks for hydrogen production. Among the promising directions, methane conversion is of particular interest [2]. However, methane decomposition is a complex process requiring significant energy input ($\Delta H$ = +74.9 kJ/mol) [2]. An effective solution in this case is the use of microwave (MW) discharge for plasma generation, which is notable for its accessibility and relatively low cost [3]. This work investigates the application of microwave discharge in combination with a catalyst for the efficient decomposition of methane. A steel cylinder (length 20 mm, diameter 25.5 mm) with the elemental composition of 30 at.% C, 26 at.% Fe, 22 at.% O, 8 at.% Cr, 5 at.% Al, and 8 at.% Ni was used as the catalyst.

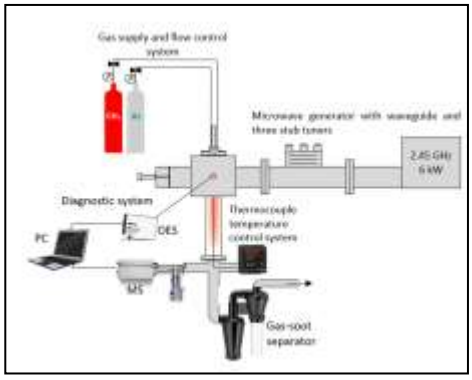



Figure 1. PM-6 applied research installation

The experiments were carried out using a PM-6 setup (Figure 1), equipped with a microwave generator with a power of up to 6 kW (frequency 2.45 GHz). The reaction chamber consisted of a quartz tube with a diameter of 30 mm fitted with a perpendicularly mounted rectangular waveguide. The working gas mixture was supplied in a swirling flow to the central part of the tube, where the plasma discharge was initiated. Analysis of the decomposition products was performed using a mass spectrometer. As a result, a technology for hydrogen production using a catalyst and microwave discharge was developed: the maximum methane conversion rate reached 31%, with hydrogen selectivity of 85% at a power of 0.6 kW.

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# $TiO_2$ - Decorated AgCl Visible-Light-Responsive Photocatalyst for Microplastic Degradation

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Microplastic (MP) pollution has emerged as one of the most pressing environmental challenges of our time. Conventional wastewater treatment systems are insufficient for complete MP removal, achieving only ~70% efficiency, necessitating the development of advanced treatment strategies [1]. Photocatalysis, leveraging reactive oxygen species (ROS) generated under solar or simulated light, represents a promising approach for MP degradation. Among candidate materials, $TiO_2$-based photocatalysts have been extensively studied; however, their wide bandgap (~3.2 eV) severely limits visible-light utilization. AgCl is known for its strong visible-light activity and plasmonic enhancement via in-situ generated $Ag^0$ nanoparticles, yet AgCl/ $TiO_2$ heterostructures have not been explored for MP degradation to date.

In this work, a series of AgCl/ $TiO_2$ heterostructure photocatalysts were synthesized via a facile mechanochemical method using a planetary ball mill. The synthesis is based on an ion-exchange reaction between $AgNO_3$ and $NH_4Cl$ in the presence of $TiO_2$ (P25), yielding AgCl/$TiO_2$ composites with mass ratios of 95/5, 85/15, 75/25, and 50/50.

Structural and surface analyses confirmed the successful formation of phase-pure AgCl/$TiO_2$ composites with intimate interfacial contact between the two phases. Optical characterization revealed progressively enhanced visible-light absorption relative to bare $TiO_2$, consistent with the bandgap narrowing arising from heterostructure formation.

The 95/5 AgCl/$TiO_2$ composite showed the highest photocatalytic activity toward LDPE microplastic degradation under visible-light irradiation, outperforming both bare $TiO_2$ and all other composite ratios. Product analysis confirmed extensive oxidative chain fragmentation of the LDPE backbone, providing direct mechanistic evidence of photocatalytic degradation.

This study presents the first application of AgCl/$TiO_2$ heterostructures for visible-light-driven MP degradation. The mechanochemical synthesis offers a scalable, solvent-free route, while the plasmonic enhancement from in-situ $Ag^0$ formation and favorable band alignment in the heterostructure enable superior photocatalytic activity under solar irradiation. These results highlight the strong potential of AgCl/$TiO_2$ composites as efficient and practical photocatalysts for environmental remediation of MP pollution.

**Keywords:** microplastics; photocatalysis; $TiO_2$; AgCl; visible light; LDPE degradation; heterostructure; mechanochemical synthesis

**Acknowledgments.** This research was funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan, grant number AP22788706

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# Sustainable Fe-Doped Carbon Electrodes from Waste Wheat Biomass for Green Electroanalysis

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Biomass-derived activated carbons have attracted considerable attention as electrode materials due to their developed porosity, electrical conductivity, low production cost, and applicability in electrochemical sensing systems [1–4]. In this work, an Fe-doped activated carbon electrode derived from waste wheat biomass was developed for the direct potentiometric and redox electroanalytical determination of pharmaceutical compounds. For this purpose, the activated carbon was synthesised via two-stage carbonisation of wheat husk, followed by $FeCl_3$ modification and thermal activation. Structural characterisation confirmed the formation of a graphite-like porous carbon matrix with uniformly distributed iron-containing particles and a specific surface area of 293.91 $m^2 \cdot g^{-1}$. Raman spectroscopy and X-ray diffraction analysis revealed partially ordered $sp^2$ carbon domains and the presence of Fe-containing phases within the carbon structure. UV-Vis spectroscopy showed an absorption maximum at 210 nm corresponding to π-π* transitions in aromatic carbon domains. The optical band gap determined by the Tauc method was 2.7 eV, indicating charge-transfer interactions between iron species and the carbon matrix.

The Fe-modified activated carbon was used to fabricate a carbon paste electrode (CPE) for potentiometric and voltammetric analyses. Electrochemical measurements demonstrated a linear response in the concentration range of $1.0 \cdot 10^{-6}$-$1.0 \cdot 10^{-1}$ $mol \cdot L^{-1}$, with a near-Nernstian slope of 54.35 $mV \cdot decade^{-1}$ and a response time below 20 s. The electrode maintained stable analytical performance in the presence of interfering ions, including $Na^+$, $Ni^{2+}$, and $Cr^{3+}$, demonstrating acceptable selectivity toward $Fe^{3+}$-containing analytes. The electrochemical behaviour of the Fe-doped activated carbon electrode was additionally evaluated in the $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$ redox system. Cyclic voltammetry revealed well-defined anodic and cathodic peaks with increasing peak currents at higher scan rates, indicating predominantly diffusion-controlled electron-transfer behaviour. A characteristic anodic peak observed at approximately +340 mV (vs Ag/AgCl) was attributed to the $Fe^{2+} \rightarrow Fe^{3+}$ oxidation process, indicating efficient charge transfer at the electrode surface. The modified electrode exhibited enhanced electrochemical response compared with the bare glassy carbon electrode, together with good electrochemical stability and reproducibility. The developed electrode also showed promising performance in direct redox potentiometric titration. Determination of hydrogen peroxide yielded an experimental value of 2.98% compared with the theoretical value of 3.00%, with RSD=0.78%. Analysis of ascorbic acid demonstrated satisfactory agreement between the experimental 11.15% and theoretical 12.60% values, with RSD=1.16%.

The obtained results show the potential of agricultural waste-derived Fe-doped activated carbon as a sustainable and efficient biomass-based electrode material for direct potentiometry and redox electroanalysis of pharmaceutical compounds.

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# Flexible Temperature Sensing Systems for Thermal Field Perception

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Flexible sensors exhibit tremendous application potential in various fields, including human-computer interaction, smart medical systems, and electronic skin. Among them, flexible temperature sensors and systems play a crucial role. They can replicate and transmit thermal sensations, thereby reflecting important temperature information of the human body, environment, and objects. However, current materials and devices still face critical challenges in practical applications: poor mechanical flexibility, limited sensitivity, complex device fabrication processes, and poor carrier transport and thermal conductivity. Based on the above, we have been proposed a facile, efficient, and low-cost in situ fabrication strategy to controllably design nickel oxide -based heterostructure devices, and the self-gated carrier devices with metal-semiconductor-metal structure were constructed, exhibiting excellent carrier transport properties and sensing performance. To further promote the flexibility of the device, we obtained flexible fiber and film-based temperature sensors through facile material synthesis and device fabrication methods, which presented excellent deformability and temperature sensing properties. Based on the flexible temperature sensors, the sensor arrays were fabricated and the sensing systems for thermal field perception were designed and used in signal monitoring and temperature warning systems, especially in the field of battery safety monitoring

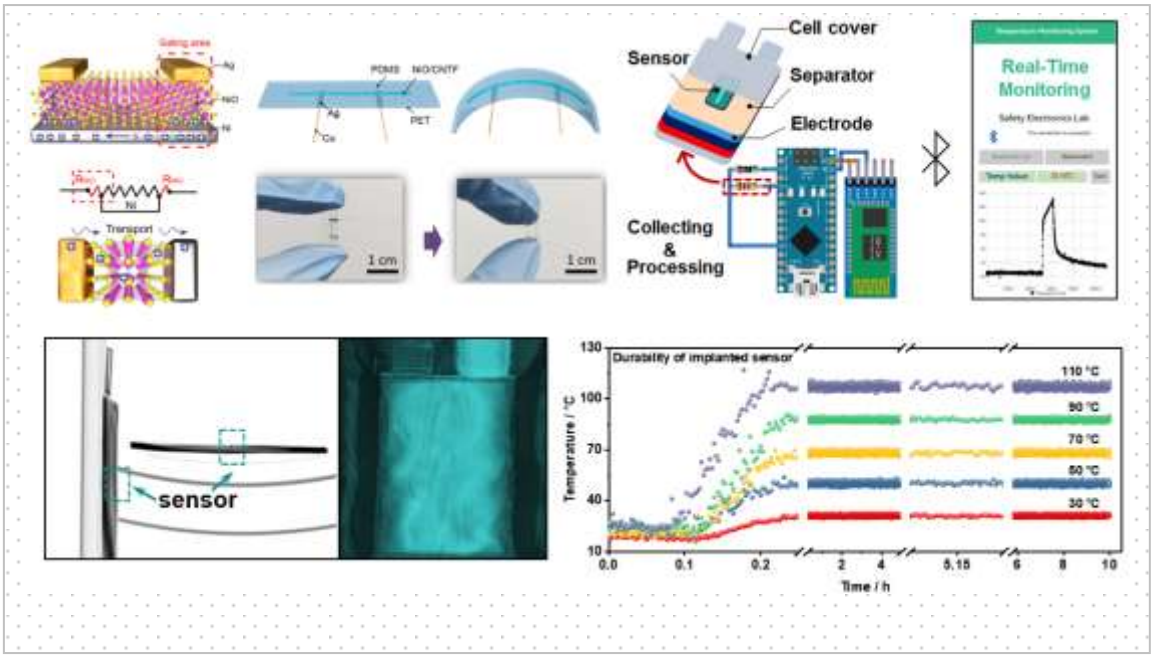



Figure 1. Flexible Temperature Sensors and Battery Safety Monitoring.

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# A Set of Interaction Potentials for Molecular Dynamics Simulation of $YPO_4$ and $ScPO_4$ Crystals

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Crystals $YPO_4$ and $ScPO_4$ are promising materials used as phosphors activated by dopants. In particular, systems such as $YPO_4:Bi^{3+}$; $YPO_4:Bi^{3+},Gd^{3+}$; $ScPO_4:Gd^{3+}$; $ScPO_4:Eu^{3+}$ can provide persistent luminescence in the ultraviolet and visible spectral regions. The intensity and duration of the luminescence of such phosphors are sensitive to the presence of impurities, vacancies, impurity-vacancy complexes, as well as extended defects and grain boundaries. For predicting the properties of a phosphor as a function of temperature, dopant composition and concentration, and crystal growth conditions, molecular dynamics simulation is relevant.

In this work, we propose an original method for the parameterization of classical interaction potentials for molecular dynamics and static simulations of $YPO_4$ and $ScPO_4$ crystals. A force field describing the $PO_4$ complex in these crystals is obtained, taking into account the screening of Coulomb interactions [1] and the reduction of dispersion attraction [2] upon the overlap of the electron shells of phosphorus and oxygen atoms. A three-particle O–P–O potential is considered, which specifies the tetrahedral mutual orientation of the P–O bonds resulting from $sp^3$ hybridization. The potential parameterization used experimental values of the force constants of the $PO_4$ complex, as well as structural data for $YPO_4$ and $ScPO_4$ crystal lattices.

The proposed sets of interaction potentials allowed us to obtain temperature dependences of the lattice constants of $YPO_4$ and $ScPO_4$ crystals that are in good agreement with experimental data [3–4]. Furthermore, the intrinsic Frenkel and Schottky disorder energies were calculated for $YPO_4$ and $ScPO_4$. The equilibrium shapes of isolated model crystallites of $YPO_4$ and $ScPO_4$, which correspond to the proposed interaction potentials, were determined.

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# Transition Metal Dopant Effects on Hydrogen Adsorption at TiFe(111): A Spin-Polarized DFT Study of Sc, V, Cr, Mn, Co, and Ni

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TiFe alloys are promising intermetallic hydrogen storage materials because they combine low elemental cost, high volumetric hydrogen storage density, reversible hydrogen uptake and release under moderate conditions, and improved safety relative to compressed hydrogen gas. However, their practical application is hindered by the severe activation treatment required before the first hydrogenation cycle. In this work, spin-polarized density functional theory calculations were used to systematically investigate the effects of six 3d transition-metal dopants, Sc, V, Cr, Mn, Co, and Ni, on $H_2$ adsorption and activation at TiFe(111) surfaces. Both Ti- and Fe-terminated surfaces were considered, and the dopant effects were evaluated through adsorption energies, adsorption geometries, bond elongation, charge transfer, and electronic structure analysis.

The results reveal a strong termination dependence of $H_2$ activation. For the Ti-terminated TiFe(111) surfaces considered here, all doped systems interact only weakly with molecular $H_2$. In contrast, doped Fe-terminated surfaces exhibit much stronger $H_2$ adsorption and H–H bond activation. Mn shows the strongest effect, leading to near-complete $H_2$ dissociation with an adsorption energy of −1.838 eV, while Co also promotes substantial H–H bond weakening. Electronic-structure analysis suggests that Mn and Co introduce dopant-derived states near the Fermi level, enhancing charge redistribution between the surface and adsorbed hydrogen. These results indicate that Fe-terminated TiFe(111) surfaces are more favorable sites for dopant-assisted molecular $H_2$ activation among the configurations studied. The findings provide atomistic insight into the beneficial role of Mn in TiFe-based hydrogen storage alloys and suggest a possible surface-activation role for Co under appropriate microstructural conditions. Future work should validate these predictions through controlled hydrogen absorption experiments and surface characterization, while extending the calculations to defective, reconstructed, and oxide-covered TiFe surfaces that better represent practical activation conditions.

# Theoretical Evaluation of Zn, Ni, and Co Based Imidazolate Frameworks for $CO_2$ reduction to CO

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The carbon dioxide reduction reaction ($CO_2$RR) has gained significant attention as a promising approach for reducing carbon emissions. Nevertheless, the design of catalysts that offer both high product selectivity and low cost remains a key challenge. In this study, density functional theory (DFT) calculations were employed to investigate the catalytic performance and reaction mechanism of $CO_2$-to-CO conversion over twelve ZIF-like catalysts. These catalysts were constructed from three metal centers, Zn, Ni, and Co, combined with four imidazolate-derived linkers: 2-methylimidazole (mIm), 2-aminoimidazole (aIm), imidazole-2-carboxaldehyde (ICA), and 2-nitroimidazole (nIm).

Analysis of the activation energy barriers revealed that Zn-aIm showed the most favorable catalytic behavior among the studied systems, exhibiting the lowest activation energy barrier of (0.21 eV). Quantum theory of atoms in molecules (QTAIM) and noncovalent interaction (NCI) analyses of the $CO_2$ activation step suggested partial covalent character and strong electrostatic interactions between $CO_2$ and the catalyst active sites. Furthermore, natural bond orbital (NBO) and electron density difference (EDD) analyses revealed notable charge redistribution and bending of the $CO_2$ molecule upon interaction with the catalyst surface. Overall, the low activation barrier and favorable electronic interaction features indicate that Zn-aIm is the most effective electrocatalytic surface among the investigated catalysts, enabling more efficient $CO_2$ activation during $CO_2$RR.

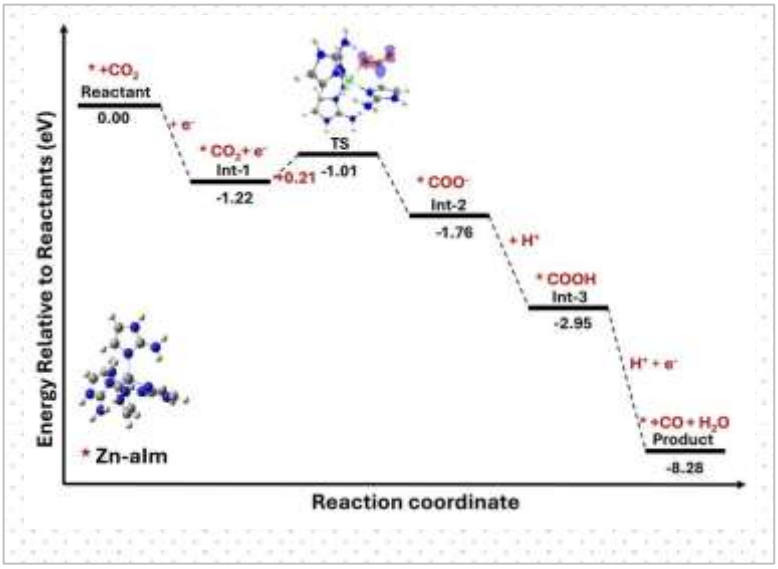



Figure 1. Energy Profile of $CO_2$ Reduction over Zn-aIm

# Addressing Data Scarcity on Fuel Cell Electric Vehicle (FCEV) Modelling

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In the era of energy and sustainability crisis, the demand for alternative sources of energy has soared globally. Harnessing wind, water and solar energy provides its own benefits to the sustainable and energy-efficient development, although it has serious limitations imposed by the environmental conditions. To circumvent these limitations, researchers propose an alternative energy source or technology – proton exchange membrane fuel cells (PEMFCs) that generate sustainable energy by converting chemical energy into electricity. PEMFCs have captured the attention of environmentalists and sustainability experts as they provide clean, cost-efficient energy producing water as the final byproduct of the electrochemical reactions. Still, this advancement requires areas of improvement for degradation, performance and aging prognosis modelling.

Therefore, researchers develop and run a diverse range of fuel cell (FC) models to tackle three aforementioned issues in the laboratory settings. Model-based approach succeeds at designing fuel cells that reflect real-world electrochemical, thermal and water transport processes, but face high computational demand. Researches that use machine learning framework report very accurate predictions on fuel cell performance with low RMSE values, although this data-driven approach suffers from a lack of realistic automotive datasets and physical interpretability. Overall, these models have proven to be accurate and robust on multiple occasions.

However, these models do not accurately reflect the degradation, performance and remaining useful life (RUL) of fuel cells under real-life operation. As high-tech companies reluctanly disclose corporate information on fuel cell electric vehicles to researchers, this presents a lack of literature on prediction models tested under the real-world vehicle driving conditions. Accelerated Stress Tests (ASTs) , for instance, use single mode evaluation that fails to account for the influence of several degradation mechanisms in the cell. Another challenge that poses a threat to accurate predictions of the model is reversible voltage loss caused by transient overloading of the engine. In particular, the robustness and accuracy of predictions in long-term are the most challenging. Data is also scarce on the aging prognosis model on fuel cells tested under automotive conditions.

This review compares the efficiency and performance of model-based and data-driven methods under idealized laboratory-based environment as well as emphasize the lack of literature on fuel cell modelling under real-world driving conditions.

# Microstructure-Driven Lithium Transport in Ni-Rich NMC811 Cathodes Revealed by Advanced Characterization and AI-Assisted Image Analysis

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Understanding the relationship between microstructure and lithium-ion transport is critical for improving the performance and durability of Ni-rich cathode materials. In this work, advanced multimodal characterization techniques, including high-resolution backscattered electron imaging, time-of-flight secondary ion mass spectrometry (ToF-SIMS), and electrochemical analysis, were combined with deep learning–based image segmentation to quantitatively investigate the microstructure of NMC811 cathodes. The AI-assisted workflow enabled rapid extraction of grain size distributions, particle morphology, and crack networks within secondary particles, providing a fast alternative to conventional microstructural analysis methods (Fig. 1).

Correlative microstructural and electrochemical investigations revealed that crack formation and electrolyte penetration into secondary particles strongly influence lithium transport kinetics. A significant asymmetry between charge and discharge diffusion coefficients was observed, with lithium diffusion during charging being approximately twenty times slower than during discharge. Quantitative image analysis showed that the internal crack surface area was substantially larger than the external particle surface area, indicating that electrolyte-accessible internal interfaces play a major role in governing lithium transport. These findings demonstrate how the combination of advanced characterization and artificial intelligence can provide deeper insights into microstructure–transport relationships and degradation phenomena, offering valuable guidance for the design of next-generation high-performance lithium-ion battery cathodes.

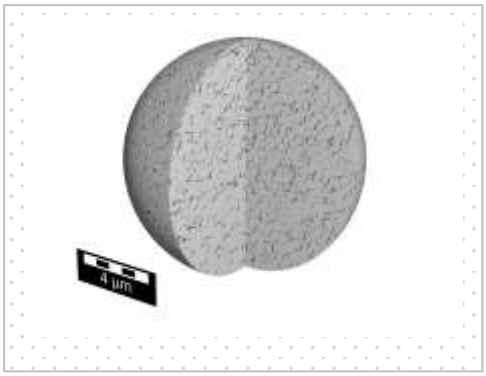



Figure 1. AI generated NMC microstructure for 3D characterization

# Modeling of Hydrogen Diffusion Kinetics and Trapping Processes in Complex Alloyed Oxide Dispersion Strengthened (ODS) Steels

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Oxide Dispersion Strengthened (ODS) steels, such as ODS-EUROFER and 14Cr ferritic ODS variants, are considered leading candidate materials for structural components in future fusion reactors and advanced fission systems due to their outstanding creep strength and radiation resistance [1]. One of the critical challenges associated with these materials is their interaction with hydrogen isotopes, where uncontrolled transport and retention may lead to hydrogen embrittlement, tritium inventory issues, and potential radiological safety concerns. The complex microstructure of ODS steels, often characterized by a bimodal grain-size distribution resulting from consolidation techniques such as Spark Plasma Sintering (SPS) or Hot Isostatic Pressing (HIP), has a significant influence on hydrogen diffusion behavior [2].

Modeling of these processes was performed using the Thermo-Calc software package with the DICTRA module. The developed model incorporated key microstructural parameters, including a bimodal grain-size distribution and a high volume density of nanoscale oxide particles acting as effective hydrogen traps and fundamentally altering the hydrogen transport mechanism. These nanoparticles, uniformly distributed throughout the matrix, create a large number of interfaces that serve as efficient trapping sites. According to the diffusion calculations, while the activation energy for hydrogen migration through the crystal lattice is approximately 30.4 kJ·mol$^{-1}$, the presence of these nano-traps with a high binding energy of 44.9 kJ·mol$^{-1}$ and a considerable concentration of about $2.0 \times 10^{25}$ m$^{-3}$ results in a substantial reduction in the overall transport kinetics and a pronounced increase in hydrogen solubility at low temperatures.

To gain a deeper understanding of how microstructural variations affect the transport properties of the material, the results of hydrogen diffusion and trapping simulations are presented and visualized in Figure 1.

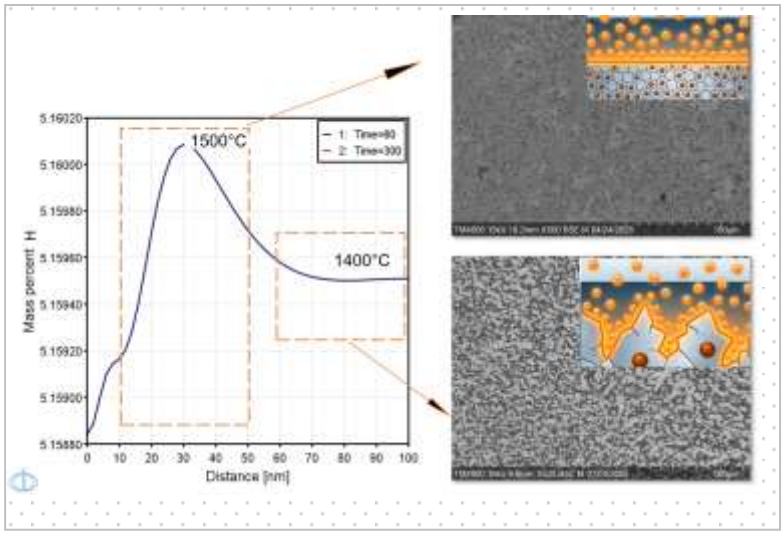



**Figure 1 - Comparative analysis of hydrogen concentration profiles and hydrogen diffusion behavior in ODS steels consolidated at 1400 °C and 1500 °C.**

The modeling results demonstrated that the presence of a high-density dispersion of oxide nanoparticles significantly reduces the effective mobility of hydrogen and promotes its retention within the material. The developed approach can be used to predict tritium transport and retention behavior in advanced ODS steels intended for next-generation fusion and fission reactor applications.

This work was financially supported by the Atomic Energy Agency of the Republic of Kazakhstan under Project BR24792713, “Development of Nuclear Energy in the Republic of Kazakhstan.”

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# Generative Reconstruction of Lithium-ion Battery Electrode Architectures for Mesoscale Electrochemical Analysis

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Over the past decades, significant advancements in battery performance have been achieved primarily through optimization of electrode microstructures and electrolyte compositions, rather than substantial changes in active material chemistry. Nevertheless, the performance of electrochemical energy storage systems is governed by mesoscale electrode morphology, including phase distribution, pore connectivity, and transport pathways. In Ni−rich layered oxide cathodes ($LiNi_xMn_yCo_zO_2$), grain orientation, particle morphology, and pore networks critically influence lithium transport and mechanical stability [1].

Recent generative AI frameworks have demonstrated significant potential for porous electrode reconstruction and optimization, including microstructure generation, transport property prediction and manufacturing-aware design workflows [2–4]. However, most existing approaches primarily focus on morphological descriptors and transport properties such as porosity, tortuosity, diffusivity, and permeability, while electrochemical phenomena are typically incorporated only indirectly through surrogate performance metrics or reduced−order simulations. For example, ElectrodeNet emphasizes anisotropic transport prediction and multiscale transport−informed optimization of porous electrodes [5], while the framework by Kench et al. focuses on manufacturing−aware microstructural optimization coupled with Bayesian analysis and cell−level simulations [2]. Similarly, Lombardo et al. optimize morphological and transport properties in latent space using GAN−based Bayesian optimization [3]. Nevertheless, explicit incorporation of electrochemical heterogeneity, reaction−distribution effects, chemo−mechanical degradation, and physics−informed electrochemical constraints into generative microstructure frameworks remains comparatively underexplored.

In this work, we integrate two−dimensional and three−dimensional microstructural imaging data with conditional generative adversarial networks (cGANs) to capture local chemo−morphological heterogeneities essential to coupled transport and electrochemical reaction processes [Fig. 1]. The purpose of this approach is to establish a data−driven, physics−informed framework that not only reconstructs realistic electrode microstructures but also embeds them into digital twin workflows and multiphysics simulations. This enables accelerated materials discovery cycles and supports degradation−aware fast charging strategies.

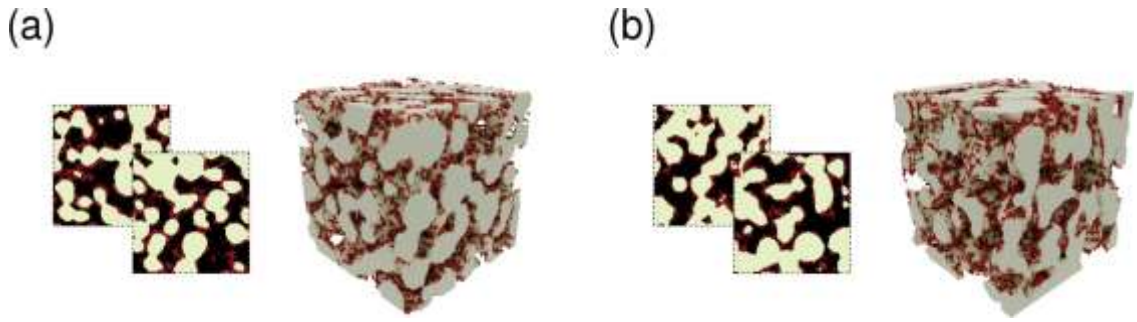



Figure 1. Representative images of NMC cathodes: (a) original 3D microstructure obtained via X−ray computed tomography; (b) AI−generated 3D reconstruction.

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# Hydrometallurgical Processing of Copper - Nickel Sulfide Concentrate to Mixed Hydroxide Precipitate for Battery Applications

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This study proposes an integrated four-stage hydrometallurgical flowsheet – comprising sulfation roasting, water leaching, pre-neutralization, and precipitation – for the conversion of copper - nickel sulfide flotation concentrate from the Maksut deposit (East Kazakhstan) into a mixed hydroxide precipitate (MHP) for battery applications.

Sulfation roasting at 650 $^0$C enabled the transformation of sulfide minerals into water-soluble sulfates while selectively oxidizing iron to hematite. Subsequent water leaching at 90 $^0$C achieved high extraction efficiencies of 86.5% Ni and 95.1% Co, while effectively retaining more than 98.1 % of iron in the solid residue.

Impurity removal was accomplished via selective pre-neutralization with $Ca(OH)_2$ at pH 4.47, leading to the removal of over 99.9% residual iron. Final precipitation using MgO at pH 7.42 yielded a dark green MHP containing 37.68 wt.% Ni and 3.53 wt.% Co, with iron levels below 0.02 ppm. XRD analysis identified jamborite as the dominant phase.

The proposed flowsheet (Figure 1) demonstrates a viable and efficient route for producing battery-grade nickel intermediates from local sulfide resources.

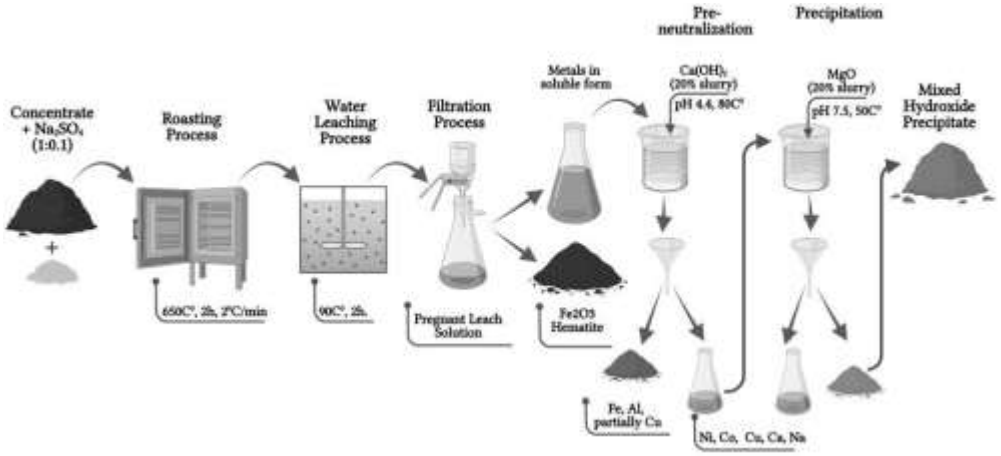



Figure 1. Experimental Flowsheet of the Four-Stage Hydrometallurgical Process for Conversion of Cu–Ni Sulfide Concentrate to MHP.

**Acknowledgementss.** This work was funded by the target program № BR21882402 (2023-2025) “Development of new material technologies and energy storage systems for a green economy” from the Ministry of Science and Higher Education of the Republic of Kazakhstan.

## POSTER SESSION

# Enhanced Ni–Rich Cathodes by Molybdenum Surface Passivation Doping for High Voltage Lithium-ion Batteries

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Increasing the cut-off voltage is important to attain the maximum capacity of Ni based cathodes for LIBs (Lithium – ion batteries). However, Ni cathodes are highly reactive at high voltages which would initiate interfacial surface side reactions on the surface of the electrodes, affects the performance of Ni-rich cathodes will be affected. To overcome this challenge, Mo doping was introduced to enhance the interface/structural stability of Li – batteries. Adding Mo ions , reduces the surface side reactions by supressing the surface active $Ni^{3+}$ species and also helps in stabilizing lattice oxygen through Mo-O bonds, thus prevents structural deformation of cathodes at high operating voltage. As expected Mo doped – Ni rich cathodes delivers the high capacity of 216 mAh $g^{-1}$ with excellent cycle stability of 85% after 150 cycles and enhanced capability at 4.5 V. This study presents a new era in designing advanced Ni based cathodes for lithium ion batteries.

**Keywords:** High voltage, Mo doping, surface passivation, LIBs.

# Development Of Gel Polymer Electrolytes Based On Graphene Oxide-Doped Track-Etched Membranes For All-Solid-State Supercapacitors

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Developing functional solid-state gel polymer electrolytes (GPEs) with high ionic conductivity and excellent mechanical integrity is essential for flexible next-generation energy storage systems [1]. Track-etched membranes (TeMs) serve as an ideal mechanically robust platform with highly uniform, continuous cylindrical nanochannels. However, their native polymeric matrices exhibit low ionic conductivity, requiring tailored chemical functionalization of the pore walls. In this study, we present a comprehensive comparative evaluation of functional GPE architectures based on polyethylene terephthalate (PET) and polycarbonate (PC) track-etched host matrices modified via UV-initiated controlled radical polymerization.

The functional hybrid matrices were fabricated using two distinct synthetic approaches. For the PET-based systems, a poly(acrylic acid) (PAA) track-etched framework was combined with electrospun composite nanofibers made from poly(vinylidene fluoride-hexafluoropropylene) (PVDF-HFP), an ionic liquid ($EMIMBF_4$), and varying concentrations of graphene oxide (GO) as a functional top coating. For the PC-based platforms, GO nanosheets were introduced directly into the polycarbonate composite precursor films prior to ion-beam irradiation and subsequent chemical track-etching. To introduce intensive and uniform ionic conductive pathways along the nanochannel interiors without initiating pore blockage, reversible addition–fragmentation chain-transfer (RAFT) graft polymerization of acrylic acid was successfully optimized for both systems. Successful surface functionalization, progressive nanochannel constriction, and homogeneous filler dispersion were verified by FTIR, XPS, SEM-EDX, and nitrogen adsorption-desorption analyses.

Electrochemical characterizations, including cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS), revealed a pronounced non-linear dependence of transport behavior on GO filler loading. A moderate GO concentration of 0.5 wt% was identified as the absolute optimum for balancing continuous interconnected pathway formation and preventing adverse filler agglomeration or channel obstruction. For the single-sided PVDF-HFP_GO@PET-g-PAA configuration, the total room-temperature ionic conductivity reached $14.83\times10^{-3}$ mS $cm^{-1}$, which further enhanced to $39.08\times10^{-3}$ mS $cm^{-1}$ when deploying a symmetric double-sided electrospun configuration. In parallel, the self-supported, completely layout-flexible PC_GO-g-PAA (0.5 wt% GO) electrolyte matrix exhibited a high specific capacitance of 60 mF $g^{-1}$ at 5 mV $s^{-1}$, combined with exceptional cycling stability characterized by negligible performance loss and a Coulombic efficiency remaining near ~100% over 1500 intensive cycles. The synergetic interaction between confined RAFT grafting networks and carefully adjusted carbonaceous nanofillers highlights the massive potential of multi-component track-etched membrane designs as durable, leakage-resistant electrolytes for supercapacitors.

**Acknowledgments**. This study (grant IRN AP 23487226) was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan.

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# Nickel-Doped Carbon Derived from PET as a Promising Host Material for Lithium–Sulfur Batteries

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Lithium–sulfur (Li–S) batteries are promising energy storage systems owing to their high theoretical capacity and low cost [1]. However, their performance is hindered by low conductivity and the shuttle effect of lithium polysulfides [2].
In this work, nickel-doped carbon was obtained from polyethylene terephthalate (PET) using nickel acetylacetonate ($Ni(acac)_2$) as a precursor (3–7 wt% Ni). The PET-derived carbon matrix is characterized by a porous structure, enabling sulfur confinement, while nickel is associated with enhanced conductivity and the formation of active sites for interaction with polysulfides.
The material is characterized by a partially ordered porous structure [3]. The incorporation of nickel is associated with accelerated polysulfide conversion and suppression of their dissolution [4].

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# Strategies for the Optimization of Electrochemical Deposition of High-Entropy Alloy CuFeCoNiZn

Bakyt Zhappassova [1], Nazym Makanova [1], Ayaulym Belgibayeva [1], Aliya Mukanova [1], Arailym Nurpeissova [1*], and Zhumabay Bakenov [1]

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High-entropy alloys (HEAs) have recently attracted significant interest and may replace conventional alloys due to their outstandi ng performance. Containing five elements within their structure, HEAs exhibit high energy because the number of possible microstates increases with the greater number of elements in the crystal lattice. Consequently, configurational entropy contributes substantially to the overall entropy. HEAs have found applications in energy-storage systems, such as anodes in lithium-ion batteries and electrodes for supercapacitors. However, the primary approach to synthesizing these materials involves mixing salts followed by calcination, which generates hazardous by-products during synthesis. One of the most convenient and straightforward one-step methods for obtaining high-entropy materials is electrochemical deposition. To date, several electrodeposition techniques for high-entropy materials have been explored, but since the constituent elements must have similar reduction potentials, it is usually difficult to obtain an alloy within a single potential or current range [1].

In this work, several electrochemical methods, including but not limited to galvanostatic and potentiostatic approaches, were employed to obtain CuFeCoNiZn HEA. Moreover, different complexing agents were utilized for deposition to monitor their ability to form an alloy, such as citric acid, sodium citrate and sodium citrate monobasic. Ni-foam was selected as the substrate for deposition, and higher mechanical characteristics were potentially achieved due to its larger surface area. The morphology and elemental composition were confirmed by SEM, EDS and XPS. Additional XRD analysis demonstrated that all metals were successfully deposited. Electrochemical tests indicated the pseudocapacitive behavior of the prepared electrode, which may be applied in the fabrication of battery or supercapacitor cells.

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# Upcycled Electrospun PET Membranes as Sustainable Separators for Lithium-Ion Batteries

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The continuous accumulation of plastic waste has become a major global environmental concern, stimulating growing interest in sustainable recycling strategies and the development of environmentally friendly functional materials [1]. Among various polymeric wastes, polyethylene terephthalate (PET) has attracted particular attention owing to its excellent mechanical durability, thermal stability, chemical resistance, and wide availability as post-consumer waste. In recent years, recycled PET has emerged as a promising material for advanced electrochemical and energy storage applications. Owing to its favorable physicochemical properties, PET-based fibrous membranes demonstrate strong potential as separator materials for lithium-ion batteries (LIBs), where high porosity, thermal reliability, and mechanical integrity are critically important [2,3].




Figure 1. Schematic illustration of the fabrication process of electrospun PET-based fibrous separators from waste plastic cups and their application in lithium-ion coin cells.

In this work, fibrous separator membranes were fabricated from recycled PET beverage cups through electrospinning, as illustrated in **Figure 1**. Waste PET was dissolved in a mixed solvent system consisting of trifluoroacetic acid (TFA) and dichloromethane (DCM), followed by electrospinning to obtain porous fibrous membranes. After thermal treatment, the membranes were punched into separator disks and assembled into CR2032 coin cells for electrochemical testing. The obtained membranes exhibited a uniform interconnected fibrous morphology favorable for electrolyte uptake and ion transport. SEM analysis revealed homogeneous fiber distribution throughout the membrane surface and cross-section. The fabricated separators possessed an average thickness of approximately 25 μm and maintained a flexible free-standing structure suitable for LIB applications. The proposed approach demonstrates the potential of converting disposable PET waste into value-added separator materials for sustainable energy storage systems.

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# Electrochemical Synthesis of Simonkolleite

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Simonkolleite ($Zn_5(OH)_8Cl_2 \cdot H_2O$) is a layered zinc hydroxide salt considered a promising precursor material for ZnO nanostructures used in photocatalysis, antimicrobial coatings, sensors, and nutritional applications [1]. Compared with conventional synthesis methods such as co-precipitation and hydrothermal treatment, electrochemical synthesis offers improved control over crystal morphology, lower energy consumption, and environmentally safer processing [2]. However, the mechanisms of electrochemical simonkolleite formation and the optimal synthesis parameters remain insufficiently studied, making this research particularly relevant. In this work, simonkolleite nanostructures were synthesized electrochemically in a $ZnCl_2$ electrolyte using zinc and copper electrodes. The electrolyte consisted of 4M $ZnCl_2$ solution with the addition of tetrapropylammonium hydroxide (TPAH). Cyclic voltammetry was performed in the potential range from −1.1 V to 2.0 V at a scan rate of 10 mV/s and frequency of 50 Hz. The effects of electrochemical parameters, including applied voltage, chloride ion concentration, deposition time, temperature, and electrolyte composition, on the formation of the deposited phase were investigated. The obtained samples were characterized by infrared (IR) spectroscopy (Figure 1). The IR spectra exhibited characteristic absorption bands associated with hydroxyl groups, adsorbed water molecules, Zn–O, and Zn–Cl vibrations, confirming the formation of layered simonkolleite structures. The bands observed at 906, 717, 620, 569, 532, 468 $cm^{-1}$ are attributed to Zn–OH and Zn–O vibrational modes characteristic of simonkolleite [3].

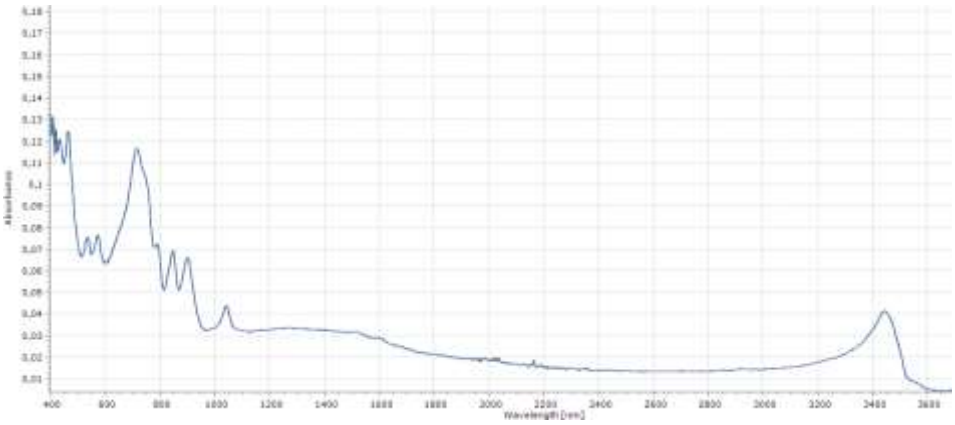


Figure 1. IR spectra of electrochemical synthesized simoncolleite

The experimental results demonstrated that electrochemical synthesis enables controlled formation of thin hexagonal simonkolleite nanostructures under optimized conditions. Excessively high potentials promoted side reduction reactions and structural instability, while moderate electrochemical conditions favored stable crystal growth. The developed electrochemical approach shows strong potential for scalable fabrication of zinc-based layered nanomaterials applicable in advanced energy storage systems and ZnO-derived function

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# The Influence of the Composition of Ni-P thin films on Their Electrocatalytic Properties.

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The hydrogen evolution reaction (HER), a fundamental step in water electrolysis, is of critical importance as hydrogen fuel is considered a clean alternative to fossil fuels for the future. From an electrochemical point of view, HER is strongly dependent on catalyst surface properties and reaction intermediates adsorption behavior. It is desirable that hydrogen be produced via carbon-free methods, utilizing only renewable energy and resources in the production process. The search for cost-effective and catalytically active electrocatalysts for HER remains at the forefront of challenges to its practical and widespread implementation. Transition metal-based compounds are among the primary and low-cost candidates for replacing platinum (Pt). Transition metal phosphides represent an important class of compounds formed by alloying metals with phosphorus. Among them, nickel phosphides ($Ni_xP_y$) stand out as cost-effective catalysts with unique properties and remarkable HER performance. Their importance has recently increased due to the growing demand for scalable hydrogen production technologies. They exhibit high stability under high current densities, which is particularly crucial for large-scale applications [1]. In $Ni_xP_y$ compounds, metallic bonds (Ni-Ni) coexist with stronger ionic bonds-specifically, the bonding between nickel and phosphorus ions. These interactions impart $Ni_xP_y$ with high thermal stability, hardness, and resistance to chemical degradation [2]. In the fabrication of electrocatalysts, phosphides are employed as effective additives that can enhance electrocatalytic performance by optimizing surface morphology and tuning the electronic structure [3]. Additionally, nanostructuring of such materials can further increase the number of active sites available for hydrogen adsorption. The phase diagram of the system includes a wide range of nickel compounds with varying phosphorus content. In this study, Ni-P thin films were synthesized via electrolysis from two different electrolytes, and their electrocatalytic properties were subsequently investigated in an alkaline medium (1 M KOH). During the deposition from an electrolyte containing $NiCl_2 \cdot 6H_2O$, $Na_2HPO_4 \cdot 2H_2O$, $NaH_2PO_4 \cdot 2H_2O$ and $H_3PO_4$, X-ray phase analysis revealed the formation of the $NiP_3$ compound (sample 1). During the electrochemical deposition of Ni-P thin films from an electrolyte containing $NiCl_2 \cdot 6H_2O$, $NiSO_4 \cdot 6H_2O$, $NaH_2PO_4 \cdot 2H_2O$, and $H_3PO_4$, X-ray phase analysis revealed that the resulting film consisted of a mixture of two compounds: $Ni_2P$ and $NiP_2$ (sample 2). Both samples were examined for their catalytic activity in the hydrogen evolution reaction (HER) under alkaline conditions. For this purpose, polarization curves were recorded in a 1 M KOH solution. The obtained experimental data are presented in the figure, which includes not only the two synthesized samples but also comparative curves of the catalytic activity of electrodes traditionally used in the HER. Such comparative analysis allows a clearer understanding of the relative efficiency of newly synthesized catalysts. Based on these polarization curves, Tafel plots were constructed in the coordinates of E(V) - lgi.

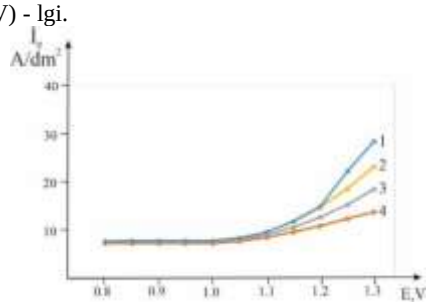



**Fig.** Electrocatalytic activity of the electrocatalysts in the HER in 1 M KOH:1 – Sample No. 1 ($NiP_3$), 2 – Sample No. 2 ($Ni_2P + NiP_2$), 3 – Steel-3, 4 – Nickel.

The slope of the Tafel plots was used to calculate the Tafel angles. The electrocatalytic activity of both samples exceeded that of pure nickel and steel, which are commonly used in industrial water electrolysis. It was found that, in an alkaline medium, the catalytic activity of sample 2, consisting of a mixture of two compounds, was lower and amounted to 203 mV/dec. The highest catalytic activity was observed for sample 1, with a Tafel slope of 135 mV/dec. This suggests a more favorable reaction pathway and faster charge transfer kinetics for the $NiP_3$-based structure.

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# UV-Crosslinked PPC-Based Polymer Electrolyte for Solid-State Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) have become the dominant energy storage technology for portable electronics, electric vehicles, and large-scale energy storage systems due to their high energy density and long cycle life [1]. As the demand for safer and higher-performance batteries continues to grow, significant attention has been directed toward replacing conventional liquid electrolytes, which suffer from safety concerns associated with leakage, volatility, and flammability. These limitations can lead to thermal runaway and restrict the development of next-generation high-energy-density batteries.

Solid polymer electrolytes (SPEs) have emerged as promising alternatives because they combine enhanced safety, good processability, lightweight characteristics, and the potential to suppress lithium dendrite growth [2]. However, the practical implementation of SPEs is still hindered by insufficient ionic conductivity at moderate temperatures, limited mechanical strength, and inadequate interfacial stability with lithium electrodes. Consequently, the design of new polymer electrolyte systems capable of simultaneously providing high ionic conductivity, thermal stability, mechanical robustness, and electrochemical stability remains a major research challenge.

In this work, a UV-photopolymerized solid polymer electrolyte based on chemically modified poly(propylene carbonate) (PPC), hydrolyzed H-MEMO, and polyethylene glycol diacrylate (PEGDA) was successfully developed for solid-state lithium-ion batteries. The prepared membranes were transparent, flexible, and self-supporting, demonstrating excellent film-forming properties. Among the investigated formulations, the SP20 electrolyte (PPC = 2:1) exhibited the highest ionic conductivity of 2.3 $\times 10^{-4}$ S $cm^{-1}$ at 80 °C. The optimized crosslinked structure also provided good thermal stability, with degradation temperatures above 270 °C, while the SP15 sample achieved a tensile strength of 5.67 MPa and an elongation at break of 132.5%. Electrochemical measurements revealed a wide stability window of up to 4.5 V versus $Li/Li^+$ and stable lithium stripping/plating behavior at current densities up to 1.0 mA $cm^{-2}$ for more than 200 h. These results demonstrate that UV-photopolymerized PPC-based electrolytes are promising candidates for advanced solid-state lithium-ion batteries, offering a balanced combination of ionic conductivity, mechanical flexibility, thermal durability, and electrochemical stability.

**Acknowledgments**
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# The Perspective of Functionalized Polylactic Acid-Based Track-Etched Membranes for the Development of Gel-Polymer Electrolytes

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Biodegradable track etched membranes (TeMs) are promising materials for various technological processes due to their high uniformity and controlled pore geometry, which ensures high selectivity and reproducibility of filtration, separation and formation of functional nanostructures [1]. The use of biodegradable polymers such as polylactic acid (PLA) reduces the environmental burden and expands the possibilities of using such membranes in biomedical technologies, tissue engineering and controlled substance delivery systems [2]. In addition, the developed surface and the possibility of chemical modification make them an effective platform for creating sensors, catalytic and composite materials. We propose the development of composite track etched membrane based on polylactice acid with electrospun fibers chitosan and PVA/KCl for its application for gel-polymer electrolyte. PLA TeMs were obtained by the solvent casting method, following this the prepared films were irradiated on DC-60 heavy ion accelerator. The irradiated films were etched in alkali solution (0.1M NaOH) for 40 min. The pore diameter was 330±10 nm. After prepreparation of polymer template the PLA TeMs were functionalized with grafting poly(acrylic) acid (PAA) by UV induced polymerization [3]. The effect of reaction time, precursor concentration, and solvent type was investigated to determine the optimal grafting conditions. According to the findings, the highest value of grafting degree 23% was achieved at monomer concentration 10% after 3h. The grafting degree was determined gravimetrically, while the presence of PAA was confirmed by FTIR and XPS analyses. The fibers of the Ch/PVA/KCl composition were applied by electrospinning at a voltage of 18 eV for 20 minutes. The fiber thickness was around 200 nm.

The electrodes were made from a mixture of 90 wt.% carbon black and 10% by weight% PVDF with the addition of N-methyl-2-pyrrolidone to the required viscosity. The resulting paste was applied to a carbon-coated aluminum foil with a layer of about 25 microns, dried at 50°C for 2 hours and then at 120°C under vacuum overnight, after which it was rolled with a roller press. Symmetrical two-electrode supercapacitors were assembled in an argon glove box using stainless steel components. Electrochemical measurements (EIS, CV, and GCD) were performed at room temperature on a VersaSTAT3 potentiostat. EIS studies of the gel polymer electrolyte were performed in the frequency range of 100 kHz–0.1 kHz. According to the Nyquist diagrams, the ionic conductivity of hybrid HMS with different GO content was calculated; the maximum conductivity was observed at a concentration of 0.5 wt% of graphene oxide. CV measurements were performed in the potential range of 0.5-1.2 V relative to OCP at scanning speeds of 5-1000 mV/s. The specific capacitance of the supercapacitor was calculated based on the obtained voltammograms.

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# Electrodeposition of Corrosion-Resistant Ni–$TiO_2$ Composite Coatings From Aqueous Sulfate Solutions

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Corrosion of metals remains one of the most significant problems of modern materials science, with direct losses estimated at 3–6% of the gross domestic product of industrialized countries. Among the available protection methods, electrodeposition of metallic coatings holds a leading position owing to precise control of coating thickness and uniformity at low process temperatures. However, conventional single-component nickel coatings are characterized by microporosity, which allows aggressive media to reach the substrate and initiate localized corrosion [1]. A promising route to overcome this limitation is the formation of composite electrochemical coatings (CEC), in which inert dispersed particles, such as titanium dioxide ($TiO_2$), are embedded into a metallic matrix, combining the mechanical strength of the metal with the functional properties of the dispersed phase [2].

Titanium dioxide is one of the most attractive dispersed phases for CEC because of its high chemical inertness over a wide pH range, hardness, and low cost. Incorporated $TiO_2$ particles fill pores and microdefects of the nickel matrix, create a physical barrier against the diffusion of aggressive $Cl^-$ ions, and act as additional nucleation centers that refine the grain structure of the deposit. The aim of this work is to determine the influence of the conditions of $TiO_2$ incorporation into the nickel matrix during electrodeposition from a sulfate electrolyte and to evaluate the corrosion resistance of the obtained Ni–$TiO_2$ composite coatings in a chloride medium.

The coatings were deposited galvanostatically at 25°C from an electrolyte containing a Watts bath and suspended $TiO_2$ (10 g/l) under magnetic stirring and cathodic current densities of 100–800 A/ $m^2$ (figure 1).

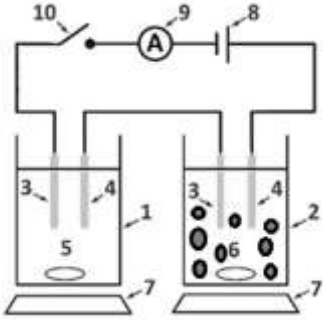



Figure 1. Schematic diagram of the setup for obtaining composite coatings: 1, 2 - electrolytic cells; 3 - anodes; 4 - cathodes; 5 - electrolyte without a dispersed phase; 6 - suspension electrolyte; 7 - magnetic stirrer; 8 - DC power supply; 9 - ammeter; 10 - switch

SEM and EDX mapping showed a uniform distribution of $TiO_2$ particles over the surface of the composite coating , which indicates a non-Faradaic adsorption-electrophoretic mechanism of $TiO_2$ incorporation into the cubic nickel matrix, described by the Guglielmi model. In a chloride medium, nickel corrosion proceeds via an anodic dissolution reaction (1) and a cathodic oxygen reduction reaction (2):

$$Ni \rightarrow Ni^{2+} + 2e^- \quad (1)$$

$$O_2 + 2H_2O + 4e^- \rightarrow 4OH^- \quad (2)$$

The Tafel extrapolation method showed that the incorporation of $TiO_2$ shifts the corrosion potential to more positive values and reduces the corrosion current density compared to pure nickel over the entire investigated range of current densities, since the standard potential of the Ti(IV)/Ti(III) couple is more positive than that of the Ni(II)/Ni(0) couple. Within the practical range of 100–300 A/$m^2$ it did not exceed 0.31 mm/year for the composite versus 0.45 mm/year for the single-component nickel coating.

Thus, the $TiO_2$ particles protect the metal surface from contact with aggressive media and thereby contribute to a decrease in the rate of anodic dissolution of nickel and its corrosion degradation. Furthermore, the introduction of a dispersed phase of $TiO_2$ particles into the coating stimulates the formation of a large number of surface corrosion microcells, in which titanium dioxide nanoparticles act as cathodic regions, while the areas of the nickel matrix act as the anode.

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# First-Principles Study of Y-Doped FeCrAl Alloys: Linking Mechanical Properties with $H_2$ and $O_2$ Surface Interactions

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FeCrAl alloys are considered promising candidates for accident-tolerant fuel cladding due to their excellent oxidation resistance and high-temperature stability; however, their performance is strongly influenced by alloying elements such as yttrium (Y). In this study, a comprehensive first-principles investigation based on density functional theory (DFT) is conducted to evaluate the effect of Y incorporation on the mechanical properties, electronic structure, and surface reactivity of FeCrAl alloys. The results show that Y doping induces lattice expansion and modifies the electronic structure through hybridization of Y-d states with Fe and Cr orbitals. Elastic analysis reveals that although both alloys satisfy mechanical stability criteria, Y addition leads to a reduction in bulk modulus, shear modulus, and hardness, accompanied by increased ductility. Electron localization function (ELF) analysis indicates the formation of localized bonding regions around Y, resulting in heterogeneous bonding and reduced mechanical strength. Surface calculations demonstrate that Y significantly lowers the (110) surface energy, enhancing thermodynamic stability. Adsorption studies reveal weak molecular adsorption of $H_2$ on both surfaces, while $O_2$ undergoes strong dissociative adsorption with substantial charge transfer. Notably, Y doping enhances oxygen adsorption strength and promotes dissociation by increasing electron donation to antibonding orbitals. These findings provide new insights into the role of reactive elements in tuning both bulk and surface properties of FeCrAl alloys, contributing to the design of advanced materials for nuclear energy applications.

# Structural and Mechanical Stability of High-Entropy Diboride under Heavy Kr Ion Irradiation

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High-entropy diborides (HEBs) are considered promising ultra-high-temperature ceramics for nuclear and aerospace applications due to their high melting point, hardness, oxidation resistance, and potential radiation resistance. In this work, the effect of heavy krypton ion irradiation on the structural-phase state and mechanical properties of the high-entropy diboride $(TiHfZrNbTa)B_2$ synthesized by spark plasma sintering (SPS) was investigated [1]. Binary diborides $NbB_2$, $TaB_2$, $CrB_2$ and $TiB_2$ were additionally studied for comparison. Irradiation was performed using 147 MeV Kr ions with a fluence of $10^{15}$ $cm^{-2}$ at the DC-60 cyclotron [2]. Crystal structure and phase composition were studied by X-ray diffraction. Mechanical properties were evaluated by Vickers microhardness measurements. Results are shown in Figure 1 and Figure 2.

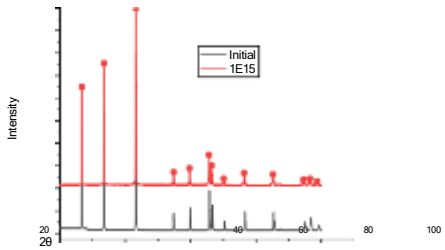



Figure 1. XRD pattern of HEB.

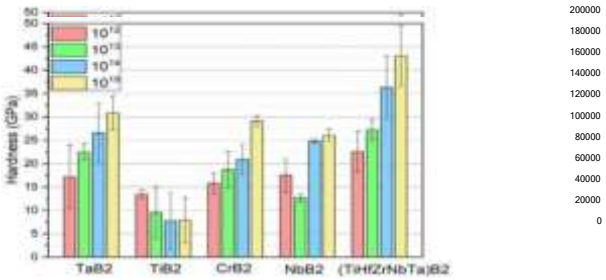



Figure 2. Microhardness evolution of HEB and borides.

XRD analysis confirmed that the HEB retained its single-phase hexagonal $AlB_2$-type structure after irradiation, with no evidence of secondary phase formation or amorphization [3]. Slight peak broadening and shifts toward lower diffraction angles were observed, indicating irradiation-induced lattice distortion and defect accumulation. The absence of radiation-induced amorphization in the HEB is consistent with literature reports indicating that high-entropy ceramics exhibit greater resistance to irradiation and better preservation of their crystalline structure compared with single-component ceramic materials.

The microhardness results demonstrate different responses of the investigated diborides to irradiation. The gradual increase in hardness of the HEB under irradiation is attributed to the accumulation of point defects acting as pinning points for dislocations within the strongly distorted high-entropy lattice, while chemical disordering and the sluggish diffusion effect create high energy barriers that suppress defect migration and prevent the agglomeration of small defects into larger defect clusters [4]. Changes in hardness may be associated with anisotropic variations in lattice parameters and the development of significant internal stresses [4]. The obtained results indicate that the high-entropy diboride retains its crystalline structure and phase composition after irradiation, while the increase in hardness may suggest higher radiation resistance compared with conventional metal diborides.

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# Radiation-Reduced Few-Layer Graphene Oxide as a Functional Nanofiller for Radiation-Resistant Polymer Coatings and Composites for Auxiliary Nuclear Power Plant Systems

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The development of radiation-resistant polymer coatings and composites is an important task for improving the durability of auxiliary systems of nuclear power plants, where materials may be exposed to ionizing radiation, thermal ageing, humidity, corrosion media and decontamination chemicals. In this work, radiation-reduced few-layer graphene oxide is proposed as a multifunctional nanofiller for protective polymer coatings and composite materials intended for non-core and auxiliary nuclear applications.

The material is obtained through a controllable route including graphite oxidation to graphene oxide, delamination to few-layer graphene oxide, and subsequent radiation-induced reduction using accelerated electron beam treatment. This approach enables the formation of reduced graphene oxide without conventional chemical reducing agents and provides an opportunity to tune the balance between residual oxygen-containing functional groups, defect structure, hydrophobicity and electrical conductivity. Such tunability is essential because different nuclear-related applications require different filler characteristics: barrier coatings require improved dispersion and tortuous diffusion pathways, radiation-resistant polymer matrices require stable interfacial interaction and reduced degradation, while diagnostic or sensing layers may benefit from controlled electrical conductivity.

The proposed research focuses on the incorporation of radiation-reduced few-layer graphene oxide into model epoxy and elastomeric polymer matrices. The structure of the nanofiller and composites is planned to be evaluated by Raman spectroscopy, X-ray photoelectron spectroscopy, scanning electron microscopy, thermal analysis and electrical conductivity measurements. Functional performance will be assessed through mechanical testing, adhesion, electrochemical impedance spectroscopy, water uptake, and comparative ageing under radiation and thermal-humidity conditions. Special attention is given to the relationship between the degree of radiation reduction and the resulting barrier, mechanical, electrical and ageing-resistant properties of the polymer system.

Compared with conventional fillers such as carbon black, mineral platelets, nanoclays and chemically reduced graphene oxide, radiation-reduced few-layer graphene oxide offers a potentially cleaner and more application-tailored route to multifunctional polymer modification. Unlike heavy-metal or boron-containing shielding materials, the proposed nanofiller is not positioned as a primary radiation shielding component, but as a low-loading functional additive for protective coatings, secondary polymer composites and condition-monitoring layers in auxiliary nuclear power plant systems. The expected advantage is the combination of enhanced barrier performance, improved resistance to radiation-induced ageing, reduced material weight and possible integration of diagnostic functionality.

The results are expected to provide a scientific basis for the application-specific design of radiation-reduced graphene oxide nanofillers for advanced polymer materials operating in nuclear and extreme energy environments. The proposed approach may contribute to the development of durable protective coatings, radiation-resistant secondary composites and smart monitoring materials for auxiliary systems of nuclear power plants.

# Classical Molecular Dynamics of Anion Diffusion in Fluorite Crystals: Potential Reconstruction and Investigation of Chlorine Diffusion in $SrCl_2$

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Fluorite-structured crystals play an important role in modern science and technology. Typical representatives of this class are nuclear fuel materials $UO_2$, $ThO_2$, and $PuO_2$, for which understanding diffusion mechanisms is essential for modeling charge and mass transport processes under neutron irradiation. Fluorite crystals also include $BaF_2$, $CaF_2$, $SrF_2$, and $SrCl_2$, whose properties as solid-state electrolytes are determined by the mechanisms of anion diffusion. $SrCl_2$ is of particular interest because consistent experimental data on ionic conductivity are available over a wide temperature range, from room temperature to the melting point [1]. In addition, the mass of the mobile anion in $SrCl_2$ differs significantly from that of oxygen and fluorine, which is likely to affect the characteristics of anion transport.

In this work, a series of interionic potentials in the Buckingham form $A \cdot exp(-Br) - C/r^6 + Qq_iq_j/r$ were reconstructed for $SrCl_2$ using two different approaches. In the first approach, the Cl–Cl interaction parameters were partially fixed using literature data [2, 3], while the remaining parameters were determined by fitting to the experimental high-temperature properties of the crystal. In the second approach, the Cl–Cl interaction calculated using the Hartree–Fock method with correlation-energy correction was employed, after which the Sr–Cl interaction was reconstructed from the temperature dependence of the lattice constant.

The obtained potentials, together with a potential previously reported in the literature, were used to calculate the temperature dependence of the diffusion coefficient by molecular dynamics simulations using the Einstein relation, $\langle a^2(t) \rangle = 6Dt$. The potential based on the Cl–Cl parameterization from Ref. [2] demonstrates good agreement with the experimental diffusion coefficient data [4] (Fig. 1). The potential based on the Hartree–Fock Cl–Cl interaction reproduces well the anion diffusion coefficient derived from experimental ionic conductivity data when normalized by the superionic transition temperature, $ln(D) = f(Ts/T)$ (Fig 2). The obtained results indicate that this approach is promising for describing anion diffusion in $SrCl_2$. Future work will focus on static calculations of defect formation energies and activation energies of various diffusion mechanisms in order to establish their relationship with different temperature regimes. The work was supported by the Ministry of Science and Higher Education of the Russian Federation, project No. FEUZ-2026-0010.

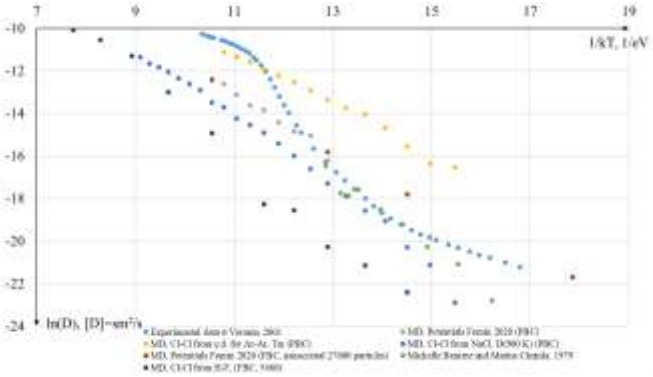



Figure 1. Temperature dependence of the diffusion coefficient of chlorine in $SrCl_2$ $ln(D)=f(1/kT)$.

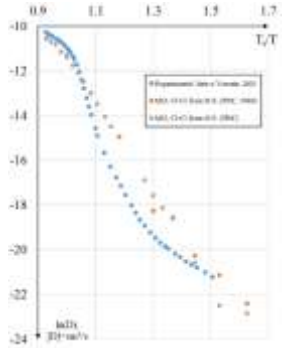



Figure 2. Dependence on the reduced temperature $lnD=f(T_s/T)$.

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# Assessment of Volumes and Radiological Characteristics of Solid Radioactive Waste Generated During the Decommissioning of the BN-350 Reactor

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The BN-350 reactor was the world's first industrial fast neutron reactor and represented a major milestone in the development of sodium-cooled fast reactor technology. The BN-350 reactor was commissioned on 16 July 1973 in Aktau, Kazakhstan. It operated successfully for approximately 20 years before it was permanently shut down in 1999 and entered the decommissioning phase [1].

The decommissioning of the BN-350 reactor was divided into five main stages. The third stage includes activities with a solid radioactive waste (SRW). The composition of BN-350 reactor SRW includes various materials accumulated both during operation and decommissioning. The conducted assessment of the quantity and composition of SRW shows that the total mass of waste in the storage facility currently amounts to more than ~7000 tons with a total activity of $5.17\times10^{14}$ Bq. Most of the total activity is associated with a relatively small fraction of high-activity waste, accounting for ~170 tons with a total activity of $4.73\times10^{14}$ Bq. The results indicated that low-level waste constitutes the majority of the accumulated SRW. A preliminary assessment showed that it accounts for approximately 89% of the total mass of solid radioactive waste [2].

To determine the appropriate ways of further handling SRW, a radiological assessment was carried out, including the identification and quantification of radionuclides with a special emphasis on gamma-emitting radionuclides. 15 samples were selected to reflect the diversity of the accumulated waste. They cover the main categories of SRW currently in storage, including building materials, metallic com-ponents, and composite structures. The selected waste is representative of the majority of the currently accumulated SRW of the BN-350 reactor.

The results showed that Cs-137 is the dominant gamma-emitting radionuclide in all studied samples. The absence of other identified radionuclides above the MDA does not exclude their presence but suggests that their contribution to external dose is second-ary under the given measurement conditions. The measured ambient dose equivalent rates (0.2–14 μSv/h at 1 m) demonstrate a wide variability in radiological hazard. These values significantly exceed public exposure limits and, in some cases, approach or exceed occupational dose constraints under con-tinuous exposure scenarios. This confirms that even low-level waste, as classified by ac- tivity concentration, may present non-negligible external radiation hazards and therefore requires controlled handling conditions, including shielding and access restrictions. An important observation is the non-uniform distribution of contamination, evi-denced by localized areas of elevated dose rates [3].

The results also support the feasibility of a differentiated waste management strategy. For low -activity waste streams, conditioning and long-term storage remain the primary approach. However, for metallic waste, the high contribution of Cs-137 suggests that decontamination techniques targeting this radionuclide can be particularly effective. In this context, remelting technologies, including electroslag and induction slag remelting, repre-sent promising solutions [4].

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# Influence of Synthesis Parameters on the Structural Formation of Oxide Dispersion-Strengthened Steel

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The development of modern nuclear power engineering is characterized by an active transition to next-generation reactor technologies, including Generation IV fission reactors and future fusion reactors. According to assessments by the International Atomic Energy Agency (IAEA), unlike conventional power reactors, these systems are expected to operate under significantly elevated temperatures, intense neutron fluxes, and increased thermomechanical loads. Such advances in nuclear reactor technology are accompanied by corresponding new requirements for structural materials [1]. Current research on structural materials is focused on the development of multifunctional materials capable of maintaining structural stability under extreme operating conditions. In this context, ferritic–martensitic oxide dispersion-strengthened steels (ODS steels) are of particular interest as promising structural materials. The enhanced performance of ODS steels is achieved through the incorporation of nanoscale yttrium oxide ($Y_2O_3$) particles, which stabilize the material microstructure, hinder dislocation motion, and act as effective sinks for radiation-induced defects [2].

The synthesis of ODS steels is carried out using powder metallurgy techniques, including mechanical alloying (MA) and subsequent sintering of the resulting powder mixture. A uniform distribution of oxide particles within the metallic matrix is achieved during the MA process. Among the existing technologies for consolidating the obtained powder mixture, spark plasma sintering (SPS) is considered a promising method. Due to the simultaneous application of electric current and pressure, this technique limits grain growth and ensures uniform densification of the material throughout its volume [3]. The conventional route for the production of ODS steels typically involves the use of pre-alloyed steel powder followed by the incorporation of yttrium oxide through mechanical alloying [4]. As a result, the strengthening dispersed phase is formed within an already established matrix, which may lead to a non-uniform distribution of oxide particles and reduce the effectiveness of their interaction with dislocations and grain boundaries.

In the present study, an alternative approach was implemented, in which the steel matrix was synthesized directly from the initial metallic component powders with the simultaneous addition of $Y_2O_3$ during the mechanical alloying stage, followed by consolidation using spark plasma sintering. This approach enables the concurrent formation of the matrix and dispersed phase, promoting a more uniform distribution of oxide nanoparticles and a controlled development of the material's defect structure.

It was established that the SPS temperature has a significant effect on the structural and phase state of the ODS steel. Throughout the entire investigated temperature range, α-Fe(Cr) remained the dominant phase, indicating the formation of a metallic matrix based on a BCC solid solution. $Y_2O_3$ reflections were detected in the samples sintered at 1000–1400 °C, confirming the retention of the oxide strengthening phase after consolidation. In the sample produced at 1500 °C, weak $Fe_3O_4$ reflections were additionally observed, which are associated with surface oxidation of the material. The results demonstrate that mechanical alloying provides effective dispersion of the powder mixture, whereas the SPS regime determines the structural and phase state of the sintered samples. The obtained findings indicate that a sintering temperature of 1400 °C provides the most favorable combination of phase composition and stability of the oxide strengthening phase, making this processing condition promising for the fabrication of radiation-resistant ODS steels.

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# Development and Performance Assessment of Uranium–Graphite Fuel Matrices for the IGR Research Reactor LEU Conversion

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The conversion of research reactors from highly enriched uranium (HEU) to low-enriched uranium (LEU) fuel remains one of the key objectives of international efforts aimed at strengthening nuclear security while maintaining the scientific and technological capabilities of existing research reactor facilities. Within this context, the conversion of the Impulse Graphite Reactor (IGR) [1-3] requires the development of a graphite-based fuel matrix capable of meeting both neutronic and engineering requirements. Unlike conventional research reactor fuels, the IGR concept relies on uranium-containing graphite elements, making the development of uranium–graphite fuel matrices a critical component of the LEU conversion.

This work summarizes recent progress in the development and characterization of uranium–graphite fuel matrices based on nuclear-grade graphites IG-110U and IG-430U. The proposed approach is based on the impregnation of graphite with uranium-containing solutions through the graphite pore structure, followed by thermal treatment to obtain stable uranium-containing phases within the graphite matrix. Particular attention was given to the influence of graphite characteristics and impregnation conditions on uranium loading efficiency, distribution uniformity, and the resulting material performance.

Experimental studies were performed on graphite specimens manufactured by Toyo Tanso Co.,Ltd., and representative graphite block fragments using both boiling- and vacuum-assisted impregnation routes. The developed matrices were characterized using a combination of gravimetric measurements, elemental analysis, optical and electron microscopy, X-ray diffraction (XRD), and thermal analysis techniques. Uranium concentration profiles were evaluated at different locations within the graphite specimens to assess loading homogeneity and the effectiveness of the impregnation procedures.

As part of the material characterization, additional performance assessments were conducted under conditions relevant to the IGR conversion program. The evaluation program comprised high-temperature thermal exposure and repeated thermal cycling in an inert atmosphere, followed by structural and mechanical characterization of the treated samples. The obtained results demonstrated successful introduction of uranium-containing phases into both graphite grades and confirmed the preservation of structural integrity after thermal treatment.

The results highlight the importance of graphite microstructure and impregnation methodology in achieving uniform uranium distribution and reliable fuel-matrix performance. The developed experimental approach provides a practical framework for further optimization of uranium impregnation processes and supports ongoing efforts toward the qualification of graphite-based LEU fuel for the IGR research reactor.

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# General Match Characteristics for MagLIF Liner Material

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The laser-ignited Magnetized Liner Inertial Fusion (MagLIF) scheme is currently one of the most promising approaches for the practical implementation of thermonuclear fusion [1, 2]. The significance of theoretical and experimental research in this area lies in finding solutions to a number of problems, such as studying of the optimal thermonuclear fuel composition, optimizing ignition conditions, developing effective nuclear physics methods for hot plasma diagnostics, designing constructional appearance and other. The nature of some effects still need further detailed studies. Successful research will allow us to advance the search for an efficient thermonuclear fusion facility and will be of great value for the future of energy.

One of the problems requiring a rational solution in MagLIF is the optimal choice of liner material, which is a structural component of the fuel capsule and plays an important role in achieving fusion fuel ignition conditions. The burning pattern will be determined by MagLIF fuel in main and adjusted by related accompanying processes, such as constructional particles involvement. In [3], promising fuel types are considered and analyzed. The traditional types are pure deuterium fuel and DT, $D^3He$ mixtures. Impurities from structural materials will inevitably be present in the fuel during the burning stage, as the entire system requires extreme conditions for thermonuclear fusion. Under these conditions, mainly defined by solid-state material densities and energies in the keV and above range, the fuel will apparently be in a plasma state. Therefore, the involvement of liner material particles and their impact on fuel burning must be thoroughly studied. An analysis of some options for liner material and other additional construction material is done in [1]. Here, we analyze the role of the liner in the operation of the MagLIF device.

The influence of several factors that must be considered when selecting a material for the MagLIF liner and choosing its optimal configuration are examined. Some characteristics include:

1) High breaking strength: to retain the fuel within until experimental work begins;
2) High electrical conductivity: to efficiently conduct the current discharge;
3) High heat capacity: to rapidly heat up and melt the liner;
4) Resistance to magnetohydrodynamic instabilities: to prevent premature failure of the system. This includes initially optimal material characteristics, such as density, uniformity of material distribution throughout the volume, etc.;
5) Participation in exothermic nuclear reactions: to actively generate additional energy output and heat the burning zone;
6) Participation in energy transfer processes: to actively exchange energy between burning zones;
7) Participation of liner particles and reaction products of fusion in thermonuclear fuel burning: to actively catalyze burning;
8) Diagnostic capabilities: to obtain reaction products that can be used to diagnose the fuel burning zone;
9) Contribution to system stability: to reduce the risks of premature Z-pinch failure;
10) Contribution to radiation losses: to minimize radiation losses due to bremsstrahlung.

In [1] the use of metallic beryllium capsule is proposed. Therefore, as an example, one of the optimal materials for the liner's shell, $^9Be$, is considered. An analysis of the element's passive participation in MagLIF thermonuclear burning is conducted based on calculations of the burning kinetics of traditional thermonuclear fuels.

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# Thermodynamic and Kinetic Basis for Mechanical Activation and SPS Densification of W–Cu Composites

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Nanostructured W-Cu pseudoalloys are promising materials for heat-loaded electrical contacts, heat-sink components and extreme-energy systems because they combine the refractory skeleton of tungsten with the high electrical and thermal conductivity of copper [1]. Their processing remains difficult because W and Cu have very limited mutual solubility, poor wettability and a strong thermodynamic tendency to remain separated, which complicates densification and microstructural homogenization [1,2].

This work presents a calculation-guided processing route for 70W-30Cu and 75W-25Cu powder compositions intended for high-energy mechanical activation followed by short-cycle spark plasma sintering (SPS) (Fig.1). Thermodynamic calculations were used to evaluate phase stability, mixing enthalpy, component activities and processing-related phase limitations. Kinetic simulations were used to estimate interfacial diffusion under short SPS thermal exposure. The results show that mechanical activation should be considered primarily as a defect- and interface-generation step rather than as a full alloying stage. Its role is to increase W/Cu contact area, refine the composite precursor and improve the probability of capillary-assisted rearrangement during SPS.

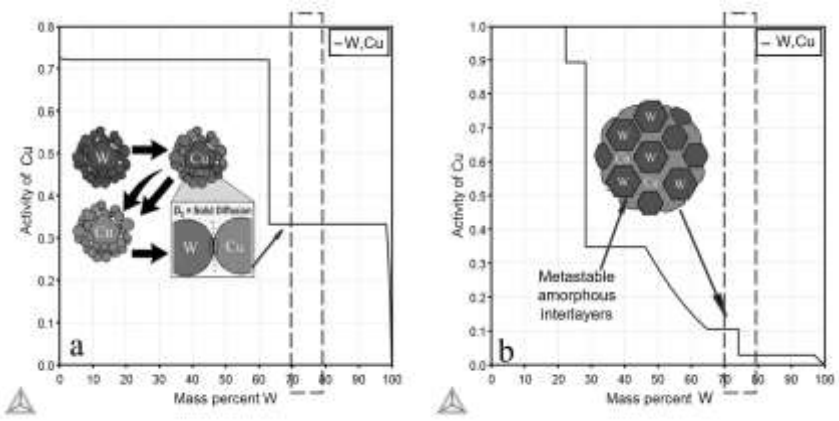



Figure 1. Calculated copper activity map in the W–Cu system combined with a schematic representation of possible nanoscale microstructural changes: (a) 950 °C; (b) 1050 °C.

The calculated thermodynamic response supports the use of short SPS cycles that enhance densification while limiting copper redistribution, tungsten grain coarsening and loss of nanoscale structural features. For the selected compositions, the expected target microstructure consists of a W-rich load-bearing framework with a connected Cu phase. A practical verification window is proposed: powder morphology and particle-size distribution after activation; oxygen content; XRD phase stability; relative density; W/Cu phase connectivity by SEM/EDS; hardness; and electrical or thermal response. The proposed route provides a basis for experimental optimization of W-Cu nanocomposites without introducing sintering activators that may degrade functional conductivity.

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# Wildfire Real-Time Power Generation and Carbon Dot Energy Storage Technology

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Wildfires are extreme natural events that cause severe environmental damage worldwide every year. However, wildfires release a large amount of thermal and chemical energy that can be captured and stored efficiently. This energy could serve as a valuable resource for power supply and post-disaster recovery in remote and fire-affected areas. Recent research has explored a range of wildfire energy capture and storage technologies, including thermoelectric conversion, fuel cells, thermoacoustic power generation, and carbon dot-based energy storage materials. Thermoelectric materials have shown enhanced heat-to-electricity conversion efficiency under high-temperature conditions. Carbon dots, an emerging class of carbon nanomaterials, have similarly attracted attention for their excellent electrical conductivity, tunable surface chemistry, and long-term cycling stability, with applications in lithium-ion batteries, sodium-ion batteries, and supercapacitors. The further integration of artificial intelligence and Internet of Things technologies into these systems offers new optimization pathways for smart energy systems, thus improving the reliability and efficiency of wildfire energy utilization.

Fresh leaves of three species, *Salix alba (*white willow), *Pyrus ussuriensis* (Manchurian pear), and *Acer negundo* (boxelder maple), were collected from the Nazarbayev University campus (Astana, Kazakhstan). The leaves were fully carbonized by open-flame combustion and diluted in autoclaved water at a 1:50 ratio. After 2 hours of equilibration at room temperature, zeta potential and particle size distribution were measured by using a ZetaView TWIN Nanoparticle Tracking Analysis instrument.

All three ash suspensions exhibited negatively charged surfaces, with zeta potential distributions ranging from approximately -53 to -3 mV (*Salix alba*), -54 to -1 mV (*Pyrus ussuriensis*), and -47 to -1 mV (*Acer negundo*), with peak frequencies between -20 and -30 mV across all samples. Particle size distributions varied by species, with *Pyrus ussuriensis* and *Acer negundo* yielding finer and more narrowly distributed particles (majority of signals below 900 nm) compared to *Salix alba* (dominant peak between 1100 and 1400 nm).

The consistent negative surface charge observed across all three species indicates good colloidal stability and electrochemical potential, supporting the viability of wildfire ash as a renewable precursor for carbon dot synthesis and subsequent energy storage applications. In a broader context, this review systematically summarizes the latest research progress in wildfire energy utilization, analyzes the applicability of different technologies and their synergy, and explores the potential of intelligent optimization in energy systems. Overall, these findings may lead to an integrated and sustainable framework for wildfire energy harvesting that could meaningfully support power supply and post-disaster recovery in remote and fire-affected regions.

# Pre-Feasibility Study of Radioisotopes Production for Nuclear Batteries at The Wwr-K Reactor

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The WWR-K reactor is a multipurpose research reactor capable of supporting a broad spectrum of scientific, technological, and industrial applications, including neutron activation analysis, materials testing, radioisotope production, and irradiation research [1-4]. As part of Kazakhstan's strategic efforts to establish domestic capabilities in advanced nuclear technologies, particular attention is being given to the development of radioisotope-based nuclear batteries utilizing locally produced radioisotopes [5]. In this context, the WWR-K reactor is considered a promising irradiation facility to produce radioisotopes required for radioisotope power sources.

This paper presents the preliminary results of a feasibility assessment of radioisotope production at the WWR-K reactor for nuclear battery applications. The study focuses on three strategically important radioisotopes: Ni-63, Sr-90, and H-3 – which are widely recognized as potential energy sources for long-life radioisotope power systems. Neutron activation and irradiation analyses were performed to evaluate the time-dependent production characteristics of these isotopes under the current operational conditions of the reactor. The corresponding irradiation curves were analyzed to determine isotope accumulation rates, achievable production yields, and the evolution of specific activity as a function of irradiation time.

Based on the results obtained, optimal irradiation conditions for each target radioisotope were identified, considering the existing neutron flux distribution and operational constraints of the WWR-K reactor. Furthermore, several technical approaches are proposed to improve production efficiency, including optimization of irradiation positions, target design, irradiation schedules, and neutron spectrum utilization. The implementation of these measures is expected to increase isotope yield and enhance the specific activity of the produced radioisotopes, thereby improving the technological feasibility of domestic radioisotope production for future nuclear battery systems. The results demonstrate the potential of the WWR-K reactor to serve as a key infrastructure element in Kazakhstan's emerging radioisotope production program and provide a basis for further optimization studies and experimental validation.

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# Modeling of Hydrogen Diffusion Kinetics and Trapping Processes in Complex Alloyed Oxide Dispersion Strengthened (ODS) Steels

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Oxide Dispersion Strengthened (ODS) steels, such as ODS-EUROFER and 14Cr ferritic ODS variants, are considered leading candidate materials for structural components in future fusion reactors and advanced fission systems due to their outstanding creep strength and radiation resistance [1]. One of the critical challenges associated with these materials is their interaction with hydrogen isotopes, where uncontrolled transport and retention may lead to hydrogen embrittlement, tritium inventory issues, and potential radiological safety concerns. The complex microstructure of ODS steels, often characterized by a bimodal grain-size distribution resulting from consolidation techniques such as Spark Plasma Sintering (SPS) or Hot Isostatic Pressing (HIP), has a significant influence on hydrogen diffusion behavior [2].

Modeling of these processes was performed using the Thermo-Calc software package with the DICTRA module. The developed model incorporated key microstructural parameters, including a bimodal grain-size distribution and a high volume density of nanoscale oxide particles acting as effective hydrogen traps and fundamentally altering the hydrogen transport mechanism. These nanoparticles, uniformly distributed throughout the matrix, create a large number of interfaces that serve as efficient trapping sites. According to the diffusion calculations, while the activation energy for hydrogen migration through the crystal lattice is approximately 30.4 kJ·mol$^{-1}$, the presence of these nano-traps with a high binding energy of 44.9 kJ·mol$^{-1}$ and a considerable concentration of about $2.0 \times 10^{25}$ m$^{-3}$ results in a substantial reduction in the overall transport kinetics and a pronounced increase in hydrogen solubility at low temperatures.

To gain a deeper understanding of how microstructural variations affect the transport properties of the material, the results of hydrogen diffusion and trapping simulations are presented and visualized in Figure 1.

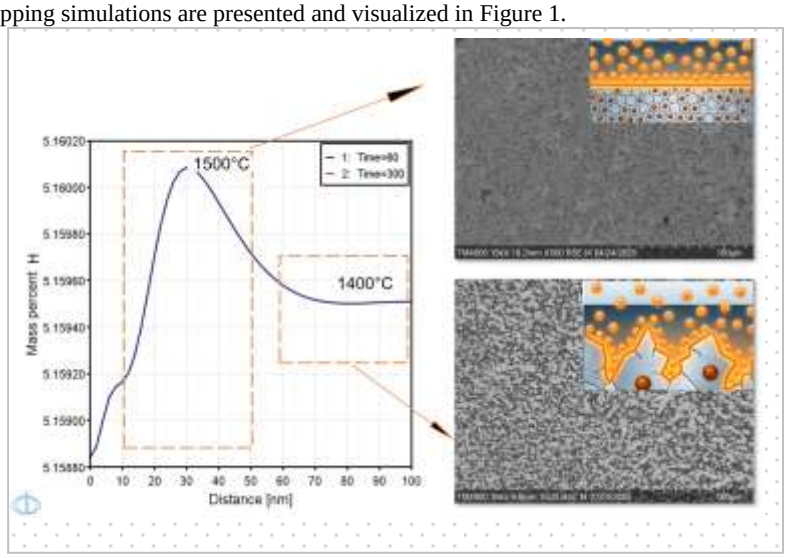



Figure 1 - Comparative analysis of hydrogen concentration profiles and hydrogen diffusion behavior in ODS steels consolidated at 1400 °C and 1500 °C.

The modeling results demonstrated that the presence of a high-density dispersion of oxide nanoparticles significantly reduces the effective mobility of hydrogen and promotes its retention within the material. The developed approach can be used to predict tritium transport and retention behavior in advanced ODS steels intended for next-generation fusion and fission reactor applications.

**Acknowledgement.** This work was financially supported by the Atomic Energy Agency of the Republic of Kazakhstan under Project BR24792713, “Development of Nuclear Energy in the Republic of Kazakhstan.”

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# Valence Electron Rules and The Expanding Family of Heusler Compounds: from Ternary to Quaternary Architectures

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Ternary intermetallic Heusler compounds constitute one of the most extensively studied families of materials, owing to their structurally simple cubic arrangements and remarkable versatility across numerous applications. A key feature enabling predictive materials design is the exceptional agreement between their electronic structure and simple valence electron counting principles, specifically the Slater-Pauling and 18-electron rules. Three primary ternary variants are well established: full Heusler
($X_2YZ$), inverse Heusler ($XY_2Z$), and half Heusler (XYZ) [1]. Despite the wealth of knowledge accumulated on these ternary systems, the exploration of quaternary Heusler compounds ($XX'YZ$) remains comparatively limited. This disparity is largely
attributed to the increased complexity inherent to the quaternary phase space, which presents both a challenge and an opportunity for discovering novel functional materials.

Recently, particular attention has turned toward lithium based quaternary Heusler compounds (XLiYZ), driven by the growing demand for lightweight, earth-abundant materials in energy-related technologies. The incorporation of Li, the lightest metal, not only significantly reduces the mass density of the alloy but also introduces unique electronic and electrochemical properties that are absent in conventional transition-metal-based Heusler phases [2]. These Li-based quaternary systems are emerging as promising candidates for next-generation lithium-ion battery electrodes, solid-state electrolytes, and spintronic devices requiring low magnetization damping. However, their experimental realization remains challenging due to lithium's high reactivity and tendency to occupy interstitial sites, while theoretical predictions using the Slater-Pauling rule for such compounds are still in their infancy. Therefore, the targeted synthesis and characterization of Li-containing quaternary Heusler alloys represent a timely and underexplored frontier, with significant potential for both fundamental understanding and applied innovation [3]. Figure 1 presents a schematic band structure of an 18-electron half-Heusler compound. As shown, the high d-type density of states near the Fermi level in the valence band leads to a large Seebeck coefficient S.

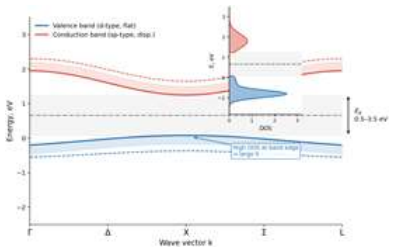


Figure 1. Schematic band structure of an 18-electron half-Heusler compound. The high density of states (DOS) of the valence band of d-type character near the Fermi level gives rise to a large Seebeck coefficient S

Among the various criteria guiding the prediction of novel compounds, thermodynamic stability remains both the most essential and the most demanding to satisfy. In the present work, this criterion is rigorously assessed along three complementary axes. First, stability is evaluated against all competing equilibrium phases existing within the quaternary Li-X-Y-Z phase space. Second, the influence of chemical disorder is examined, considering both disorder localized within a single rock-salt sublattice and disorder distributed between two distinct rock-salt sublattices. Third, for any fixed composition XLiYZ, the relative stability of competing quaternary crystal structures is systematically compared. This multi-tiered approach provides a robust framework for identifying thermodynamically viable lithium-containing quaternary Heusler compounds and avoiding metastable or decomposable candidates [4].

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# Physics-Constrained Generative AI for Reconstruction and Design of SOFC Electrode Microstructures

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Solid oxide fuel cells (SOFCs) are promising electrochemical energy conversion devices due to their high efficiency, fuel flexibility, and potential for integration into sustainable energy systems. However, their performance and durability are strongly governed by mesoscale electrode morphology, including pore connectivity, phase distribution, and transport pathways. In addition, thermally activated degradation phenomena such as Ni coarsening, TPB loss, and phase redistribution significantly affect transport processes and electrochemical activity during operation [1, 2].

Traditional simulation and reconstruction approaches for SOC electrode microstructures are computationally expensive and difficult to scale for large parametric studies, uncertainty quantification, and optimization tasks. In this work, we propose a computational framework for realistic reconstruction and controllable generation of SOC electrode microstructures using physics-constrained neural networks (PCNs) and conditional generative adversarial networks (cGANs). Unlike conventional generative approaches that primarily focus on morphological similarity [3], the proposed framework incorporates physics constraints associated with transport-relevant structural descriptors.

By integrating microstructural datasets into data-driven generative pipelines, the framework captures heterogeneities governing coupled mass, charge, and ionic transport processes. Furthermore, the proposed approach enables conditioned generation of porous electrode architectures with targeted structural and electrochemical characteristics, supporting inverse microstructure design and virtual optimization. The generated microstructures can be directly coupled with pore-scale simulations, digital twin workflows, and multiscale electrochemical models for rapid virtual testing, degradation analysis, and performance prediction. The proposed PCN-cGAN framework demonstrates the potential of physics-aware generative artificial intelligence and computational modelling for scalable, electrochemically informed design and optimization of next-generation SOFC electrodes.

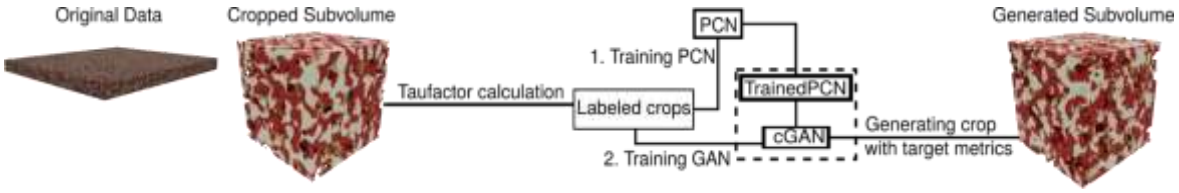



Figure 1. Computational workflow for reconstruction and design of porous SOFC electrode microstructures using physics-constrained neural networks (PCNs) and conditional generative adversarial networks (cGANs)

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# Modeling of Perovskite Solar Cells with a Hybrid Electrode Structure

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Hybrid organic-inorganic perovskites are among the most promising and cost-effective materials due to their outstanding optoelectronic properties, including a high absorption coefficient, long electron and hole diffusion lengths, high charge-carrier mobility, a narrow band gap, and good stability [1-4]. However, the fundamental optical properties of perovskites, such as absorption, parasitic absorption, reflection, and transmission, remain insufficiently studied, despite being important parameters for assessing their suitability for high-efficiency optoelectronic devices.

In this work, in addition to the optical properties, the electrical characteristics of the device, including current-voltage characteristics and the effects of defect density, bulk defect density, and surface recombination, were investigated. The optical and electrical characteristics were studied using COMSOL Multiphysics based on the drift-diffusion model. Poisson's equation, the charge-carrier continuity equations, and the current-density equations were solved. The model accounted for the major recombination mechanisms. Figure 1 shows the structure of the QIBC hybrid model used in this study and its corresponding energy-band diagram.

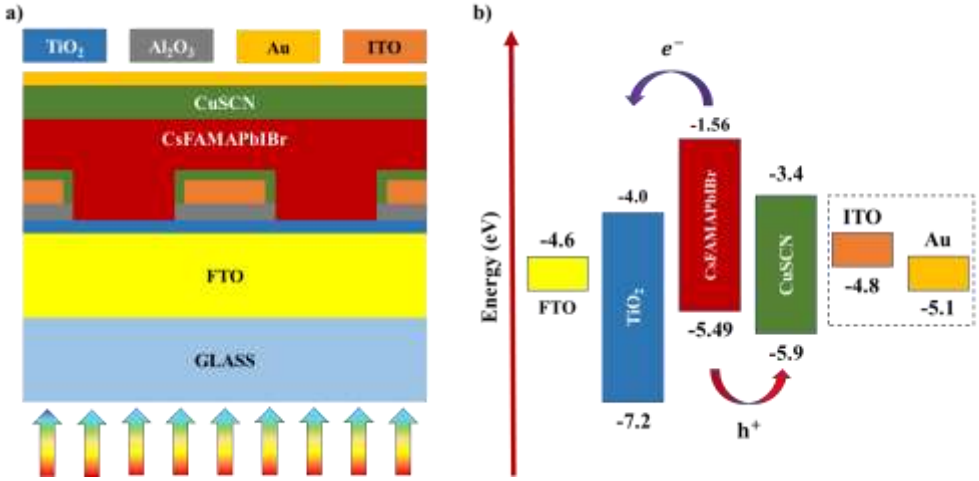



Figure 1. a) structure of the hybrid QIBC model and b) energy band diagram.

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# Numerical Simulation of Thermophysical Processes in a Metal Hydride Hydrogen Storage System and Analysis of Methods for Enhancing Heating Uniformity

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The research focuses on thermophysical processes in metal hydride hydrogen storage systems, which are considered one of the most promising solid-state energy storage technologies. One of the major challenges in this field is the low heat transfer efficiency in the porous medium, resulting in non-uniform temperature distribution throughout the metal hydride material and consequently reducing the rates of hydrogen absorption and desorption [1]. The aim of this study is the numerical simulation of thermophysical processes and the development of design solutions to improve the heating uniformity of a metal hydride container [2]. A comparative analysis of four configurations was carried out: a short heater, a heater positioned 10 mm higher, and systems equipped with steel and aluminum fins designed to enhance heat removal from the heating element and promote more uniform heat distribution throughout the intermetallic material. The numerical simulation results demonstrated a significant influence of the heating system configuration on the thermal behavior of the metal hydride container. When the heater was positioned at the same level as the intermetallic region, heat transfer was less efficient: the average heater temperature reached 275.8 °C, while the temperature difference within the intermetallic material was 29.8 °C. In addition, local overheating was observed in the lower part of the container. Raising the heater by 10 mm improved the heating intensity of the intermetallic material and increased its average temperature. However, during further heating of the entire intermetallic volume to the operating temperature range of 250–300 °C, local overheating may occur in the lower section of the container, which is undesirable for the metal hydride system under consideration [1]. The use of thermally conductive fins further improved heat distribution throughout the container volume while simultaneously reducing local overheating of the heating element by transferring part of the thermal energy into the intermetallic material. The average temperature of the porous medium reached 255.6 °C and 254.3 °C for steel and aluminum fins, respectively, confirming the effectiveness of these design solutions for thermal energy redistribution. The most uniform temperature field was achieved with aluminum fins, where the temperature difference across the intermetallic volume was only 23.5 °C. These results indicate that the implementation of fins enhances the heating uniformity of the metal hydride material and reduces temperature gradients. Therefore, the most promising design solution for achieving a uniform thermal regime is the use of aluminum fins combined with an optimized heater position.

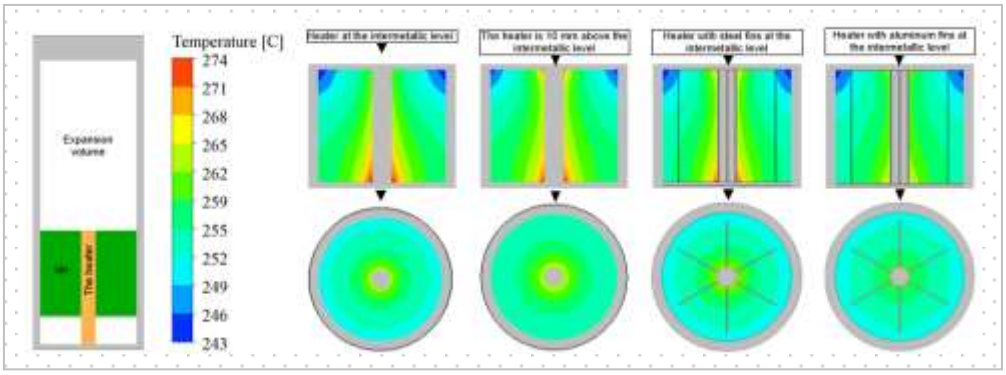



Figure 1. Temperature distribution in the intermetallic material for different heating system configurations.

The obtained results can be applied to the design and optimization of ampoule-type hydrogen storage and transportation systems, where precise control of temperature gradients is essential for ensuring operational reliability and extending equipment service life.

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# A Method of Crystal Lattice Recognition Using AI/ML. A Case Study of Uranium Carbides and Nitrides

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Uranium carbides and nitrides are a potential type of nuclear fuel for Generation IV reactors [1]. To date, these materials have been studied for their thermodynamic, chemical, metallic, and magnetic properties – which is sufficient for the construction of demonstration reactors (e.g., within the framework of the «BREST» project). However, unlike the more thoroughly studied MOX fuel, this information is insufficient for implementation in operating nuclear power plants. Open questions remain regarding the study of vacancy formation mechanisms, collision cascades, and the behavior of mixed carbonitride fuel.

It is known from experimental data that upon reaching the melting temperature, «nuclei» – alternative carbide and nitride phases: $U_2C_3$, $UC_2$, $U_2N_3$, $UN_2$ – emerge in microcrystals initially consisting of uranium monocarbides or mononitrides. The process of capturing the emergence of these «nuclei» (clusters of alternative phases) and their evolution is challenging under experimental conditions; therefore, numerical simulation is employed. The primary method is molecular dynamics simulation [2-5]. To detect the emergence of nuclei, the use of artificial intelligence and machine learning (AI/ML) technologies is proposed. The development of the necessary algorithms and their adaptation to the specific material became the target objective.

At the first stage, we determined the crystal type based on nearest-neighbor analysis. A dataset was created containing information on the radial distribution of crystal ions. Considering that real monocrystals do not possess an ideal shape, the dataset was expanded by adding artificial perturbations (a 15% deviation in crystal lattice length units). Using machine learning methods, kernel density estimates of the ion distribution probability were analyzed. The proposed solution is implemented as the CRIS software application (Crystal Recognition & Identification System). However, a drawback of this model is that it only allows us to estimate the probability of an ion belonging to a specific phase, but does not determine the spatial location of the nuclei.

At the second stage, we addressed a similar task using the PointNet neural network architecture. The system constructs a point cloud and analyzes it, comparing it with dataset information on the shape of crystal structures. An initial drawback was its reliance on static crystal shapes (neglecting thermal expansion and ion vibrations). However, this issue was resolved – the system learned to recognize different types of crystal structures within a macrocrystal.

Ultimately, we propose a comprehensive algorithm: molecular dynamics simulation is performed, and every 100 time steps, information on the positions of ions is saved to files. Each file is then processed by the PointNet architecture, which identifies regions of different crystal structures, generating a hypothesis regarding the affiliation of a group of ions to a particular phase. The information is stored in separate lists, which are then individually passed to the CRIS application for hypothesis verification, after which a report is generated for the user.

**Acknowledgement.** This work was supported by a grant from the Ministry of Science and Higher Education No. FEUZ-2026-0010.

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# An Open-Source Computational Workflow for AI-Ready Particle Morphology Characterization via Elliptic Fourier Analysis

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Particle morphology governs critical functional properties of granular materials across engineering and scientific domains, including flowability, packing density, permeability, heat transfer, and mechanical strength, making its accurate quantification essential for process design, predictive simulation, and materials informatics. In energy relevant systems such as catalyst beds, battery electrode powders, granular heat transfer media, and nuclear fuel particles, morphology directly influences mass and energy transport at the particle scale, yet is frequently reduced to a single scalar index. Conventional shape descriptors (circularity, sphericity, aspect ratio) are inherently incapable of resolving the multiscale geometric complexity of irregular particles: they discard contour information above the global form level, conflate distinct morphological features, and lack the dimensionality required to serve as meaningful feature vectors for machine learning (ML) models. Elliptic Fourier Analysis (EFA) addresses these limitations by decomposing closed particle contours into a hierarchical set of normalised harmonic descriptors that capture morphological information from macroscale form to microscale surface texture. Each harmonic order contributes an independent geometric component, producing a high dimensional, scale invariant descriptor vector that is intrinsically suited for data driven classification, clustering, and property prediction. Despite its strong analytical foundation, EFA has seen limited adoption in engineering workflows because existing implementations rely on scripting environments, require programming expertise, lack integrated visualisation, and do not support high throughput batch analysis, leaving a clear gap for an accessible, reproducible, and scalable characterisation tool.

This work presents the first open source, browser accessible GUI platform for fully automated EFA based particle shape characterisation, requiring no programming experience (Fig. 1). Developed in Python Streamlit, the application integrates the complete analytical pipeline: contour preprocessing, harmonic decomposition, normalisation, shape descriptor computation, harmonic sensitivity analysis, multivariate statistics, and reproducible exportable outputs, within a single unified workflow. Three interconnected modules guide users from single particle contour reconstruction with interactive harmonic order control (Module 1) through dataset level descriptor stabilisation for data driven harmonic order selection (Module 2) to population level multivariate statistical interpretation with Pearson correlation matrices (Module 3). Pixel to physical unit conversion enables scale independent analysis across nano to macroscale systems. The platform is freely accessible at https://efa-gui.streamlit.app/, distributed via PyPI (pip install efa-gui), and its source code is publicly available on GitHub under the MIT licence [1].



Fig. 1. Streamlit GUI platform: (a) Module 1: single particle contour reconstruction with interactive harmonic order control and real time accuracy metrics; (b) Module 2: dataset level harmonic sensitivity analysis and descriptor stabilisation; (c) Module 3: population level multivariate shape statistics and Pearson correlation matrix.

Platform capability was validated in a controlled laboratory study with 22 senior chemical engineering students; mean Likert scores of 4.18 to 4.50 (scale 1 to 5) confirmed high usability, workflow clarity, and analytical effectiveness [1]. From a materials informatics perspective, the platform functions as a scalable feature extraction engine: each particle contour yields a standardised descriptor vector: encoding elongation ratio, asymmetricity, polygonality, surface roughness, and higher-order harmonic indices, directly compatible with downstream ML classification, clustering, and property prediction pipelines. Standardised outputs facilitate construction of large scale morphology databases linking particle geometry to macroscopic functional behaviour, supporting digital twin integration and AI assisted optimisation of particulate processes. Future development will couple the platform with automated image segmentation pipelines for direct microscopy input and incorporate built in ML classifiers, further reducing the barrier between raw imaging data and AI ready shape features.

**Keywords:** open source GUI; particle morphology; Elliptic Fourier Analysis; materials informatics; AI ready feature extraction;

**References**

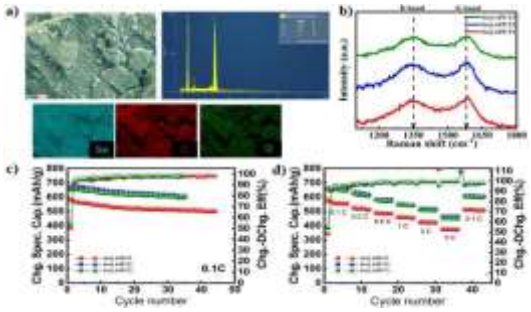
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# Upcycled PET-Derived Porous Carbon as a High-Capacity Anode for Low-Temperature Sodium–Selenium Batteries

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Waste PET plastic is building up faster than we can manage it, and global plastic production is expected to nearly double by 2100 [1]. In this work, we turned used PET bottles into a porous activated carbon material and tested it as an anode host for sodium–selenium (Na–Se) batteries. The whole synthesis was done in a single step. KOH was used to break down the PET, while at the same time the carbon was activated and carbonized during heating no separate processing stages were needed. By changing the KOH to PET ratio, we were able to control the porosity and degree of structural disorder in the final carbon. This was confirmed by Raman spectroscopy, where the D/G band ratio shifted across the three prepared materials (APET1, APET2, APET3). Selenium was then loaded into the carbon pores by melt-diffusion, which is known to promote uniform Se distribution and limit polyselenide dissolution [2,3]. SEM and EDS mapping showed that Se was spread evenly through the carbon host, which we believe contributed to the stable electrochemical performance. The best electrode, Se@APET2, delivered an initial capacity of 674 mAh $g^{-1}$ at 0.1 C and kept 614 mAh $g^{-1}$ after 35 cycles (~91%), with Coulombic efficiency staying above 98%. At higher rates, capacity retentions were 94.9%, 88.2%, 82.7%, 78.3%, and 70.3% at 0.2, 0.5, 1, 2, and 5 C, and recovered to 606 mAh $g^{-1}$ when returned to 0.1 C. Over 150 cycles at 0.5 C, the capacity went from 614 to 512 mAh $g^{-1}$, which means 83.4% retention and CE above 99%. These results show that waste PET can be a useful and affordable starting material for making carbon hosts in sodium-based batteries.



**Acknowledgements.** This research was funded by the Research Targeted Programs" BR24992766 "Development of methods and technologies for environmentally friendly "green" processing of polymer waste for energy storage" from the Ministry of Science and Higher Education of the Republic of Kazakhstan.

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# Nickel and Titania Co-decorated Carbon Nanofibers: a Novel Scaffold for High-Loading Lithium Polysulfide Catholytes

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Lithium-Sulfur (Li-S) batteries offer high energy density and affordability, but their commercial application is limited by the poor kinetics of intermediate lithium polysulfides (LiPSs)[1-2]. To address these obstacles, this study presents a free-standing current collector composed of carbon nanofibers decorated with nickel and titanium dioxide nanoparticles Ni(1.0%)/TiO2@CNF with a high sulfur loading of 2 mg*cm$^{-2}$. As shown in **fig. 1d**, the Ni(1.0%)/TiO2@CNF electrode delivers a high initial specific capacity of over 1150 mAh*g$^{-1}$ at a 0.5C rate, demonstrating robust capacity retention and stability over 200 cycles, which is further supported by the voltage profiles in **fig. 1c** that exhibit stable and well-defined discharge plateaus. Cyclic Voltammetry (CV) at varying scan rates in **fig. 1f** and over initial cycles in **fig. 1c** confirms rapid, highly reversible LiPS conversion. Furthermore, SEM and TEM analyses in **fig. 1a** and 1**b** reveal that the Ni and $TiO_2$ nanoparticles are uniformly distributed across the conductive CNF network, providing abundant catalytic active sites. These results highlight that the synergistic effect of metal and metal oxide nanoparticles effectively accelerates sluggish electrochemical kinetics, making Ni(1.0%)/TiO2@CNF a highly promising composite for high-performance Li-S batteries.

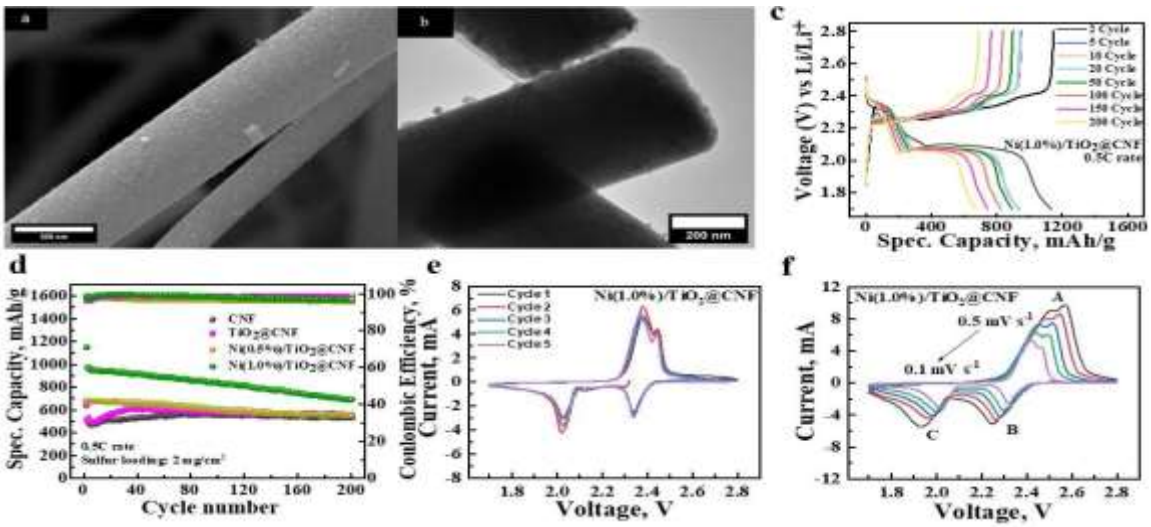



Figure 1. Morphological characterization of Ni(1.0%)/TiO2@CNF: (a) SEM image; (b) TEM; electrochemical performance: (e) voltage profile; (d) 0.5C rate long-term cyclability; (e) cyclic voltammetry; (f) cyclic voltammetry at different scan rates

**Acknowledgment**

This work was supported by the Research Grant AP22788422 "Advancing the Frontiers: High-Performance Anode-Free Lithium-Sulfur Batteries" funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan under the Competition for grant funding of young scientists for scientific and (or) scientific and technical projects for 2024–2026.

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# Beyond Batteries: Solid-State Materials for Integrated Energy Storage, Gas Separation

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Modern energy systems are undergoing a paradigm shift from centralized, fossil-based infrastructures toward distributed and renewable-driven architectures. While batteries have emerged as a cornerstone for short-term energy storage due to their high efficiency and rapid response, their limitations in long-duration storage, safety, and operational stability necessitate complementary technologies. In this context, hydrogen-based systems, gas separation processes, and advanced sensing platforms are increasingly integrated to enable flexible, scalable, and resilient energy solutions.

This talk explores the role of solid-state porous materials, particularly metal–organic frameworks (MOFs) and zeolites, as multifunctional platforms that bridge these domains. Owing to their tunable porosity, high surface area, and chemical versatility, these materials serve as highly effective adsorbents for hydrogen storage**,** selective membranes for gas separation**,** and active layers in gas sensing devices. Their integration into energy systems enables efficient hydrogen production and purification, safe and compact storage, and real-time monitoring of gas composition and system integrity.

By coupling these functionalities with battery technologies, it becomes possible to design hybrid energy storage systems that operate seamlessly across multiple timescales, where batteries handle transient loads and porous-material-enabled hydrogen systems provide long-term storage and energy buffering.

The presentation will highlight recent advances in the design and deployment of different families of porous materials for adsorption and separation. These materials contribute to improving the efficiency, safety, and adaptability of battery-centered systems, ultimately paving the way toward more robust and sustainable energy infrastructures.

# Improving Performance and Stability of Perovskite Solar Cells

Yugesh Kumar, Saurabh Srivastava, Sudhir Ranjan, Raju Kumar Gupta, Anand Singh, Ashish Garg
Department of Sustainable Energy Engineering, IIT Kanpur

Since their emergence in 2009, perovskite solar cells have come a long way with top efficiencies approaching 27%. Despite all the high-efficiency claims, its commercial implementation has not been possible, primarily because of poor atmospheric stability, driven by multiple factors. This talk will focus on strategies to improve the stability of perovskite solar cells and on detailed investigations of the underlying physical mechanisms.

# Green Nanomaterials for a Zero-Emission Future

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The global transition toward a zero-emission future demands sustainable energy storage systems that combine high performance, long-term stability, low cost, and environmental compatibility. Biomass-derived activated carbon has emerged as a promising green electrode material owing to its renewable origin, high surface area, hierarchical porosity, rich surface functionality, and excellent electrochemical durability. In this context, the integration of biomass-derived carbon with redox-active nanomaterials provides an effective strategy to overcome the limited energy density of conventional carbon-based supercapacitors. This presentation focuses on the rational design of biomass-derived activated carbon and its advanced composites with sulfur, nickel cobalt layered double hydroxide (NiCo-LDH), and polyaniline for next-generation supercapacitor electrodes. The synergistic combination of porous carbon frameworks and faradaic redox-active components enables rapid ion transport, improved charge storage, enhanced capacitance, superior rate capability, and remarkable cycling stability. Particular attention is given to solid-state supercapacitors, where these green nanocomposites support safe, flexible, efficient, and durable device architectures. By correlating synthesis approaches, structural features, interfacial chemistry, and electrochemical behavior, this work highlights the potential of biomass-based carbon/redox-active nanocomposites as scalable and sustainable materials for high-efficiency energy storage technologies.

# Magnetron Sputtering of $YBa_2Cu_3O_{7-x}$ Thin Films on Biaxially Textured Flexible Substrates (Under Industrial Conditions) in a Reel-to-Reel Deposition System

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Industrial production of second-generation high-temperature superconducting tapes (2G-HTS) commonly employs pulsed laser deposition (PLD), chemical vapor deposition (CVD), reactive co-evaporation (RCE) or solution-based process (MOD) for the fabrication of superconducting $REBa_2Cu_3O_{7-x}$ (REBCO) layer [1]. While PLD is the "gold standard" for high-quality REBCO epitaxial growth [2], magnetron sputtering offers a potentially more scalable alternative for industrial applications. In this work, we deposited YBCO thin films onto the biaxially textured flexible substrates using direct current (DC) and radio-frequency (RF) magnetron sputtering. We used industrial multilayer buffer substrate tapes of the following architecture $Al_2O_3$ / $Y_2O_3$ / IBAD-MgO / epitaxial MgO /LMO (IBAD = ion-beam-assisted deposition). It has both out-of-plane and in-plane orientation and serves as a texture template for $YBa_2Cu_3O_{7-x}$ (YBCO) sputter deposition with optimized process parameters. X-ray diffraction (XRD) confirmed the formation of required YBCO phase and strong c-axis texture with in-plane alignment. Common issues in YBCO magnetron sputtering include maintaining correct stoichiometry due to selective sputtering and oxygen depletion, negative ion bombardment causing re-sputtering and plasma instability are discussed. Prospect of increasing nanoparticles formation likelihood for pining centers densification in YBCO thin films by utilization deposition techniques with a higher ionization degree like cathodic arc (CA) ablation and high-power impulse magnetron sputtering (HiPIMS) is also discussed.

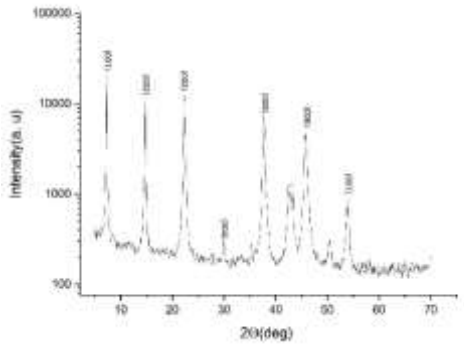



Fig.1 XRD patterns of the YBCO layer.

**Acknowledgements.** This research was supported by Faraday Factory Japan LLC and the targeted program no. BR21882402 (2023–2025) from the Ministry of Science and Higher Education of the Republic of Kazakhstan.

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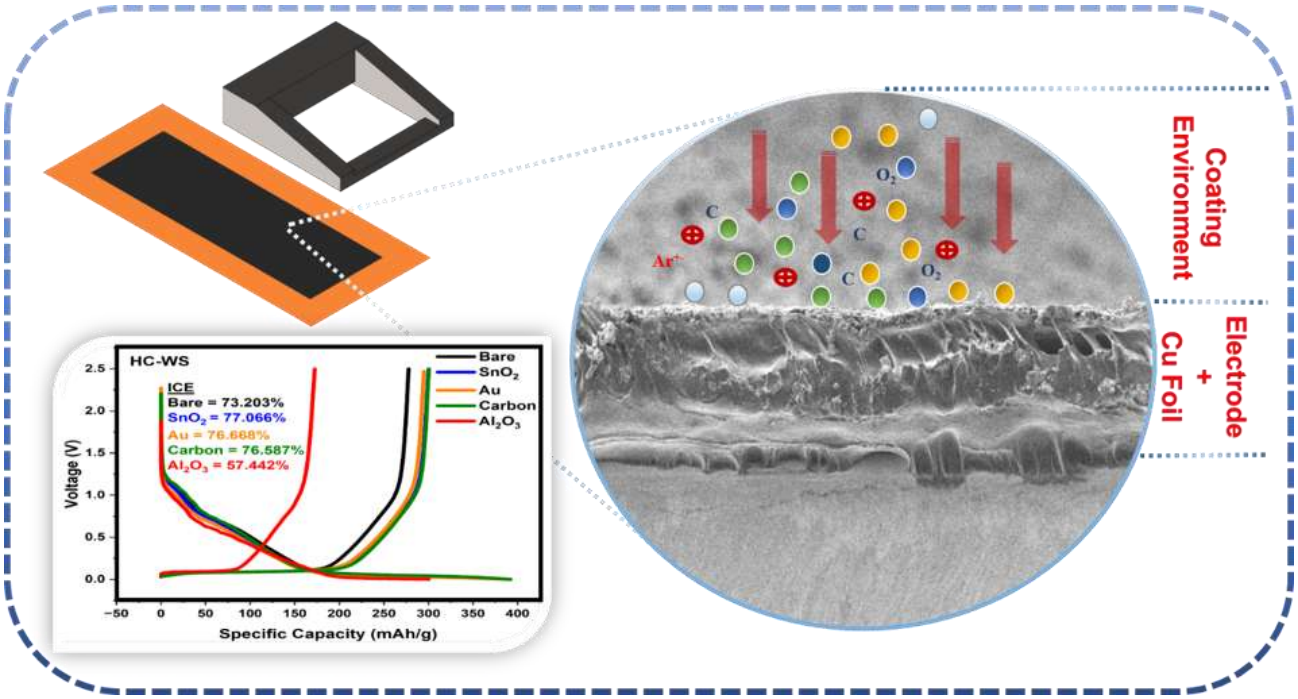
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# Advanced Surface Engineering Strategies to Enhance Initial Coulombic Efficiency of Biowaste-Derived Hard Carbon Anodes for Sodium-Ion Batteries

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Biowaste-derived hard carbon (HC) has emerged as a sustainable and low-cost anode material for sodium-ion batteries (SIBs), offering a circular economy alternative to graphite, which is unsuitable for sodium storage due to the larger ionic radius of $Na^+$. In this study, walnut shells were utilized as a renewable precursor to synthesize HC, providing a high-carbon-content feedstock with intrinsic porosity. Despite these advantages, HC suffers from poor cycling stability and low initial Coulombic efficiency (ICE), primarily caused by parasitic surface reactions and excessive solid electrolyte interphase (SEI) formation. To overcome these limitations, four advanced surface engineering strategies were systematically applied: SnO2 coatings via magnetron sputtering, Au coatings via Q150T ES sputtering, Al2O3 coatings via atomic layer deposition (ALD), and amorphous carbon coatings via an Agar Scientific carbon coater. Each coating was designed to address specific inefficiencies of bare HC—SnO2 and $Al_2O3$ provided chemical stabilization, Au enhanced electronic conductivity, and carbon delivered scalable passivation. Comprehensive structural and surface analyses confirmed uniform and conformal coatings, while electrochemical testing demonstrated significant improvements in ICE, reversible capacity, and cycling stability compared to uncoated HC. Among the strategies, $SnO_2$ and Au coatings yielded the most pronounced ICE enhancement, carbon coatings improved conductivity and interfacial stability, whereas Al2O3 coatings showed limited effectiveness under the tested conditions. This comparative framework establishes rational surface engineering as a viable pathway to tailor the interfacial chemistry and electrochemical performance of biowaste-derived HC, advancing its potential as a sustainable anode material for next-generation sodium-ion batteries.

**Keywords:** Biowaste-derived hard carbon; Sodium-ion batteries; SnO2 coating; Au coating; Carbon coating; Al2O3 coating; Initial Coulombic efficiency (ICE); Surface engineering; Solid electrolyte interphase (SEI)

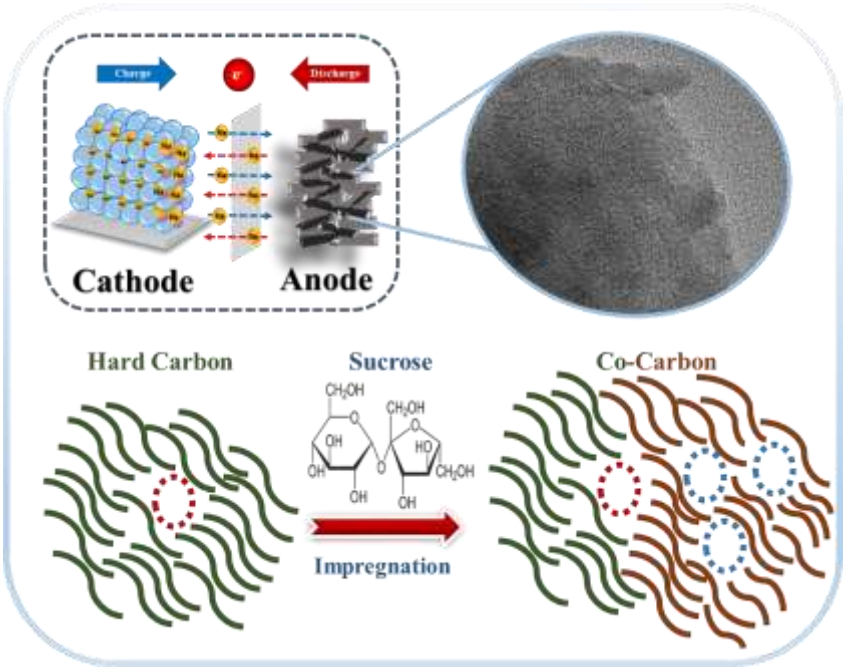


# Sucrose-Impregnated Biowaste Hard Carbon Synthesised Through Co-Carbon Strategy for Advanced Sodium-Ion Battery Applications

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Biomass-derived hard carbon is a promising and eco-friendly anode material for sodium-ion batteries, but its electrochemical efficiency is frequently constrained by limited closed pore development. In this research, hard carbon derived from walnut shells (HC-WS) was enhanced via sucrose impregnation and subsequent pyrolysis, creating soft carbon domains that produce a large number of closed pores. This transformation results in a co-carbon structure, where the rigid hard carbon backbone is enhanced by sucrose-derived soft carbon, leading to greater pore accessibility and better sodium-ion storage performance. Thorough analysis through XRD and Raman spectroscopy verified that sucrose treatment adjusts interlayer spacing, stacking arrangement, and defect density, balancing structural disorder with improved graphitic coherence. SEM and TEM analyses showed gradual increases in porosity and defect sites, while EDS mapping indicated consistent oxygen incorporation. XPS analysis also validated the increase of oxygen functionalities that stabilize the solid electrolyte interphase (SEI) and enhance electrode–electrolyte interactions. Electrochemical testing indicated that sucrose treatment greatly enhances sodium storage capabilities. The 0.25 M sucrose-treated sample exhibited the highest initial coulombic efficiency (≈80%), enhanced cycling stability, clearer differential capacity characteristics, and outstanding rate capability at varying current densities. Higher concentrations (0.5–1 M) improved performance relative to unmodified HC-WS, yet excessive disorder and oxygen incorporation weakened conductivity and long-term reliability. This study shows that sucrose treatment converts biowaste-derived hard carbon into a co-carbon framework featuring numerous closed pores and enhanced surface chemistry. Moderate impregnation strikes the ideal balance among structural order, defect density, and conductivity, presenting a scalable route to high-performance anodes for sodium-ion batteries.

**Keywords:** Sodium-ion batteries, Hard carbon, Biowaste valorization, Co-carbon strategy, Sucrose impregnation, Sustainable anode materials and electrochemical performance.



# Effect of Mechanical Activation on Selective Leaching Behavior of Nickel Sulfide Concentrate

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Nickel sulfate is a key precursor for NCM cathode material production and is traditionally obtained from nickel sulfide concentrates (NSC) via energy-intensive smelting or high-pressure leaching. In this work, an acid-free mechanochemically assisted atmospheric leaching approach is investigated to enhance the extraction of nickel and cobalt under mild conditions.

Mechanical activation (MA) was performed at 200-800 rpm for 60 min under dry and wet conditions (Figure 1). Subsequent leaching was conducted using ferric sulfate solution at 90 °C with a solid-to-liquid ratio (S/L) of 1:20. The results demonstrate that MA significantly modifies the reactivity of NSC. Wet activation improves leaching performance, with nickel and cobalt recoveries reaching ~65% at 200 rpm with no any additivies, compared to ~55% for the untreated concentrate, while dry activation shows lower efficiency.

Ferric sulfate leaching at an optimum concentration of 0.25 mol/L $Fe_2(SO_4)_3$ resulted in a substantial increase in extraction efficiency, with nickel recovery reaching ~88% and copper recovery reaching ~98% within 120 min at 90°C. In this system, $Fe^{3+}$ acts as the primary soft oxidizing agent via the mechanism $Fe^{3+} + MeS \rightarrow Fe^{2+} + Me^{2+} + S^0$, facilitating sulfide oxidation and suppressing passivating elemental sulfur layer formation on mineral surfaces.

Overall, the results demonstrate that mechanochemical pre-treatment combined with ferric sulfate leaching provides a promising low-temperature and atmospheric-pressure alternative to conventional high-temperature processing routes for nickel sulfide concentrates.

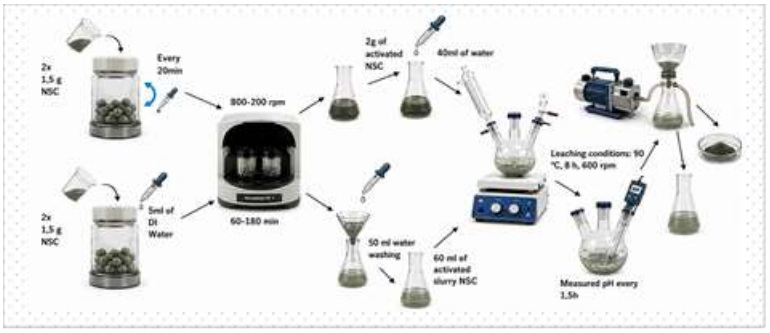



Figure 1. Schematic diagram of dry and wet mechanical activation procedures and subsequent leaching setup.

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# Scale-Up of Solid-State $LiFePO_4/C$ Synthesis by Using Roll Ball Milling

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Lithium iron phosphate ($LiFePO_4$, LFP) remains a key cathode material for cost-effective and safe lithium-ion batteries, however simple and scalable solid-state routes based on low-cost precursors are still required. In this work, a solid-state mechanochemical approach for LFP/C synthesis is demonstrated using chemically pure-grade $Fe_2O_3$ and $Li_2CO_3$ precursors and locally sourced phosphoric acid (85% $H_3PO_4$, Kazphosphate, Kazakhstan), combined with an in-situ carbon coating strategy.

The batch size was systematically increased from 10 g to 100 g (Figure 1). Roll ball milling was performed for 4 h using 10 mm $ZrO_2$ balls with ball-to-powder ratio 1:20 to ensure homogeneous mixing and reaction. The process was successfully scaled up to 100 g while maintaining constant milling parameters, thereby preserving comparable energy input and collision conditions.

The obtained LFP/C materials exhibit a phase-pure olivine structure, good crystallinity, and controlled particle morphology at both 10 g and 100 g scales. These results confirm the reproducibility of the method and its potential for further scale-up to kilogram-level production without compromising material quality. The novelty of this work lies in the combined use of chemically pure reagents, a scalable mechanochemical approach, and a domestic phosphorus source, demonstrating the feasibility of localized and industrially relevant LFP production.

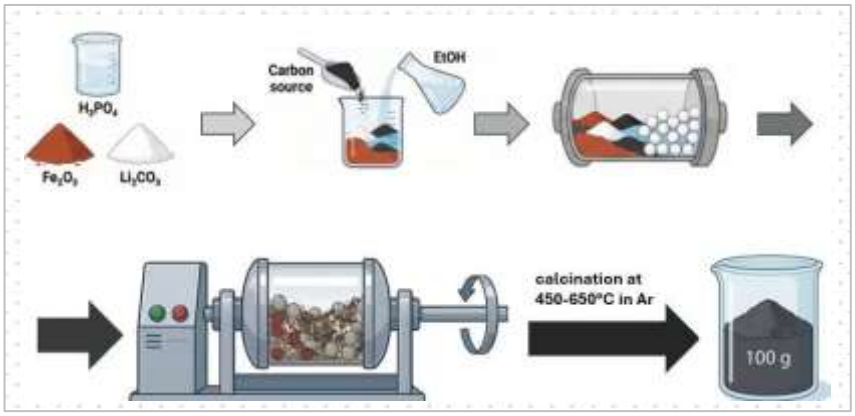



Figure 1. Schematic Workflow for the 100 g Scale Synthesis of $LiFePO_4/C$.

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# Boron-Doped $LiCoPO_4$ as a High-Voltage Cathode for Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) require high-energy and thermally stable cathode materials for next-generation applications. Olivine-type $LiCoPO_4$ (LCP) is a promising candidate due to its high operating voltage (~4.8 V vs. $Li/Li^+$) and structural stability [1]. However, its practical use is limited by low electronic conductivity and slow lithium-ion diffusion.

In this work, boron-doped $LiCoPO_4$ (LCP-B) was synthesized via a two-step solid-state method combining planetary ball milling and thermal treatment. X-ray diffraction confirmed the preservation of the orthorhombic olivine structure (Pnma) without secondary phases, while slight peak shifts indicate lattice distortion induced by boron incorporation. Scanning electron microscopy revealed a reduction in particle size from ~200-500 nm (pristine) to ~100-300 nm (LCP-B), suggesting improved surface area and shortened diffusion pathways.

Electrochemical characterization demonstrated enhanced performance of the doped material. Cyclic voltammetry showed improved redox reversibility, while electrochemical impedance spectroscopy indicated reduced charge-transfer resistance and enhanced lithium-ion diffusion. The initial discharge capacity increased from ~40 to ~58 $mAh \cdot g^{-1}$, with improved capacity retention after 20 cycles (~43 $mAh \cdot g^{-1}$ for LCP-B vs. ~25 $mAh \cdot g^{-1}$ for pristine LCP). Coulombic efficiency also increased to ~78-81%.

These improvements are attributed to the combined effects of lattice distortion and reduced particle size, which facilitate charge transport and interfacial kinetics. Although the capacity remains below the theoretical value due to high-voltage instability, boron doping represents a promising strategy for enhancing LCP-based cathodes. The electrochemical performance was evaluated by galvanostatic charge–discharge (GCD) cycling, as shown in Fig. 1a–d.

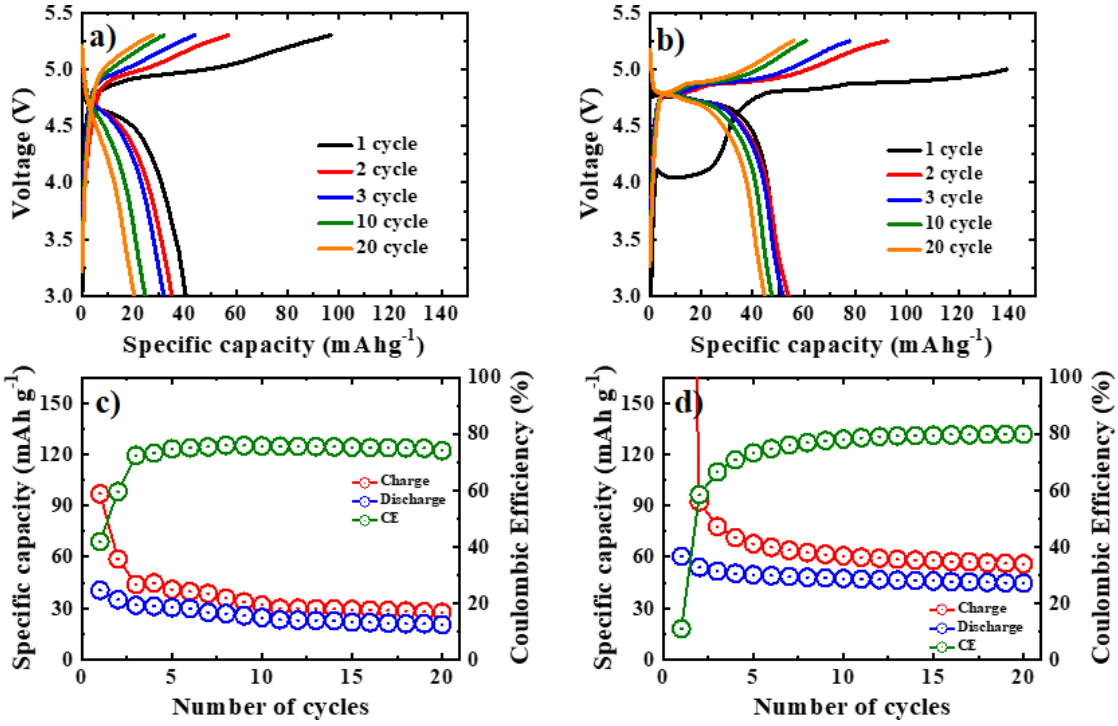



Fig. 1. GCD curves and cycling stability profiles of (a, c) pristine LCP and (b, d) B-doped LCP (LCP-B) at a 0.1C rate.

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# Mechanochemical-Assisted HF-Free Etching of $V_2AlC$ for Tuning Interlayer Spacing and Electrochemical Behavior of $V_2CT_x$ MXene Anodes

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MXene, a two-dimensional family of transition metal carbides, exhibits exceptional conductivity, rich surface chemistry, and structural tunability, making it a prime candidate for next-generation LIBs [1]. There is a lack of systematic comparison between mechanochemical and hydrothermal HF-free etching methods for synthesizing $V_2CT_x$ MXene, particularly in terms of how they influence structure, defects, and lithium storage performance. The use of corrosive HF as the etching agent makes the MXene synthesis process toxic and hazardous to the environment and hinders exploration of its use in various other applications [2].
This report presents a method of mechanochemical etching without the use of HF for the synthesis of $V_2CT_x$ MXene from $V_2AlC$ using the NaF/HCl system, which is systematically compared with the traditional hydrothermal approach. Ball grinding etching significantly increases the efficiency of aluminum extraction, reduces the content of the residual phase MAX and leads to a violation of the structure, which leads to an increase in the distance between the layers and an increase in the number of active surfaces. The optimized BM-48 sample exhibits the lowest MAX/MXene intensity ratio (28.9%), enlarged c-lattice parameter, and highly fragmented layered morphology. Electrochemically, BM-48 delivers an initial charge capacity of 276 mAh $g^{-1}$ and maintains 244 mAh $g^{-1}$ after 30 cycles at 0.1 C, demonstrating superior rate capability with 100 mAh $g^{-1}$ at 1 C with lithium storage dominated by pseudocapacitive and surface-controlled mechanisms. Conversely, hydrothermal samples exhibit a more organized lamellar structure and increased structural activation during cycling, while showing reduced initial productivity.

**Acknowledgements**. This research was funded by the Research Targeted Programs" BR24992766 "Development of methods and technologies for environmentally friendly "green" processing of polymer waste for energy storage" from the Ministry of Science and Higher Education of the Republic of Kazakhstan.

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# Porous Carbons from Renewable Biomass for Cryogenic and Ambient Hydrogen Storage

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As an energy carrier, hydrogen is distinguished by its exceptional physical properties. Being the lightest chemical element, it delivers a superior gravimetric energy density of 140 MJ $kg^{-1}$, nearly triple that of conventional gasoline (44 MJ $kg^{-1}$) [1]. Furthermore, its combustion yields only water vapor, establishing hydrogen as a premier solution for the decarbonization of heavy, energy-intensive industrial sectors. Data from the Hydrogen Council indicates a robust expansion of the global clean hydrogen sector, now encompassing over 1,700 initiatives. Recent figures show that 510 of these projects have secured final approval, including a significant influx of 80 new projects within the past year. This sector has maintained a consistent upward trajectory since 2020, with annual investment growth exceeding 50% and a record $35 billion capital injection recorded in 2025 [2]. Despite the potential of hydrogen, its broad industrial application is hampered by a complex array of challenges regarding secure, economical, and high-performance storage and transport. Consequently, modern materials science has shifted its focus toward engineering sophisticated materials that function at near-ambient conditions, aiming to eliminate the dependency on high-pressure tanks and cryogenic cooling.

This research presents a systematic optimization of KOH-activated rice husk carbon for maximized hydrogen sequestration. By precisely controlling the activation temperature and chemical ratios, a material with an ultra-high surface area (3802 $m^2$ $g^{-1}$) and total pore volume (2.10 $cm^3$ $g^{-1}$) was produced. The resulting sorbent exhibited significant hydrogen storage capacities of 1.05 wt.% (25 °C) and 10.9 wt.% (-196 °C). The practical potential of the porous carbon was investigated through kinetic studies and cycling stability tests. Kinetic analysis determined the $H_2$ loading rates and the limiting diffusion steps within the pore network, while repetitive cycling confirmed the framework's robustness and capacity reversibility. These parameters are key indicators of the material's performance in dynamic storage applications, bridging the gap between material properties and industrial requirements. These results underscore the viability of biomass-sourced carbons as scalable, high-efficiency candidates for next-generation hydrogen fuel systems, ready for further functionalization.

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# Interfacial Engineering of $SnO_2$ Thin-Film Anodes via LiPON Surface Coating for Enhanced Electrochemical Performance in Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) are among the most widely adopted electrochemical energy storage technologies, owing to their high energy density, long cycle life, and broad applicability across electric vehicles, portable electronics, and grid-scale energy systems [1-2].

Tin dioxide ($SnO_2$) has emerged as a highly promising anode material for next-generation LIBs, offering an exceptional theoretical specific capacity of 1494 mAh $g^{-1}$ – significantly surpassing that of conventional graphite anodes – while being naturally abundant, cost-effective, and environmentally benign [3-4]. Nevertheless, severe volume expansion during lithiation/delithiation and the formation of an unstable solid electrolyte interphase (SEI) remain critical barriers to its practical implementation, leading to rapid capacity fading and poor long-term cyclability [5].

To address these challenges, lithium phosphorus oxynitride (LiPON) was employed as an ultrathin artificial surface coating on $SnO_2$ thin-film anodes, simultaneously serving as a pre-formed SEI, a surface passivation barrier, and a mechanical buffer against volumetric strain [6-7].

$SnO_2$ thin films and LiPON coatings of varying thicknesses (5, 10, and 15 nm) were deposited by RF magnetron sputtering and evaluated in both as-deposited and thermally annealed conditions. Structural and morphological properties were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). Electrochemical performance was assessed by galvanostatic charge-discharge cycling over 100 cycles at 0.1C using a multichannel battery testing system (Neware BTS).

The results demonstrate that annealed samples consistently outperform as-deposited ones, confirming that thermal treatment enhances interfacial bonding and promotes stable SEI formation. This work establishes ultrathin LiPON coating combined with thermal annealing as an effective interfacial engineering strategy for high-performance $SnO_2$-based thin-film anodes.

**Acknowledgment.** This research was funded by the Small Grant NU (2026-2028) project “From Thin Films to Continuous Power: Building the Scientific Basis for Long-Length Microbatteries” (Funder Project Reference: 110326FD3226).

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# Densification and Conductivity Improvement of LLZO by Additive Design

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In recent years, solid-state lithium-ion batteries have attracted significant attention due to their enhanced safety, high energy density, and suitability for applications from portable electronics to electric vehicles. A key component is the solid electrolyte, which enables efficient lithium-ion transport while maintaining electrochemical stability at the electrode–electrolyte interface [1]. Among various materials, garnet-type lithium lanthanum zirconium oxide (LLZO) is considered one of the most promising due to its high ionic conductivity, wide electrochemical stability window, and good compatibility with lithium metal anodes [2,3]. However, its practical application is still limited by insufficient densification and high grain boundary resistance.

In this work, the effect of sintering additives, namely CuO, ZnO, and $Al_2O_3$, on the structural and electrochemical properties of LLZO electrolytes derived from commercial powders is systematically investigated. The incorporation of these additives aims to promote densification and optimize lithium-ion transport by modifying the microstructure of the material [4, 5].

Several metal oxide additives, including CuO, ZnO, and $Al_2O_3$, were used as sintering agents. Commercial LLZO powder (MTI Corp) served as the starting material. The powders were thoroughly mixed to ensure homogeneous distribution of the additives, then dried and pressed into pellets using a conventional pressing method. The pellets were subsequently calcined at elevated temperature to achieve densification and phase formation. The prepared pellets were characterized by scanning electron microscopy (SEM) and electrochemical impedance spectroscopy (EIS). Impedance measurements were performed in the frequency range from 1 MHz to 1 Hz with an applied amplitude of 0.01 V.

Among the investigated additives, CuO demonstrated the best overall performance, resulting in the highest densification (~83.0%) and enhanced ionic conductivity, which can be attributed to improved grain boundary contact and reduced porosity. These findings highlight the critical role of sintering additives in tailoring the microstructure and electrochemical performance of LLZO solid electrolytes.

**Acknowledgment.** This research was funded by the research project 110326FD3226 “From Thin Films to Continuous Power: Building the Scientific Basis for Long-Length Microbatteries”, Small Grant of Nazarbayev University (2026–2028)

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# Synergistic Integration of a $Li_2S$-PPy Cathode and Ni/$TiO_2$@CNF Interlayer for High-Performance Lithium-Sulfur Batteries

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Anodeless (or anode-free) batteries utilizing $Li_2S$-based cathodes are a highly promising approach to maximizing volumetric and gravimetric energy density by eliminating excess lithium metal[1-2]. However, their practical performance is fundamentally limited by the sluggish activation of the insulating $Li_2S$ lattice and the detrimental polysulfide shuttle effect. To overcome these challenges, we introduce an anodeless full-cell configuration comprising a $Li_2S$-polypyrrole ($Li_2S$-pPy) composite cathode on an Al foil, an etched Cu foil current collector, and an electrospun Ni/$TiO_2$@CNF interlayer, all operating within a 1M LiTFSI in DOL/DME + 2% $LiNO_3$ electrolyte. As depicted in the schematic cell assembly, the Ni/$TiO_2$@CNF interlayer acts as a highly conductive and catalytic framework that captures migrating polysulfides and accelerates their electrochemical conversion. Furthermore, the combination of this functionalized interlayer with the protective electrolyte additives suppresses uncontrolled dendritic growth on the etched Cu surface, ensuring highly stable lithium stripping and plating. This synergistic configuration significantly improves the electrochemical reversibility and capacity retention of the anode-free cell, offering a viable and scalable pathway toward next-generation high-energy-density energy storage systems

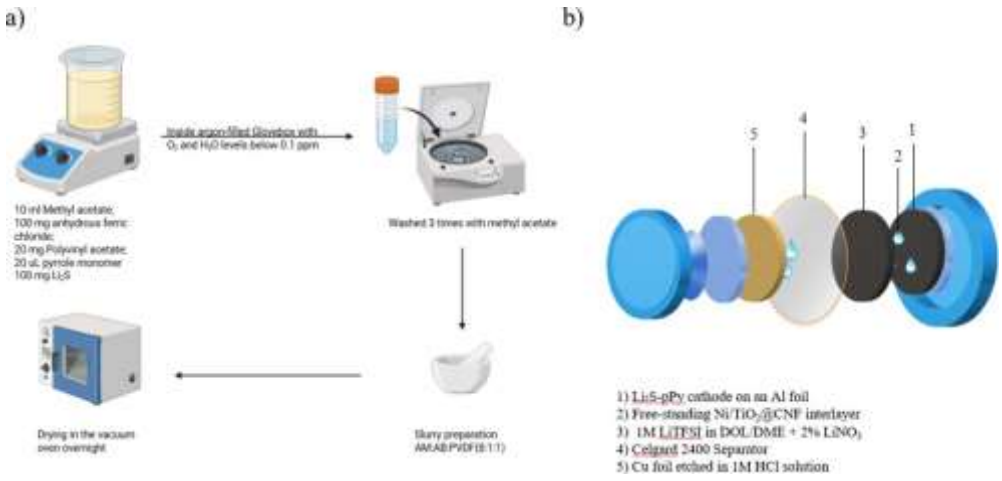



Figure 1.: (a) Synthesis process; (b) cell configuration

**Acknowledgment**

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# New 1d Nickel-Rich NCA Cathode Materials for the Lithium-Ion Battery: Synthesis and Cyclic Stability

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Lithium-ion batteries (LIBs) remain the leading energy storage technology owing to their high energy density, long cycle life, and reliable performance, and they are central to the wider adoption of electric vehicles (EVs) and renewable-energy storage. Among LIB cathodes, nickel-rich layered oxides such as $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811) and $LiNi_{0.8}Co_{0.1}Al_{0.1}O_2$ (NCA811) have attracted considerable attention because of their high specific capacity (≈200 mAh $g^{-1}$) at an average voltage of ≈3.6 V [1,2]. However, conventional electrode fabrication relies on slurry casting with electrochemically inactive PVDF binder and carbon black dispersed in toxic NMP, which adds dead mass, raises interfacial resistance, and limits the attainable energy density [1,3].

The present study reports a binder-free, free-standing one-dimensional (1D) NCA811 cathode fabricated by electrospinning followed by a multi-step thermal treatment, offering a flexible alternative to conventional slurry-cast electrodes [3,4]. A polymer–salt precursor solution containing the Ni, Co, and Al sources at a Ni:Co:Al ratio of 8:1:1 was electrospun into a continuous fibrous mat and subsequently subjected to a tailored two-stage calcination protocol: first in air and then in an oxygen-rich atmosphere to crystallize the layered oxide phase while suppressing oxygen deficiency and minimizing Ni/Li cation mixing.

Scanning electron microscopy (SEM) revealed uniform precursor fibers of submicron diameter that retained a continuous, network-like morphology after calcination (Figure 1). Energy-dispersive X-ray spectroscopy (EDS) mapping confirmed a homogeneous distribution of Ni, Co, and Al throughout the fibers. X-ray diffraction (XRD) confirmed the formation of a pure layered α-$NaFeO_2$-type phase (space group R-3m), with characteristic (006)/(102) and (108)/(110) peak splitting and an I(003)/I(104) intensity ratio of 1.7, which is above the 1.2 threshold commonly used to assess cation disorder, indicating well-ordered $Li^+/Ni^{2+}$ layering.

Coin-type half-cells assembled with lithium-metal anodes were cycled between 2.7–4.3 V at 0.1 C. The free-standing NCA811 cathode delivered an initial specific capacity of ≈120 mAh $g^{-1}$ and retained ≈80 mAh $g^{-1}$ after 100 cycles, with the coulombic efficiency stabilizing near 100% after the first formation cycles. The free-standing electrodes is a promosing material to outperform their slurry-cast counterparts in initial capacity, formation behaviour, and polarization. At the same time, the gradual capacity fade observed on extended cycling indicates that further optimization, for example of densification, calcination, and cell-assembly conditions are required to fully suppress structural coarsening and interfacial side reactions within the porous fibrous network.

Despite these limitations, the findings demonstrate that electrospinning provides a viable, binder-free pathway to high-Ni NCA811 cathodes with an increased active-material fraction and encouraging electrochemical behaviour. With further refinement, this approach represents a promising direction for morphology control and structural optimization of next-generation EV-relevant LIB cathodes.

**Keywords:** electrospinning, NCA811, free-standing cathode, lithium-ion battery, nanofibers.

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# Synthesis of Mesoporous Carbon from PMMA via $ZnCl_2$ Activation for Lithium-Ion Battery Applications

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The increasing demand for advanced energy storage systems necessitates the development of high-performance and cost-effective electrode materials. Poly(methyl methacrylate) (PMMA) is a common plastic waste, and its conversion into valuable carbon structures represents a sustainable recycling strategy [1, 2]. In this study, we demonstrate a facile approach for the synthesis of mesoporous carbon from PMMA using zinc chloride ($ZnCl_2$) as a dual-function catalyst and activating agent [3].

The synthesis began with the complete dissolution of PMMA in ethyl acetate (EA), followed by the addition of $ZnCl_2$. After drying to evaporate the solvent, the precursor was carbonized in a tubular furnace at 750 °C under an argon atmosphere. To optimize the particle size and surface area, the carbonized product underwent high-energy ball milling. The milled powder was washed with hydrochloric acid (HCl) to remove unreacted zinc and inorganic residues, then thoroughly neutralized with hot deionized water. Finally, the synthesized mesoporous carbon was mixed with a binder and a conductive additive to prepare an electrode slurry, which was cast onto a current collector for lithium-ion battery assembly.

Thermogravimetric analysis (TGA) was used to investigate the carbonization mechanism. As shown in Figure 1, pure PMMA almost completely decomposes by 420 °C with a carbon yield of less than 1%. However, the introduction of $ZnCl_2$ significantly alters the thermal degradation pathway, acting as a dehydrating agent that prevents total volatilization. This enables a stable carbon yield at the target temperature of 750 °C, facilitating the formation of a porous carbon network suitable for lithium-ion storage.

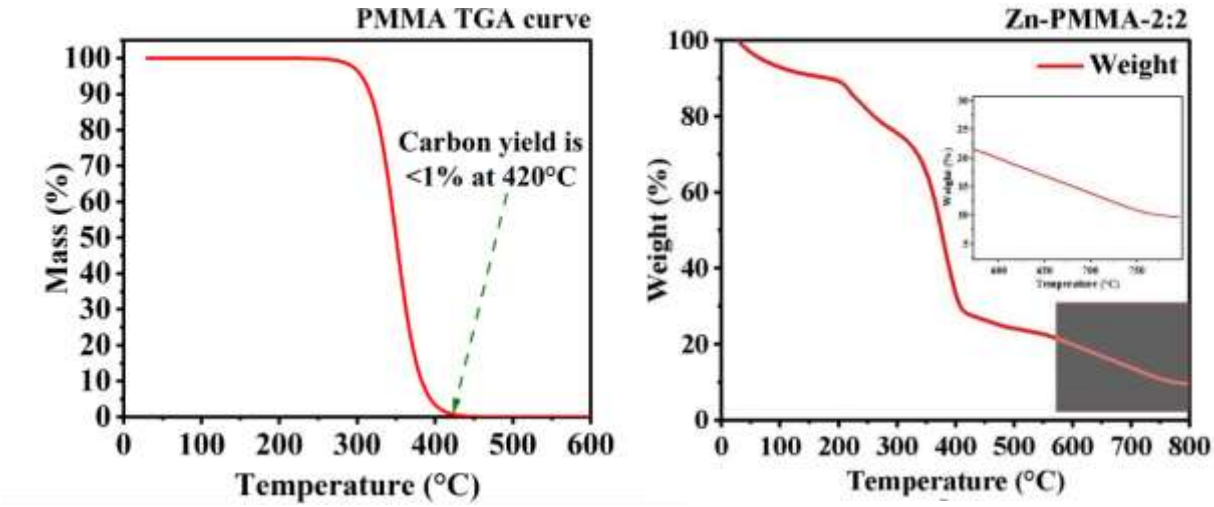



Figure 1. TGA curves of pure PMMA (a) and Zn-PMMA (b) precursor.

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# Ni and Zn Co-Doped $LiFePO_4$/C Cathode Materials Synthesized by Mechanochemical Activation for High-Performance Lithium-Ion Batteries

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Lithium iron phosphate ($LiFePO_4$, LFP) is a highly promising cathode material for lithium-ion batteries (LIBs) owing to its high operating voltage (~3.4 V), outstanding theoretical specific capacity (170 mAh $g^{-1}$), and excellent cycling stability [1]. However, its intrinsic low electronic conductivity (~$10^{-9}$ cm $s^{-1}$) and slow lithium-ion diffusion ($10^{-13}$ to $10^{-16}$ $cm^2$ $s^{-1}$) significantly hinder electrochemical performance [2, 3]. Various strategies have been adopted to overcome these limitations, including particle size reduction via mechanochemical activation, conductive carbon coating, and supervalent cation doping at the Fe site [4, 5]. While Ni and Zn have each been individually reported to enhance conductivity and structural stability of LFP [6, 7], their synergistic co-doping effect has not been extensively explored.

In this study, Ni and Zn co-doped LFP/C cathode materials were synthesized via high-energy planetary ball milling (mechanochemical activation) followed by two-stage calcination under argon atmosphere (350°C/2 h and 550°C/3 h). Five compositions were prepared: LFP/C (undoped), LFP/C–2%Ni, LFP/C–2%Zn, LFP/C–1%Ni 1%Zn, and LFP/C–2%Ni 2%Zn. Sucrose was used as the carbon source. Structural and morphological characterization was performed by X-ray diffraction (XRD), scanning electron microscopy (SEM-EDS), FT-IR and Raman spectroscopy, thermogravimetric analysis (TGA/DSC-MS), and X-ray photoelectron spectroscopy (XPS). Electrochemical performance was evaluated in CR-2032 coin half-cells using galvanostatic charge-discharge cycling and cyclic voltammetry (CV) between 2.5 and 4.2 V.

XRD confirmed phase-pure orthorhombic olivine $LiFePO_4$ structure in all samples with no impurity peaks. Small peak shifts in the 35-38° region indicated successful Fe-site substitution and lattice modifications consistent with Vegard's law [8]. SEM analysis revealed that Ni doping produced finer, more uniform particles (up to 200 nm), while Zn doping and co-doping resulted in broader size distributions (200-1500 nm). FT-IR and Raman spectroscopy confirmed complete precursor decomposition, retention of the olivine phosphate framework, and the presence of both disordered (D band, 1350 $cm^{-1}$) and graphitic (G band, 1580 $cm^{-1}$) carbon in all calcinated samples.

Electrochemical results demonstrated that moderate co-doping at 1% Ni and 1% Zn ($LiFe_{0.98}Ni_{0.01}Zn_{0.01}PO_4$/C) yielded the most balanced performance, achieving charge/discharge capacities of 145 mAh/g at the first cycle, near-99% coulombic efficiency, and minimal capacity fading over 100 cycles. CV curves confirmed reduced polarization and excellent electrochemical reversibility for this composition. In contrast, higher co-doping (2% Ni, 2% Zn) introduced structural strain, hindering $Li^+$ diffusion and reducing long-term capacity retention. The synergistic effect of $Ni^{2+}$, which enhances electronic conductivity and reaction kinetics, and $Zn^{2+}$, which reinforces the olivine structural integrity, demonstrates that moderate co-doping is the optimal strategy for developing high-rate, durable LFP-based cathodes for next-generation LIBs.

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# Electrospun PVDF-HFP/$LiClO_4$ Composite Membranes as Solid Polymer Electrolytes for All-Solid-State Lithium Batteries

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Compared to traditional lithium-ion batteries that use flammable liquid electrolytes, all-solid-state lithium batteries (ASSLBs) are considered to be an attractive next-generation energy storage technology. Among various polymer-based electrolytes, poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) has received significant attention due to its high dielectric constant, good mechanical strength, and good electrochemical stability [1]. However, its usage as a solid polymer electrolyte is limited since its ionic conductivity at room temperature is still insufficient for practical applications.

The goal of this work is to improve electrolyte uptake and increase ionic conductivity by creating PVDF-HFP/$LiClO_4$ electrospun membranes as part of a composite polymer electrolyte method. The electrospun membranes were fabricated using a 7:3 DMF/acetone solvent system, with PVDF-HFP as the host polymer and $LiClO_4$ as the lithium salt. The electrospinning parameters were optimized to achieve uniform, flexible, non-woven fibrous membranes.

Structural and morphological characterization by scanning electron microscopy (SEM) confirmed the formation of randomly oriented fibers with an interconnected porous network and fiber diameters in the nanoscale range (90–130 nm). There were some bead-like flaws found, suggesting that more optimization is required to increase fiber uniformity. Solid polymer electrolyte performance depends on high electrolyte absorption and effective lithium-ion transport, both of which are made possible by the porous structure [2].

Future research will concentrate on using succinonitrile (SN) as a plasticizer to improve ionic conductivity and increase the amorphous phase, as well as conducting electrochemical characterization using cyclic voltammetry (CV) and impedance spectroscopy (EIS) to assess membrane performance for high-energy and safe ASSLB systems.

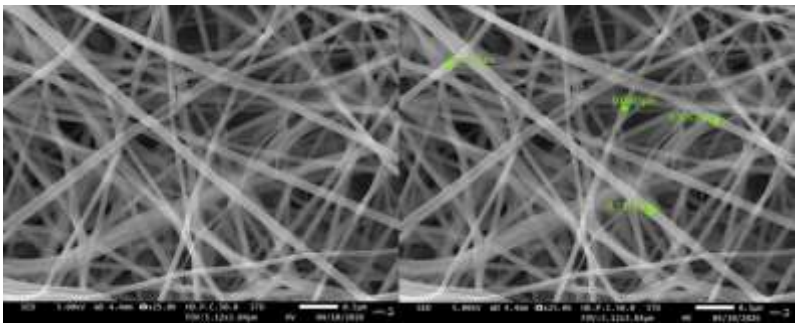


Figure 1.SEM images of the PVDF-HFP/$LiClO_4$ membrane .

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# Optimization of Ball Milling Pretreatment for Hydrothermal Synthesis of $V_2C$ MXene Toward Lithium-Ion Battery Anodes

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The development of efficient and scalable strategies for the synthesis of high-quality MXenes remains a critical challenge for their practical application in energy storage systems. In this work, a ball milling pretreatment approach is introduced to enhance the selective etching of Al from $V_2AlC$ MAX phase for the synthesis of $V_2C$ MXene via a hydrothermal route using HCl and LiF. The influence of ball milling duration on the structural evolution and etching efficiency is systematically investigated. An optimal milling time of 3 h is identified, which significantly improves the accessibility of the MAX phase to the etching solution. Subsequent hydrothermal treatment under varying durations reveals that the pretreated samples exhibit more effective Al removal compared to untreated counterparts.

Structural and morphological analyses confirm the enhanced exfoliation and formation of $V_2C$ MXene after pretreatment. When evaluated as anode materials for lithium-ion batteries, the pretreated MXene demonstrates improved electrochemical performance, including higher specific capacity and better cycling stability. The improved performance is attributed to increased surface area, facilitated ion transport, and more efficient removal of the Al layers.

This study highlights the critical role of mechanical pretreatment in optimizing MXene synthesis and provides a simple yet effective route to enhance the electrochemical properties of $V_2C$-based anodes for advanced lithium-ion batteries.

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# Mechanisms of Proton And Deuteron Emission from $^{59}$Co and $^{60}$Ni Induced by Deuterons at Medium Energies

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Deuteron-initiated nuclear reactions play an important role in nuclear physics, fusion technologies, activation analysis, and the production of medical isotopes due to complex interaction mechanisms associated with the deuteron's weak binding energy. Since the deuteron consists of a proton and a neutron bound by an energy of only about 2.2 MeV, decay processes (breakup), nucleon transfer, and pre-equilibrium radiation significantly affect reaction cross sections even at relatively low incident particle energies. As a result, deuteron-initiated reactions differ significantly from those induced by protons and neutrons, especially at energies near and above the Coulomb barrier [1].

Nickel and cobalt isotopes are of significant interest in both fundamental and applied research, as they are widely used as s tructural materials in accelerators, fusion systems, and advanced energy technologies. Such research is particularly relevant in the context of developing materials and technologies for advanced energy systems, including fusion reactors and accelerator-controlled neutron sources. High-energy deuterons can significantly activate materials, alter their radiation properties, and generate complex secondary particle spectra. Therefore, a correct description of deuteron-initiated reactions is necessary for calculating the radiation hardness of materials, predicting induced activity, and developing new functional materials for energy applications [2, 3].

In addition, modern nuclear reaction computational codes, such as TALYS and EMPIRE, still face difficulties in describing cluster emission processes and breakup mechanisms for deuterons. Therefore, a systematic study of (d,xp) and (d,xd) reactions on $^{59}$Co and $^{60}$Ni nuclei in the energy range up to 100 MeV is of interest both for testing theoretical models and for developing computational methods for modeling nuclear processes in next-generation energy systems. Studying proton and deuteron radiation in (d,xp) and (d,xd) reactions provides information on compound nucleus decay mechanisms, direct reactions, nucleon transfer processes, and the contribution of breakup processes[4, 5].

In this paper, deuteron-induced reactions on $^{60}$Ni and $^{59}$Co targets at incident particle energies of 14, 23, and 25 MeV are investigated using theoretical calculations of nuclear reactions. Several reaction channels are analyzed using the TALYS nuclear reaction code.

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# Electrochemical Deposition of CdS Thin Films in an Ethylene Glycol Electrolyte

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Energy scarcity is one of the key problems limiting global economic development. The limited availability of fossil fuels and their adverse environmental impacts have increased interest in renewable energy sources, particularly solar energy. Hydrogen production via photoelectrochemical (PEC) water splitting based on solar energy is considered a promising approach.

Chalcogenide-type semiconductors, particularly II–VI group CdS, are distinguished by their high photocatalytic activity under visible light. CdS is widely used both as a buffer layer in photovoltaic devices and as an efficient photoelectrode material for PEC water splitting. It also has applications in optoelectronic devices.

CdS thin films are prepared by various methods, including chemical vapor deposition, chemical bath deposition, vacuum evaporation, electrodeposition, and spray pyrolysis. Among these techniques, electrodeposition is considered advantageous due to its simplicity, low energy consumption, and high material utilization efficiency. CdS films can be obtained from both aqueous and non-aqueous electrolytes. In non-aqueous media, dimethyl sulfoxide (DMSO), dimethylformamide (DMF), and ethylene glycol are widely used [1–3].

The electrodeposition method in a non-aqueous electrolyte medium was used for the preparation of cadmium sulfide (CdS) thin films. The electrolyte solution was based on ethylene glycol. During the preparation of the electrolyte, elemental sulfur was first dissolved in ethylene glycol at a temperature of 363 K, after which $CdCl_2 \cdot H_2O$ was added as the cadmium source. To enhance the electrical conductivity of the solution, $NH_4Cl$ was introduced into the electrolyte.

Electrochemical studies were conducted to investigate the characteristics of the co-deposition process of cadmium and sulfur. During the experiments, the main factors affecting the deposition process—namely the concentration of cadmium ions and temperature—were examined. The concentration of cadmium in the electrolyte was varied in the range of 0.002–0.005 M, while the electrolyte temperature was maintained between 333–363 K. It was found that in ethylene glycol media with high viscosity, ion diffusion is weak at lower temperatures, which in turn slows down the co-deposition process.

CdS thin films were deposited in galvanostatic mode. The deposition process was carried out from an electrolyte containing 0.03 M $CdCl_2 \cdot H_2O$, 0.002 M S, and 0.01 M $NH_4Cl$. The surface morphology and elemental composition of the obtained thin films were investigated, and they were found to possess a homogeneous structure. The conducted studies demonstrated that the selected electrolyte composition and electrolysis conditions enable the stable and high-quality formation of CdS thin films.

Cadmium chalcogenides, particularly CdS, are notable for their broad optical absorption spectrum, high optical stability, and wide range of technological applications. These materials are extensively used in photovoltaic devices and nonlinear optical systems. In addition, the electrocatalytic activity of CdS thin films has been investigated in the electrocatalytic reduction of carbon dioxide.

In this study, a CdS thin film prepared on a copper substrate via electrochemical deposition was investigated as an electrocatalyst for the $CO_2$ reduction reaction ($CO_2RR$). Electrochemical measurements were carried out in a 0.1 M NaCl solution, where the CdS electrode served as the cathode, a platinum electrode was used as the counter electrode, and a silver/silver chloride electrode was used as the reference electrode. The obtained results enable the evaluation of the electrochemical behavior and catalytic activity of the CdS thin film in the $CO_2$ reduction process.

In addition, CdS thin films can be successfully used in the fabrication of solar cells. The CdS/CdTe solar cell has a significant share in the photovoltaic market due to its relatively low cost, high efficiency, and wide range of application possibilities. In this heterojunction solar cell, CdS (band gap 2.42 eV) is used as a “window” layer. CdTe, with a band gap of 1.5 eV, strongly absorbs the solar spectrum and acts as an efficient absorber material due to its high charge carrier mobility.

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# Development of High-Performance Mn-Based Layered Positive Electrodes for Sodium Batteries

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Over the past decade, rapidly increasing global demand for lithium-ion batteries (LIBs) has caused significant fluctuations in lithium prices and raised concerns regarding long-term resource availability and supply-chain stability. Consequently, the development of alternative battery technologies that reduce dependence on non-abundant elements has become increasingly indispensible. In this context, sodium-ion batteries (SIBs) have emerged as promising energy-storgae devices complementary to LIB technologies across a wide range of applications.[1] Practical SIBs have recently entered the market; however, nickel-containing layered oxides, such as $NaNi_{1/3}Fe_{1/3}Mn_{1/3}O_2$, are commonly employed as positive electrode materials, limiting the cost advantage of SIBs compared with $LiFePO_4$/graphite systems widely used in low-cost LIBs. In contrast, Mn-based layered oxides, $Na_xMnO_2$, are particularly attractive because of their low cost and large reverisble capacities. Nevertheless, further improvement in cycling stability and compensation of deficient sodium contents remain necessary for practical battery applications. In this study, the factors affecting the electrochemical performance of P'2-type $Na_{2/3}MnO_2$ [2] are systematically examined, and promising strategies for improving its electrochemical reversibility and long-term cycling stability are discussed.

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# Upcycling Waste PET into N-, and N,S-Co-Doped Porous Carbon Anodes for Lithium-Ion Batteries

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The accumulation of poly(ethylene terephthalate) (PET) waste-persistent across nearly every environmental compartment and lacking genuinely sustainable disposal routes [1] motivates strategies that transform discarded plastic into materials of practical value. Carbon remains a cornerstone of lithium-ion battery (LIB) electrodes [2–4], which makes PET-derived carbon an attractive target for waste valorisation. This work proposes a route to upcycle waste PET into heteroatom-doped porous carbon as an anode material for LIBs and to establish how doping chemistry shapes its electrochemical potential. The approach combines KOH-assisted saponification of PET with controlled pyrolysis under argon, followed by heteroatom doping using two accessible precursors: urea for nitrogen doping and thiourea for nitrogen/sulfur co-doping. A direct comparison of these two configurations is the central aim of the study. Nitrogen is expected to contribute pyridinic and pyrrolic sites favourable for $Li^+$ adsorption, while the additional sulfur introduced by thiourea is expected to expand the interlayer spacing and ease ion transport; the co-doped carbon is therefore of particular interest as a test of whether the two heteroatoms act synergistically rather than merely additively. A preliminary, exploratory assessment of low-temperature behaviour is also considered within the present scope. By treating activation conditions and doping configuration as the key tunable parameters, this work sets out a systematic framework for comparing nitrogen- and nitrogen/sulfur-doped plastic-derived carbons and articulates a green, low-cost pathway from PET waste toward functional anode materials for energy storage.

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# Synthesis of Holey Heteroatom-Doped Graphene via Controlled Exfoliation for Lithium-Ion Battery and Sensor Applications

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The development of advanced carbon-based materials is essential for improving the performance of lithium-ion batteries and next-generation sensing devices. In this work, we propose a strategy for the synthesis of holey heteroatom-doped graphene through controlled exfoliation of pre-existing graphene materials followed by post-treatment modification. Few-layer graphene is subjected to chemical and thermal exfoliation processes to further delaminate the structure and activate defect sites suitable for pore formation.

Subsequent controlled oxidative etching is employed to introduce nanopores within the graphene basal plane, yielding a holey graphene architecture with increased surface area and shortened ion diffusion pathways. In parallel, heteroatom doping (e.g., nitrogen or sulfur) is introduced via thermal annealing in the presence of dopant precursors, aiming to modulate the electronic structure and enhance electrical conductivity.

Although electrochemical performance has not yet been evaluated, the designed material is expected to exhibit improved lithium storage capability due to the synergistic effects of increased active edge sites, defect engineering, and enhanced charge transfer properties. In addition to battery applications, the material may also be suitable for chemical and electrochemical sensors because of its high surface area, tunable electronic properties, and enhanced sensitivity toward analyte adsorption.

This study outlines a scalable approach for engineering functional graphene-based materials for next-generation lithium-ion battery electrodes and sensing platforms.

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# Impact of Silicon Composite Microstructure on Electrochemical Stability and Mechanical Integrity of Li-Ion Battery Anodes

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Silicon composites design is a promising strategy for advancing anode materials in next-generation lithium-ion batteries (LIBs). Silicon, with its high theoretical specific capacity of 3579 $mAh \cdot g^{-1}$ (for the most lithiated $Li_{14}Si_5$ phase), offers an alternative to graphite (372 $mAh \cdot g^{-1}$) for LIBs with high energy density. However, the practical application of silicon in negative electrodes (anodes) is hindered by several critical challenges, primarily the enormous volume expansion/contraction during lithiation/delithiation, causing particle pulverization, loss of electrical contact and continuous degradation of the solid electrolyte interphase (SEI) layer. These changes, in turn, cause rapid material degradation and reduction in mechanical integrity of anodes. Therefore, recent research efforts have increasingly focused on the design of silicon-based composites with more complex structural organization.

Among commercially available silicon-based composites, silicon/carbon (Si/C) composites and magnesium-doped non-stoichiometric silicon oxide (Mg-$SiO_x$) have attracted the greatest practical interest. These two types of silicon-based composites share a same concept for mitigating volume expansion, which involves the encapsulation of silicon nanoparticles within an electrochemically inactive matrix. In Si/C composites, the buffer matrix is formed by carbon, whereas in Mg-$SiO_x$, it consists of magnesium silicate. The latter material is produced industrially by physical vapor deposition of non-stoichiometric silicon oxide where magnesium use to decrease the $SiO_2$ content.

In this study, a comprehensive analysis was performed and correlations between the structural features of Si/C and Mg-$SiO_x$ composites, their electrochemical properties, the processes of SEI layer formation, and the volume changes occurring in the anodes were established. The results demonstrated the superior electrochemical performance of the Si/C composite compared to Mg-$SiO_x$. The low oxidation degree of silicon in Si/C reduces irreversible capacity, while the small size of silicon nanoparticles (4±1 nm) encapsulated within the carbon buffer matrix ensures the absence of electrode volume changes. Moreover, post-mortem analysis demonstrated that the stable SEI layer was formed on the carbon matrix in Si/C, which prevents continuous interaction between the silicon nanoparticles and the electrolyte. In contrast, degradation of the Mg-$SiO_x$ material is caused by significant volume changes that hinder the formation of a stable SEI layer and lead to continuous oxidation of the silicon nanoparticles (16±4 nm) during electrolyte decomposition. These observations explain the dramatically different capacity retention of the two composites: 93% for Si/C versus only 14% for Mg-$SiO_x$ after 500 cycles at a 1C rate in full-cells. Thus, silicon-based anode materials must consist of a stable buffer matrix mitigating the volume expansion of silicon nanoparticles and minimizing their interaction with the electrolyte, thereby preventing material degradation.

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# A Comprehensive Investigation of Multilayer $Ti_3C_2T_x$ Mxene for Supercapacitors in Alkaline and Acidic Media

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Multilayer $Ti_3C_2T_X$ MXene has emerged as a highly promising two-dimensional material for electrochemical energy-storage applications owing to its metallic conductivity, hydrophilic surface chemistry, and tunable layered structure. Nevertheless, the electrochemical behavior of MXene-based electrodes is strongly influenced by electrolyte composition and ion-transport kinetics, which remain critical factors governing capacitive performance in aqueous systems [1] [2].

In the present work, multilayer $Ti_3C_2T_X$ MXene was successfully synthesized from $Ti_3AlC_2$ Max phase via selective hydrofluoric acid etching followed by a gentle shaking-assisted delamination process (Figure 1). Structural and surface analyses confirmed the efficient removal of Al atomic layers and the formation of a well-defined accordion-like layered architecture with enlarged interlayer spacing of approximately 1.2–1.3 nm. X-ray diffraction analysis (XRD) revealed a pronounced shift of the characteristic (002) reflection toward lower diffraction angles, indicating successful exfoliation and interlayer expansion. SEM-EDS and TEM observations demonstrated the transformation of compact MAX-phase particles into expanded multilayer nanosheets, while XPS measurements confirmed the presence of Ti, C, O, and F surface terminations together with the effective elimination of residual aluminum species [3]. The novelty of this work lies in the implementation of a mild shaking-assisted delamination stage after HF etching, which enabled controlled interlayer expansion without harsh ultrasonication or additional intercalation agents. This newly introduced step contributed to the preservation of the multilayer structure, minimized structural defects, and improved ion-accessible pathways within the MXene framework.

The electrochemical properties of $Ti_3C_2T_X$ MXene were systematically evaluated in symmetric two-electrode supercapacitor cells employing alkaline and acidic aqueous electrolytes. Cyclic voltammetry, galvanostatic charge–discharge, and electrochemical impedance spectroscopy revealed that electrolyte chemistry plays a decisive role in governing charge-storage behavior and electrochemical kinetics. In concentrated alkaline electrolyte (6 M KOH), the MXene electrode exhibited quasi-rectangular cyclic voltammetry profiles, highly symmetric charge–discharge curves, reduced internal resistance, and enhanced ion-transport characteristics. The maximum specific capacitance reached approximately 72 F/g at low scan rates in 6 M KOH, significantly surpassing the values obtained in 1 M KOH and 1 M $H_2SO_4$ electrolytes. In contrast, the acidic medium demonstrated increased polarization effects and diffusion limitations, indicating less favorable charge-transfer kinetics. The enhanced electrochemical performance in concentrated alkaline electrolyte is attributed to improved ionic conductivity, reduced charge-transfer resistance, and facilitated ion transport within the expanded MXene interlayers. These results demonstrate the strong potential of multilayer $Ti_3C_2T_x$ MXene for aqueous supercapacitor applications.

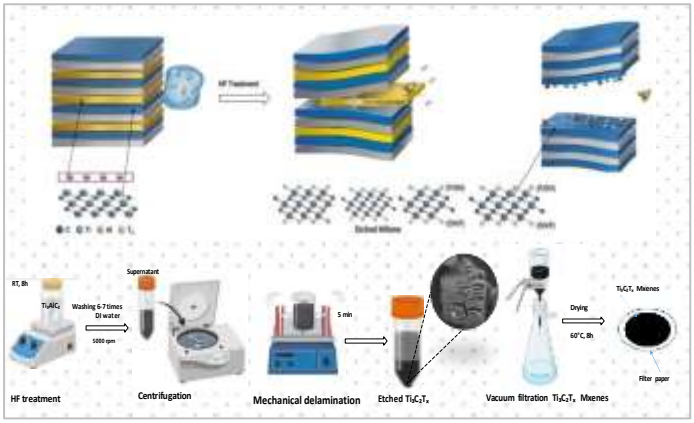



Figure 1. Methodology scheme of synthesis $Ti_3C_2T_X$ Mxene powder

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# Development of Hydrophobic Nanoparticle Coatings for Protection of Next-Generation Energy Systems

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Nowadays, hydrophobic coatings are a vital industrial tool, drawing significant interest due to their ability to repel water, prevent contamination, and protect surfaces from environmental damage. The advancement of such technologies is particularly critical for the development of hydrophobic nanoparticle coatings for the protection of next-generation energy systems, where improving operational stability under harsh weather conditions is essential. Due to their exceptional performance in self-cleaning, corrosion resistance, and anti-icing technologies, superhydrophobic surfaces have become a major focus of modern research [1]. Among the various materials used for the fabrication of such surfaces, silica-based nanoparticles have gained particular interest due to their tunable surface properties, chemical stability, and ease of functionalization.

This work focuses on the synthesis and surface modification of $SiO_2$ nanoparticles for the fabrication of hydrophobic coatings tailored for overhead power transmission line conditions. To achieve this, different sized (30 nm and 350 nm) silica nanoparticles were synthesized using the sol-gel method and further modified with hydrophobic agents to decrease surface energy and improve coating performance. Then, the morphology and particle size distribution of the synthesized nanoparticles were analyzed, demonstrating the formation of uniform particles without significant agglomeration. Specifically, modified $SiO_2$ nanoparticles were subsequently incorporated into a PDMS matrix to fabricate hydrophobic composite coatings on aluminum cables, ensuring enhanced surface protection under operational conditions [2].

The wetting behavior of such fabricated surfaces is typically evaluated via water contact angle measurement, which is a fundamental and widely accepted technique for quantifying the wetting behavior of solid surfaces [3]. In this work, the experimental results demonstrated a strong dependence of the hydrophobic properties of the coating on the curing temperature. At room temperature (~25 °C), low WCA values (approximately 25-30°) were observed, indicating a hydrophilic surface and insufficient formation of a low-surface-energy matrix. Increasing the curing temperature to 40 °C resulted in a significant increase in WCA to ~95°, confirming the formation of a more uniform hydrophobic coating with reduced surface energy.

Building upon promising wetting results, the next phase investigated operational durability under simulated overhead power transmission line conditions. The coatings were evaluated for low-temperature resistance (freezing at - 43 °C with subsequent icing), mechanical stability and UV durability. Mechanical testing via sliding abrasion showed a partial loss of superhydrophobicity, with the WCA decreasing to ~100-110 °C after 10-15 cm. However, tape-peeling tests demonstrated robust adhesion, as the WCA stabilized at ~105-115 °C even after 4-9 cycles. Additionally, a 4-hour UV irradiation caused a slight WCA decrease to ~157 °C, indicating the onset of surface degradation. Because coating stability depends heavily on the deposition technique, a pendulum-like spraying method was optimized. Visual and functional analysis confirmed that this approach produces highly uniform coatings with stable WCA along the entire surface of aluminum cables. Finally, to simulate precipitation exposure (rain/wet snow followed by icing), coated and uncoated cables were pre-cooled in a freezer for 30 minutes at 0 °C, - 5 °C, - 10 °C, and - 15 °C to ensure uniform temperature distribution.

The outstanding performance of the coatings under different conditions clearly establishes modified $SiO_2$ nanoparticles as a promising material for broad practical applications. Crucially, these findings open new avenues for the development of hydrophobic coatings for the protection of next-generation energy systems, demonstrating strong potential for industrial implementation. In electronics, hydrophobic protection is particularly important for flexible and wearable devices that are sensitive to moisture exposure. Additionally, implementing such advanced protective coatings on solar panels and wind turbine components can minimize the accumulation of water, ice, and dust, thereby reducing surface degradation and maintaining energy efficiency under unfavorable weather conditions across various regions of Republic of Kazakhstan. These protective properties ultimately contribute to lower maintenance costs and increased durability of these renewable energy systems.

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# Sodium-Ion Batteries with NaPF6/NaOTf Dual-Salt in Ether Based Electrolytes for Wide-Temperature Operation

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With the growing demand for energy storage systems, sodium-ion batteries (SIBs) have attracted considerable attention as a more affordable alternative to lithium-ion batteries due to the high prevalence of sodium in the earth's crust and the expected reduction in cost [1]. Despite significant progress in the development of SIBs, their practical application is still accompanied by several challenges, including limited cycling stability and deterioration of electrochemical performance at temperatures deviating from room temperature[2]. The properties of the electrolyte and the formation of interfacial layers on electrode surfaces play a crucial role in these processes. Therefore, the development of electrolyte systems capable of ensuring efficient battery operation over a wide temperature range is of particular interest.

In this work, binary ether electrolytes based on mixtures of $NaPF_6$ and NaOTf (1M:0M, 0,5M:0,5M, 0,9M:0,1M, 0M:1M) in glyme solvents of different chain lengths (1G – 1,2-dimethoxyethane – monoglyme; 2G – bis(2-methoxyethyl) ether – diglyme; 3G – triethylene glycol dimethyl ether – triglyme; 4G – tetraethylene glycol dimethyl ether – tetraglyme) are investigated. Ether-based electrolytes are of particular interest because of their wide electrochemical stability window and operational temperature range, as well as their ability to form solvate complexes and a thin, stable solid electrolyte interphase (SEI) layer [1,4]. $NaPF_6$ provides stable cycling behavior and effective SEI formation at room and elevated temperatures, while NaOTf improves low-temperature performance [2]. The combination of these salts is expected to improve the electrochemical stability and wide-temperature performance of sodium-ion batteries. A hard carbon (HC) anode, characterized by its ability to reversibly insert and extract sodium ions, was used in this work [3].

In this work, the physicochemical properties and electrochemical performance of ether-based sodium-ion battery electrolytes were systematically investigated using impedance spectroscopy, conductometry, Raman spectroscopy, DSC, and galvanostatic cycling in the temperature range from −30 to +40 °C. The studied parameters included ionic conductivity, solvation structure, electrochemical stability, and charge-storage behavior in Na/HC half-cells.

Electrochemical testing of Na/HC half-cells demonstrated that at +25 °C all electrolytes delivered high reversible capacities (180–280 mAh $g^{-1}$) showing the best performance for systems containing 1 M NaOTf or 1 M $NaPF_6$. At +40 °C, a small addition of NaOTf (10%) enhanced capacity from ~200 mAh $g^{-1}$ (for pure 1 M $NaPF_6$) to ~250 mAh $g^{-1}$, while higher NaOTf contents resulted in accelerated capacity fading and the battery itself due to corrosion of aluminum current collectors. At −30 °C, electrolytes based solely on $NaPF_6$ failed to support stable cycling, whereas NaOTf-containing systems enabled reversible capacities up to ~160 mAh $g^{-1}$ (4G and 2G). These results confirm that dual-salt systems significantly extend the operational temperature window of sodium-ion batteries, enabling retention of up to ~60% of capacity at low temperatures and ~80% at elevated temperatures.

Overall,the combined analysis demonstrates that electrolyte performance is determined by a balance between ionic conductivity, solvation structure, and interfacial layer stability. The optimal composition obtained in this study is 0.9 M $NaPF_6$ + 0.1 M NaOTf in G2, which provides a favorable compromise between conductivity, low-temperature ion transport, and high-temperature stability, making it a promising electrolyte formulation for wide-temperature sodium-ion batteries.

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# PLA-Based Biodegradable Printed Circuit Boards as a Regenerable Composite Platform for Green Electronics

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Electronic waste is one of the fastest-growing environmental challenges of modern technological civilization, and printed circuit boards are among its most difficult-to-recycle components because they are commonly based on thermoset epoxy or phenol-formaldehyde binders. In this work, we present a biodegradable and regenerable printed circuit board based on polylactic acid (PLA) as an environmentally safer alternative to conventional FR2/FR4-type materials. The developed PLA-based composite substrate can be processed into a functional printed circuit board, withstand key technological operations, and serve as the basis for a simple working electronic device (Figure 1A). At the end of its life cycle, the board can be separated into valuable components, including polymer matrix, reinforcing material, copper conductors, and electronic elements (Figure 1B), enabling recovery of more than 95% of the initial material mass and 100% of the electronic components. This approach demonstrates a new design principle for green electronics: electronic materials should be engineered not only for performance during service, but also for recovery, regeneration, and responsible end-of-life management within a circular economy [1-3].

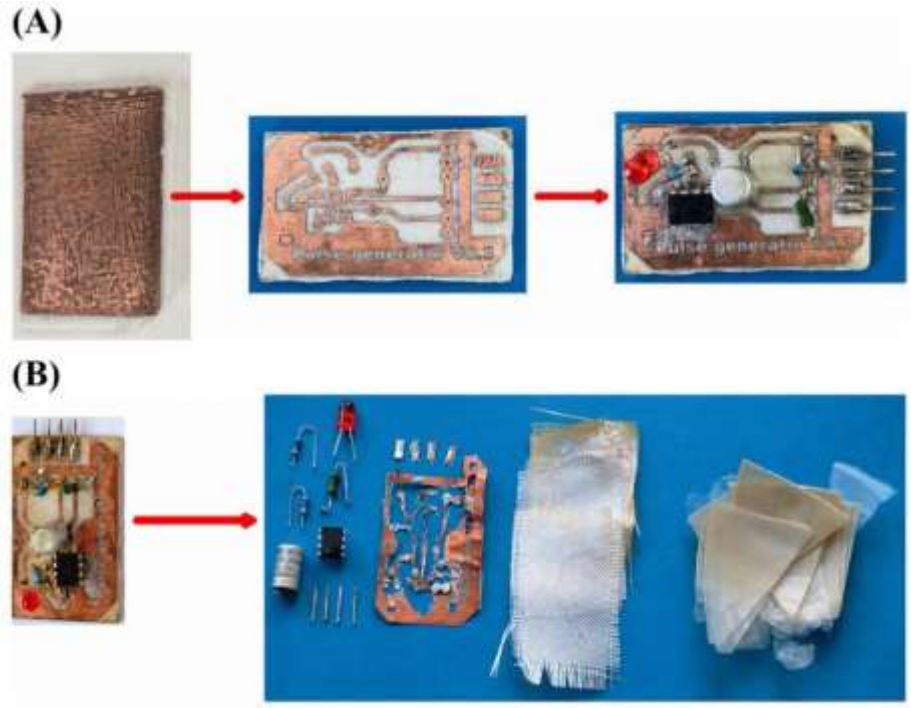



Figure 1. Life cycle of a PLA-based printed circuit board: (A) fabrication of a functional electronic device; (B) end-of-life separation into reusable components.

The study demonstrated the full life-cycle concept of a PLA-based printed circuit board: fabrication of a working electronic device, followed by end-of-life separation and recovery of valuable components. This confirms the potential of PLA-PCB technology as a regenerable composite platform for green electronics.

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# Waste Polyethylene as a Sustainable Source of Conductive Carbon Additive for $LiFePO_4$ Cathodes

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The rapid growth of lithium-ion battery production demands cost-effective and sustainable conductive additives for cathode materials, while simultaneously the global accumulation of polyethylene (PE) plastic waste presents both an environmental challenge and an underutilized carbon-rich resource. This work demonstrates a viable pathway for converting low-density polyethylene (LDPE) and high-density polyethylene (HDPE) plastic waste into functional conductive carbon materials for application as additives in $LiFePO_4$ (LFP) cathodes.

Carbon materials were synthesized via a three-stage thermochemical process. In the first stage, sulfonation with concentrated $H_2SO_4$ (98 wt%) introduced sulfonic acid groups ($–SO_3H$), hydroxyl groups, and conjugated C=C bonds into the polymer backbone, rendering the thermoplastic material infusible through radical chain crosslinking [1]. The diffusion-controlled nature of sulfonation resulted in substantially higher carbon yields for HDPE-S (33.41%) compared to LDPE-S (8.7%) at 1300 °C, attributable to the higher crystallinity of HDPE restricting acid penetration into crystalline domains while enabling denser crosslinking in amorphous regions. In the second stage, pre-carbonization at 350 °C under argon atmosphere completed desulfonation — releasing $SO_2$ and $H_2O$ via a radical chain mechanism that dominates below this temperature and maximized crosslink density, establishing a thermally stable aromatic framework [2]. The choice of 350 °C as the pre-carbonization temperature is chemically justified as the natural boundary between the radical desulfonation mechanism and the internal five-centered elimination ($E_i5$) mechanism, below which the majority of non-carbon heteroatoms are released [3]. In the third stage, carbonization was carried out at temperatures from 600 to 1300 °C, with dehydrogenation above 600 °C yielding $H_2$ as the key indicator of graphitization and $sp^2$-carbon network formation [4].

Systematic structural characterization of the carbonized series revealed a clear evolution toward graphitic order with increasing temperature. XRD analysis showed a progressive decrease in interlayer spacing $d_{002}$ and growth in lateral crystallite size $L_a$, reaching 5.34 nm (LDPE) and 4.70 nm (HDPE) at 1200 °C. Raman spectroscopy confirmed increasing $sp^2$ carbon content, with $I_D/I_G$ ratios of 1.08 and 1.01 for LDPE-C-350/1200 and HDPE-C-350/1200 respectively. XPS analysis demonstrated near-complete removal of sulfur and oxygen heteroatoms at 1200 °C, with carbon content exceeding 95 at.%. Electrical conductivity measurements identified 1200 °C as the optimal carbonization temperature, yielding conductivity values comparable to commercial Super P carbon black.

LFP cathodes incorporating LDPE-C-350/1200 and HDPE-C-350/1200 as conductive additives were evaluated electrochemically and benchmarked against Super P. Cyclic voltammetry revealed well-defined and reversible $Fe^{2+}/Fe^{3+}$ redox couples, while galvanostatic charge-discharge measurements demonstrated competitive specific capacities across a wide range of C-rates. Electrochemical impedance spectroscopy confirmed reduced charge transfer resistance compared to reference electrodes, consistent with the high electrical conductivity of the PE-derived carbons. Long-term cycling stability further validated the practical applicability of these materials.

This work establishes a sustainable waste-to-battery concept, demonstrating that commodity plastic waste can be directly converted into high-performance conductive carbon additives, offering a cost-effective and environmentally responsible alternative to conventional carbon blacks in lithium-ion battery cathodes.

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# Upcycling Waste PET into Porous Carbon Hosts for Synergistic Li–$Se_xS_y$ Cathodes Probing the Se:S Ratio as a Performance-Governing Parameter

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The convergence of two pressing challenges the unsustainable accumulation of poly(ethylene terephthalate) (PET) waste [1] and the demand for cathode platforms that transcend the limitations of single-chalcogen chemistries [2,3] motivates the present study. Lithium–sulfur batteries offer compelling theoretical energy density (2600 Wh $kg^{-1}$) yet remain constrained by sluggish redox kinetics and the polysulfide shuttle effect rooted in the near-insulating character of elemental sulfur [4]. Selenium carries electronic conductivity orders of magnitude superior to sulfur and facilitates faster charge-transfer kinetics, but its lower gravimetric capacity and high polyselenide solubility impose their own ceiling [3,5]. The binary $Se_xS_y$ strategy, in which the two chalcogens act cooperatively rather than as independent phases, has demonstrated that selenium can accelerate redox conversion while sulfur anchors volumetric capacity - provided an adequate confinement host suppresses dissolution of mixed intermediates [2,5].This work proposes a dual-value route that simultaneously addresses plastic waste and cathode engineering: waste PET is converted into hard porous carbon (HPC) through alkaline saponification followed by controlled pyrolysis under argon, yielding a hierarchically porous, defect-rich scaffold suited to chalcogen confinement. The $Se_xS_y$ active phase is introduced by melt-diffusion, and the central variable is the Se:S molar ratio, evaluated across three compositions $Se_1S_9$ (10 mol% Se), $Se_3S_7$ (30 mol% Se), and $Se_1S_1$ (50 mol% Se) spanning the transition from a sulfur-dominant, capacity-prioritising regime to one in which selenium's conductivity contribution becomes governing. The hypothesis is that an intermediate selenium fraction will produce a non-additive synergistic enhancement of specific capacity and cycling stability relative to either chalcogen-only endpoint, identifiable through rate capability, Coulombic efficiency, and capacity retention across the composition series. By treating waste PET as a functional precursor and Se:S stoichiometry as the principal design lever, this study advances a green, low-cost, and compositionally tuneable cathode strategy for lithium–chalcogen energy storage.

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# Engineering the Adhesive Architecture of Flexible Lithium-Ion Microbatteries

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The flexible Li-ion microbatteries are being developed as compact energy-storage systems for flexible and wearable electronics. Their practical realization requires not only electrochemically active thin-film components, but also mechanically stable interfaces between the flexible substrate and deposited functional layers. One of the promising substrates is widely-used polyimide tape, since it combines high mechanical flexibility, thermal stability, and chemical resistance, which are important for microbattery fabrication. However, its chemically inert surface can result in weak adhesion with deposited metal and oxide layers. Based on our experimental work and literature analysis, weak adhesion between polyimide substrate and deposited thin-film layers was identified as a key limitation in the development, leading to delamination, non uniform deposition, and possible short circuit formation. Therefore, improving the Kapton surface before placing the components of the battery on it is an important step toward reliable flexible microbattery architectures.

In this work, Kapton substrates were chemically activated by potassium hydroxide (KOH) treatment to modify the surface chemistry and improve compatibility with deposited metal and oxide layers. The treatment approach was selected based on previous studies of polyimide metallization, where alkaline modification promotes imide-ring opening and forms a more reactive surface layer [1-2]. The treated and untreated Kapton films were characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), and Raman spectroscopy to evaluate morphological and chemical changes induced by the treatment.

FTIR analysis confirmed surface modification after KOH exposure. The weakening of imide C=O bands at approximately 1775 and 1720 $cm^{-1}$ indicates partial imide-ring cleavage, while the appearance of and amide C=O band near 1650 $cm^{-1}$ and $COO^-$ stretching around 1420 $cm^{-1}$ suggests the formation of carboxylate containing surface groups. These chemical changes are consistent with the formation of a polyamic acid like surface layer, which can enhance interaction with deposited thin films. SEM and Raman analyses were used to further assess the surface morphology and structural changes after treatment.

The obtained results show that KOH treatment is a promising surface engineering route for preparing Kapton substrates for flexible microbattery fabrication. This approach provides a foundation for improving interfacial adhesion, reducing delamination related failure, and developing mechanically reliable flexible microbattery systems.

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# Optimization of Lead-Free Double Perovskite Sandwich Solar Cell Characteristics

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In recent years, halide perovskites have gained significant attention as promising materials for next-generation photovoltaics due to their exceptional optoelectronic properties [1-4]. However, the high toxicity of lead and the instability of traditional perovskite compounds remain critical barriers to their large-scale commercialization.

This study investigates a multilayer sandwich solar cell structure, Glass/ITO/$SnO_2$/Double Perovskite/NiO/Ag, in which the environmentally friendly double perovskite $Rb_2TlRhF_6$ is employed as the active layer [5]. The research includes a comprehensive analysis of the device's optical properties (absorption, reflection, and parasitic absorption) and electrical characteristics, as well as an evaluation of the influence of electrode material properties on overall device performance. Using numerical modeling techniques, key structural parameters were identified to maximize the power conversion efficiency. The obtained results provide a framework for determining the optimal conditions for enhancing the operational performance of the developed photovoltaic devices.

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# Performance Optimization of Monolithic All-Perovskite Triple-Junction Solar Cells

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All-perovskite tandem solar cells (TSCs) have achieved a power conversion efficiency (PCE) of 30.1% [1]; however, significant optical losses still prevent them from approaching the theoretical efficiency limit of 45% [2-3]. Among these losses, reflection-induced energy dissipation is particularly detrimental. Previous studies have shown that, for a representative all-perovskite TSC architecture, optical losses account for approximately 31.15% of the total energy loss, while reflection losses alone contribute up to 19.64% [2]. These reflections not only reduce the photon flux reaching the absorber layers but also represent a major bottleneck to achieving higher device efficiencies.

Multijunction solar cells based on epitaxial III–V semiconductors have demonstrated very high PCEs; however, their widespread terrestrial deployment is limited by high manufacturing costs. In contrast, multijunction solar cells fabricated using low-cost solution-processing techniques offer a promising pathway toward high-efficiency and economically viable photovoltaic technologies. Recent advances have demonstrated efficient all-perovskite triple-junction solar cells employing optimal-bandgap perovskite absorbers. These developments represent an important step toward realizing highly efficient all-perovskite multijunction solar cells. Reducing reflection losses through advanced optical management strategies is therefore essential for further improving device performance and approaching the theoretical efficiency limit.

**Acknowledgments.** This research was also funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan, grant number AP32727319.

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# Development of GCN-Modified PVA-Based Gel Polymer Electrolytes for High-Stability Lithium-Sulfur Batteries

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Lithium-sulfur (Li-S) batteries have emerged as a leading alternative for next-generation energy storage, effectively addressing the performance bottlenecks of current technologies. With a theoretical specific capacity of 1675 mAh $g^{-1}$ and, Li-S systems significantly outperform traditional lithium-ion batteries in energy storage potential [1,2]. Despite these advantages, the commercialization of Li-S technology is severely hindered by the "polysulfide shuttle effect" - the dissolution and migration of lithium polysulfides between the cathode and anode - which leads to rapid capacity degradation and low coulombic efficiency [3]. A critical strategy for addressing these fundamental challenges involves replacing the conventional liquid electrolyte (LE) with a solid-state or gel polymer electrolyte (GPE). By substituting the LE, the mobility of polysulfides can be physically and chemically restricted, providing a more robust environment for stable cycling [4,5].

Building upon previous research into dual-crosslinked PVA-based electrolytes, this study introduces a novel modification: the incorporation of graphitic carbon nitride (GCN) into a PVA-based GPE matrix. The composite AB@S cathode was synthesized via a melt diffusion process at 155° C, ensuring a high sulfur loading of ~60% within an acetylene black conductive host. The GPE membranes were fabricated using a double ultra- and thermo-crosslinking/electrospinning method, resulting in a nanofibrous structure doped with GCN concentrations ranging from 0% to 15%. Structural characterization through FTIR and SEM confirmed successful chemical crosslinking and a uniform dispersion of GCN particles throughout the ~50 μm thick membrane.

The integration of GCN proved essential for performance enhancement, as the 15% GCN sample exhibited an electrolyte uptake of 1256%, a significant increase over the 543% observed in the pristine GCN 0 membrane. Electrochemical testing demonstrated that the 15% GCN cell achieved a high initial discharge capacity of 1014.70 mAh $g^{-1}$ and maintained a superior capacity retention of 763.30 mAh $g^{-1}$ after 100 cycles at 0.1C. In comparison, the LE control cell experienced much faster degradation, retaining only 519.96 mAh $g^{-1}$. This performance boost is attributed to a synergistic mechanism where the electrospun PVA nanofibers act as a physical barrier, while the polar triazine rings of the GCN provide chemical anchoring sites to trap polysulfides. These results confirm that replacing LE with a GCN-modified GPE is a highly effective and scalable solution for achieving stable, high-capacity Li-S battery technology.

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# In Situ Gel Electrolytes and Interfacial Engineering for Extrem-Temperature Lithium Metal Batteries

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Lithium metal batteries are promising candidates for high-energy-density storage systems, yet their stable operation over a wide temperature range remains limited by sluggish ion transport, electrolyte instability, and uncontrolled lithium deposition. These issues are particularly severe under extreme temperatures, where ion migration in the electrolyte bulk and $Li^+$ transfer across the lithium metal interface are simultaneously impeded. Therefore, understanding and regulating ion transport mechanisms in both the bulk electrolyte and the interfacial desolvation region is essential for developing wide-temperature lithium metal batteries. Here, we present a gel-electrolyte/interfacial engineering strategy to improve the thermal adaptability and interfacial stability of lithium metal batteries, with emphasis on the regulation of low-temperature $Li^+$ desolvation dynamics at the lithium metal anode.

The key design is a multifunctional grafted interphase constructed on lithium metal, which integrates an organic ion-selective matrix, an electron-blocking LiCl/LiF-rich layer, and a lithiophilic Li–Ga alloy layer. This hierarchical interphase enables pre-desolvation of $Li^+$, promotes selective ion transport, homogenizes $Li^+$ flux, and guides uniform lithium deposition. PFG-NMR measurements, together with theoretical calculations and molecular simulations, confirm that the engineered interface significantly alters the interfacial transport pathway and lowers the $Li^+$ desolvation energy barrier. As a result, lithium symmetric cells with the grafted anode achieve stable cycling for over 1000 h at −20 °C, showing markedly enhanced stability compared with bare lithium. The interfacial design also improves the low-temperature cycling durability of lithium–air batteries by suppressing dendrite growth, parasitic corrosion, and interfacial polarization. Supported by in situ gel electrolyte chemistry that stabilizes the electrolyte environment and improves electrode/electrolyte contact, this work demonstrates that wide-temperature lithium metal batteries require coordinated regulation of both electrolyte bulk transport and desolvation-dominated interfacial ion transfer. This principle provides a practical pathway for developing high-energy batteries under harsh thermal conditions.

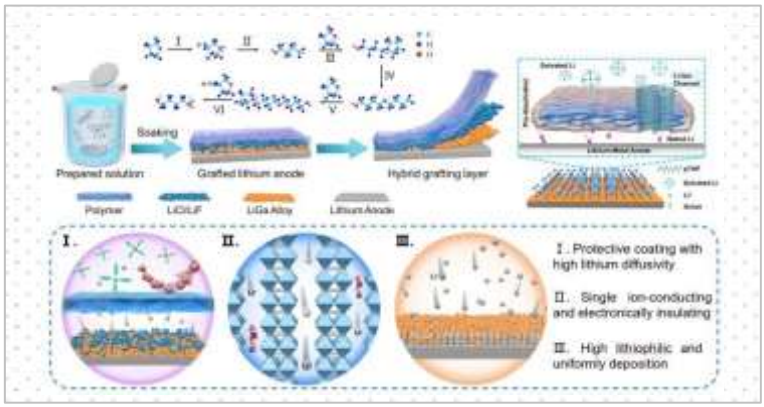



Figure 1. The preparation process of grafting layer and the design concept of multifunctional components.

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# Vinylimidazole Anchored Flexible Polyionic Liquid gel Electrolyte for High-Performance Rechargeable Zn Batteries

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The growing demand for sustainable and safe energy storage systems, driven by rapid growth in human population and increased living standards, has accelerated the exploration of alternatives to conventional lithium-ion batteries. In this context, rechargeable zinc batteries have emerged as a promising candidate due to their inherent safety, low cost, and environmental compatibility. However, the development of efficient electrolytes with high ionic conductivity, wide electrochemical stability, and robust mechanical integrity remains a critical challenge. Herein we report the design and synthesis of a novel polyionic liquid-based hydrogel electrolyte via UV crosslinked in situ polymerization of vinylimidazole monomers and polyethylene glycol diacrylate in the presence of $Zn(ClO_4)_2$. The resulting crosslinked polymeric network provides the advantage of ionic liquid and solid electrolytes, and provides continuous ion conduction pathways and enhanced interfacial stability. The imidazolium framework facilitates the efficient $Zn^{2+}$ transport, and the PEGDA backbone gives the mechanical strength and flexibility to the material. The developed hydrogel electrolyte exhibits an ionic conductivity of 0.61 x $10^{-3}$ S $cm^{-1}$ at 75 °C, indicating efficient ion transport within the crosslinked network. Furthermore, Zn/Zn symmetric Zn cells demonstrate stable cycling performance for over 300 cycles, confirming good interfacial stability and suppression of dendritic growth. These results highlight the potential of the proposed system for application in safe and high-performance zinc-based energy storage devices.

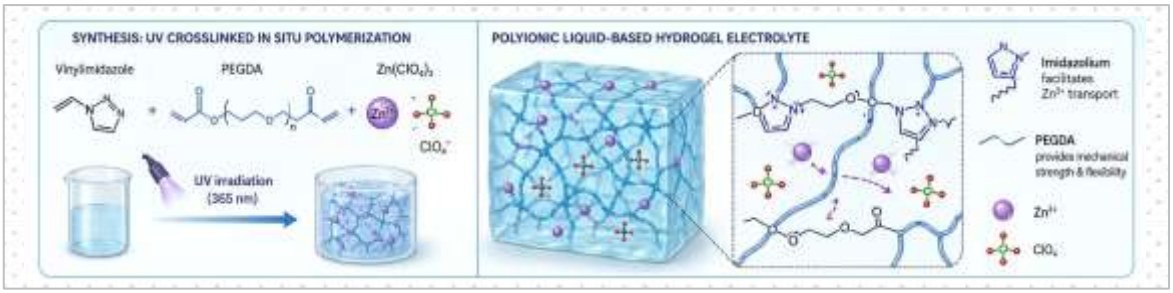



Figure 1. Schematic representation of the PIL gel electrolyte formation.

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# Redox-Active, Water-Soluble Microgels and Branched Polymers: Synthesis and Electrochemical Characterization

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Polymer-based aqueous redox flow batteries (RFBs) are attracting increasing attention as a promising next-generation energy storage technology due to their potential for low cost and environmental friendliness. Polymers with densely populated redox sites feature high charge-transport and charge-storage capacities. The incorporation of a redox unit into the polymer chain often improves cycling stability and helps overcome technical issues related to cell design. More importantly, it prevents the movement of redox species across the membrane, which can lead to severe capacity loss and make the cell more demanding on the type of membrane separating the anode and cathode compartments.

From the structural point of view, both linear and branched (crosslinked) polymers can be considered as the carriers for redox-active groups. Recently, a few works appeared that deal with more complicated polymer structures such as microgels, i.e., the weakly cross-linked submicron-size polymer meshes. The branched systems possess a lower viscosity than the linear polymers of the similar molecular weight, while the concentration of the redox-active centers can be as high as that for the linear polymer-based systems, which are favorable for use in RFBs.

In response to this need, we have synthesized and tested a range of new water-soluble redox-active TEMPO and s-tetrazine derivatives, including both low molecular weight compounds and polymers with different architectures. We have successfully modified linear polyacrylic acid, branched polyacrylic acid and poly(N-isopropylacrylamide-co-acrylic acid) microgels with pendent redox groups [2]. Electrochemical testing has shown that the new water-soluble redox polymers, both linear and microgel, demonstrate chemical reversibility in an aqueous solution. This expands the range of water-soluble cathode and anodic materials suitable for water-based organic RFBs.

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# Mechanochemical Synthesis of $LiFePO_4$ Cathode Material for Sub-Zero Temperature Lithium-Ion Batteries

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Low-temperature-tolerant lithium-ion batteries are attractive power sources due to their high energy density, low self-discharge, long cycle life, and ability to operate under diverse environmental conditions [1]. As the cathode significantly influences the cost, weight, and electrochemical performance of lithium-ion batteries, the selection of an appropriate cathode material is crucial. Polyanionic olivine-type $LiFePO_4$ is a promising candidate owing to its low cost, safety, and cycling stability. However, its practical application is hindered by poor $Li^+$ diffusivity and low electronic and ionic conductivity [2]. In this work, these limitations are addressed through a mechanochemically assisted solid-state synthesis strategy for $LiFePO_4$, specifically designed for sub-zero temperature applications.

The proposed one-pot, scalable synthesis of nanosized $LiFePO_4$/C is a solvent- and surfactant-free process. Ammonium dihydrogen phosphate is employed as both the phosphate source and the nitrogen-doping precursor. Furthermore, the relatively low calcination temperature contributes to reduced overall processing costs. The synthesized material was systematically characterized and compared with a benchmark commercial cathode ($LiFePO_4$/C (com.)). Scanning electron microscopy revealed a reduced particle size distribution for the synthesized sample ($LiFePO_4$/C (s.)), while transmission electron microscopy, Raman spectroscopy, and X-ray photoelectron spectroscopy confirmed the presence of an N-doped amorphous carbon layer. Nitrogen adsorption-desorption analysis indicated a threefold increase in specific surface area compared to the commercial counterpart.

At −20 °C and 0.1 C, the synthesized $LiFePO_4$/C (s.) delivered a discharge capacity of 108.04 mAh $g^{-1}$ and maintained 100% coulombic efficiency over 100 cycles, with reduced polarization (Figure 1a). Under identical conditions, the commercial $LiFePO_4$/C (com.) exhibited a lower discharge capacity of 92.88 mAh $g^{-1}$ and a coulombic efficiency of 95.08% (Figure 1b). Rate capability tests at −20 °C further confirmed the superior performance of $LiFePO_4$/C (s.) (Figure 1c). This enhancement is attributed to the optimized carbon content, the presence of an N-doped amorphous carbon coating, reduced particle size, and increased specific surface area.

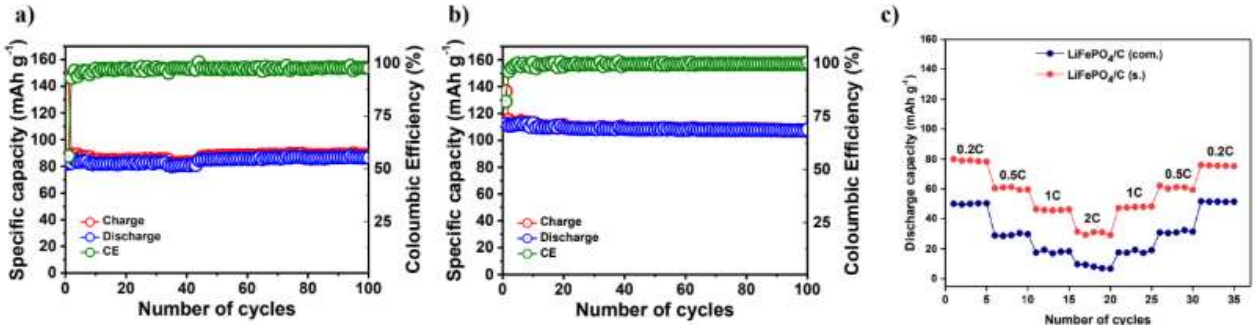



**Figure 1.** Cyclic performance at 0.1 C and -20 °C of a) $LiFePO_4$/C (s.) and b) $LiFePO_4$/C (com.); c) rate capability of $LiFePO_4$/C (s.) and $LiFePO_4$/C (com.) at -20 °C.

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# High Entropy Layered Oxide Cathodes for Sodium-Ion Batteries

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O3-type layered high-entropy sodium cathode materials are promising candidates for Na-ion batteries due to their composition flexibility and enhanced structural stability. The incorporation of multiple transition metals into a single lattice increases the overall configurational entropy, which contributes to the stabilization of the O3 layered structure during cycling. This high configurational entropy helps suppress undesirable phase transitions, such as O3–P3, that typically occur during sodium extraction and insertion, while each constituent metal plays a complementary role: Ni and Cu contribute to redox capacity, Fe enhances structural integrity, Mn promotes stability at high voltages, and Ti acts as a structural pillar to mitigate volume change.

In this work, $NaNi_{0.3}Cu_{0.1}Fe_{0.2}Mn_{0.3}Ti_{0.1}O_2$ ( NNCFMTO) and $Na_{0.95}Li_{0.05}Ni_{0.3}Cu_{0.1}Fe_{0.2}Mn_{0.3}Ti_{0.1}O_2$ ( NLNCFMTO) were investigated to evaluate the electrochemical performance and determine the optimal operating voltage range. A solid-state synthesis method was utilized. X-ray diffraction confirmed well-developed layered structures with varying degrees of stacking and transition metal ordering in both compositions.

Li-doping was introduced to optimize the structure of the high-entropy cathode. The $Li^+$ ion forms stronger Li-O bonds compared to typical transition metal-oxide bonds, helping to maintain the integrity of the alkali metal layer. Furthermore, Li-doping enhances the sodium-ion diffusion coefficient and ionic conductivity, thereby alleviating the kinetic limitations inherent to sodium-ion batteries.

Both compositions demonstrated reversible specific capacity—NNCFMTO of 140 mAh $g^{-1}$ and NLNCFMTO of 150 mAh $g^{-1}$,with cycle stability of 70 and 100 cycles, respectively, at the optimum voltage range of 2.0-4.0 V. These results highlight the significance of high-entropy design and Li-doping strategies in achieving competitive specific capacity and cycle performance, providing valuable insights into the development of high-performance sodium-ion battery cathodes.

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# Aqueous Sodium-Ion Batteries Based on High-Performance Advanced Materials

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Aqueous sodium-ion batteries (ASIBs) represent a path toward low-cost and safe grid-scale energy storage. Manganese-based Prussian blue analogues (MnPBA) offer high theoretical capacity and earth-abundant composition. However, progressive dissolution of $Mn^{2+}$ driven by $Mn^{3+}$ disproportionation is the main obstacle to industrialization.

In this work, we report the development of MnPBA// $Na_3Ti_2(PO_4)_3$ (NTP) full-cell system in a 17 M $NaClO_4$ water-in-salt (WiS) electrolyte. Sodium citrate-mediated co-precipitation was employed to synthesize MnPBA with controlled morphology and reduced structural vacancies, delivering an initial discharge capacity of ~140 mAh/g. The electrochemical evidence of Mn dissolution, discoloration of electrolyte, and electrodeposition of dissolved Mn ions on counter electrodes guided the development of a cathode stabilization strategy.

Aqueous batteries suffer from absence of CEI/SEI layers due to nature of water's decomposition products. Unlike organic solvents used in standard lithium-ion batteries - which decompose at extreme voltages to form a solid, ionically conductive, and electronically insulating protective layer - water decomposes into gases. Coating of the material with inorganic material, $Ni(OH)_2$ showed better cycling stability with 80% capacity retention after 200 cycles, proving that artificially created CEI layer contributes to longer life cycle of battery. The cyclic voltammetry, galvanostatic charging, and dQ/dV analysis were employed to evaluate the contribution of the strategy. This study demonstrates that interfacial engineering, combined with WiS electrolyte, offers a viable route to long-cycling, safe ASIBs.

# Free-Standing $MnO_2$/PEDOT/PET Nanofibrous Cathodes Derived from Recycled PET Bottles for Aqueous Energy Storage

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Polyethylene terephthalate (PET) is one of the most widely used thermoplastic polymers; however, discarded PET bottles present a significant environmental challenge due to their extremely slow degradation. Transforming waste PET into functional electrode materials offers a sustainable strategy for plastic waste valorization while supporting the development of environmentally friendly energy-storage technologies. In this work, free-standing PET nanofibrous mats were fabricated by electrospinning using recycled PETE-grade plastic bottles. The PET nanofibers were subsequently coated with the conductive polymer poly(3,4-ethylenedioxythiophene) (PEDOT) via in-situ chemical polymerization, followed by the deposition of $MnO_2$ as the electrochemically active material.

As shown in Figure 1, SEM analysis confirmed the successful formation of a hierarchical $MnO_2$/PEDOT coating on the PET nanofibers, while cyclic voltammetry exhibited the characteristic redox behavior of $MnO_2$, indicating its electrochemical activity. The resulting free-standing electrode eliminates the need for polymer binders and metallic current collectors while maintaining structural flexibility. Ongoing work focuses on optimizing the $MnO_2$ loading and conductive PEDOT layer to enhance the electrochemical performance of the electrode for aqueous energy-storage applications.

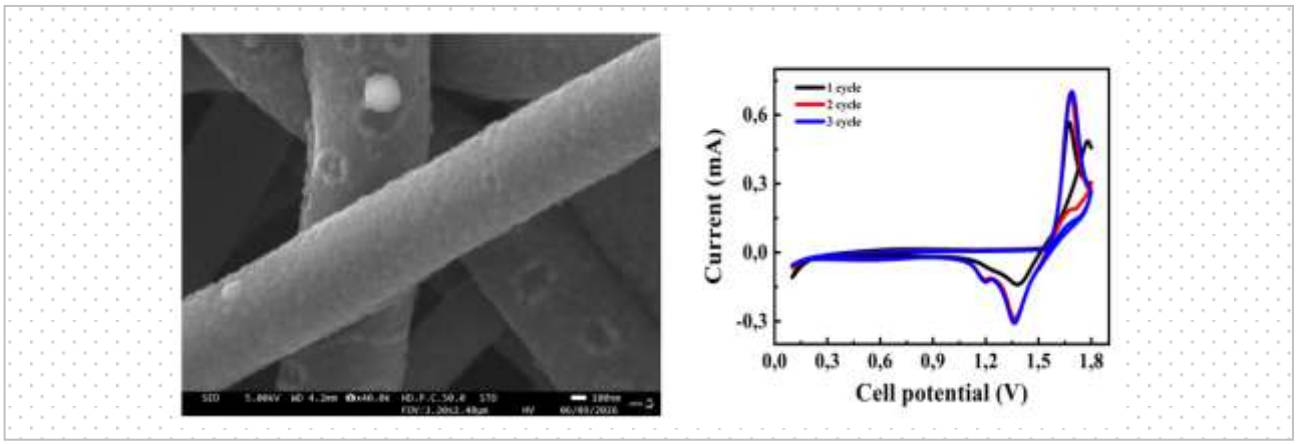



**Figure 1.** (a) SEM image and (b) CV curves of MnO2/PEDOT/PET nanofibers.

**Acknowledgements**

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# Investigation of the Effect of a Carbon Cathode with Controlled Porosity on Degradation Processes and Cycling Stability in Li-S batteries Under Variable Load Conditions

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Lithium-sulfur batteries (LSBs) are promising next-generation energy storage devices, outperforming existing lithium-ion batteries in energy density (2600 $Wh \cdot kg^{-1}$) and theoretical specific capacity (1675 $mAh \cdot g^{-1}$). As the increasing variability of electricity consumption and generation creates a growing need for flexible energy storage solutions, stationary battery energy storage systems can be integrated into distribution networks to reduce peak loads, shift electricity consumption from peak to off-peak periods, and improve the balance between electricity supply and demand [1]. However, a critical barrier to their widespread adoption remains the pronounced degradation processes that lead to rapid capacity fading and low cyclic stability [2-4]. In this work, a fundamental investigation was carried out on the effect of the porous structure of a carbon matrix with controlled pore size on the formation of sulfur cathodes and their electrochemical stability under various current regimes.

Comprehensive physicochemical characterization revealed that the specific surface area of the materials, determined by the Brunauer-Emmett-Teller (BET) method, exceeds 1100 $m^2 \cdot g^{-1}$ and can be further tuned by adjusting the precursor-to-template ratio. Both predominantly microporous structures with pore diameters below 2 nm and micro-mesoporous materials with pore size distributions starting from 1.2 nm were successfully obtained. Scanning electron microscopy (SEM) confirmed the formation of a well-developed hierarchical porous structure that ensures efficient sulfur infiltration, electrolyte transport, and partial retention of polysulfides.

Electrochemical tests were performed under long-term cycling and stepwise current density variation in the range of 0.1-2C. This testing approach was used to evaluate the response of the batteries to changes in operating intensity, which may occur in stationary energy storage systems during load leveling, peak shaving, and load shifting operations in distribution networks. Such conditions require energy storage devices to maintain stable performance during variations in charge-discharge rates. It was found that upon increasing the current density, all samples exhibit a capacity decrease; however, the extent of degradation strongly depends on the pore structure. For purely microporous materials, the discharge capacity at 2C drops to values below 400 $mAh \cdot g^{-1}$, indicating diffusion limitations and deteriorated reaction kinetics. In contrast, micro-mesoporous materials demonstrate 600-700 $mAh \cdot g^{-1}$ higher capacity values at high currents.

The most significant differences appear upon returning to a low current density (0.1C): the capacity recovery for micro-mesoporous structures exceeds 80% varying between 900-1000 $mAh \cdot g^{-1}$, whereas microporous materials show an additional loss of 5-10%, indicating enhanced irreversible degradation processes. Therefore, the obtained results demonstrate that optimizing the pore architecture of carbon cathodes is an effective approach to improving the electrochemical stability and cycling performance of lithium-sulfur batteries under variable operating conditions. Micro-mesoporous structures show particular promise for further development of stationary energy storage technologies in modern electric power systems.

**Keywords:** Lithium-sulfur batteries, porous carbon, variable load conditions, cycling stability, electrochemical degradation, stationary energy storage systems

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# Synthesis and Characterization of Electrospun PAN/LLZTO/$LiClO_4$ Composite Polymer Electrolyte

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Solid-state electrolytes are generally classified into inorganic solid electrolytes (ISEs) and solid polymer electrolytes (SPEs). Although ISEs offer high ionic conductivity and safety, their brittleness and poor interfacial compatibility limit practical application. In contrast, SPEs provide superior flexibility and processability but suffer from low ionic conductivity and limited mechanical stability [1]. To overcome these limitations, composite polymer electrolytes (CPEs) incorporating inorganic fillers such as LLZTO have emerged as an effective strategy to enhance ionic conductivity, structural stability, and interfacial performance.

Among these systems, PAN/LLZTO composite membranes have attracted considerable attention. PAN provides high thermal stability and good oxidation resistance, while electrospun PAN/LLZTO membranes form continuous conductive pathways that facilitate $Li^+$ ion transport and improve mechanical strength [2]. However, the polar nitrile groups (–C≡N) in PAN may react with lithium metal, forming a passivation layer that increases interfacial resistance. Therefore, incorporating LLZTO into PAN-based systems is considered an effective approach to improve ionic conductivity and reduce interfacial limitations [3].

In this study, LLZTO solid electrolyte was synthesized using the conventional solid-state reaction method with different lithium precursors, followed by calcination and sintering to obtain the garnet-type structure with enhanced phase purity. To overcome the limitations of conventional polymer electrolytes, particularly low ionic conductivity and interfacial instability, LLZTO was incorporated into electrospun PAN membranes to improve ionic transport, flexibility, and interfacial compatibility. The synthesized LLZTO powder was characterized using X-ray diffraction (XRD), while LLZTO pellets and PAN/LLZTO composite membranes were analyzed using scanning electron microscopy (SEM) and energy-dispersive spectroscopy (EDS) to investigate their structural and morphological properties. Electrochemical impedance spectroscopy (EIS) was employed to evaluate ionic conductivity.

A comparative study was conducted to assess the structural, morphological, and electrochemical properties of LLZTO synthesized using different lithium sources, as well as to examine the effect of polymer–ceramic composite design on ionic transport behavior. The results demonstrated that synthesis conditions, lithium precursor selection, and composite membrane fabrication significantly influence phase formation, microstructure, and ionic conductivity.

This research presents LLZTO-based composite electrolytes as promising materials for next-generation solid-state lithium-ion batteries. The obtained materials demonstrate strong potential for improving ionic transport, interfacial stability, and overall safety in advanced energy storage systems.

**Acknowledgement**
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# Electrochemical Properties and Structural Evolution of Ni/Mn-based O3-type Layered Oxides for Sodium-ion Batteries

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In recent years, rechargeable sodium-ion batteries composed of earth-abundant elements have been attracted considerable attention as energy storage devices free from material resource constraints. Among various positive electrode materials for sodium-ion batteries, layered transition metal oxides are promising materials due to their large reversible capacity. Sodium-containing layered metal oxides are divided into two major groups with different layered stacking manners: O3-type and P2-type. Compared to P2-type oxides, O3-type oxides possess larger theoretical capacities based on Na ion contents in the host layered structures. In this study, a series of $O_3$-type layered oxides, $NaNiO_2$, $NaMnO_2$, and $NaNi_{0.5}Mn_{0.5}O_2$,[1-3] are revisited, and the impacts of nickel and manganese ions on the electrochemical properties and phase transition behavior of these materials are carefully examined. Since both $Ni^{3+}$ and $Mn^{3+}$ ions are Jahn-Teller active, $NaNiO_2$ and $NaMnO_2$ adopt distorted O'$_3$-type layered structures with a in-plane distortion. In contrast, $NaNi_{0.5}Mn_{0.5}O_2$, containing Jahn-Teller inactive $Ni^{2+}$ and $Mn^{4+}$ ions, crystallizes into an O3-type layered structure without distortion. The cyclability of $NaNiO_2$ and $NaNi_{0.5}Mn_{0.5}O_2$ is significantly enhanced by limiting the upper cut-off voltage to 3.8 V, whereas the electrode reversibility of $NaMnO_2$ is less affected by the state of charge. *In-situ* X-ray diffraction measurements reveal that pronounced shrinkage of the interlayer distance, associated with the O3/P3 phase transition upon charging above 3.8 V, is observed for $NaNiO_2$ and $NaNi_{0.5}Mn_{0.5}O_2$, but not for $NaMnO_2$. Furthermore, the reveribility of structural changes strongly depends on the upper cut-off voltage. These results indicate that precise control of the state of charge is effective in achieving higher electrode reversibility of nickel-containing layered oxides. Based on these findings, the effects of nickel and manganese ions on the electrochemical properties and phase transition behavior of O3-type layered oxide materials will be discussed in detail. The impact of electrolyte solutions[4] and material synthesis conditions on electrochemical properties will also be presented.

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# Synthesis and Electrochemical Properties of Molybdenum-Based Positive Electrode Materials

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To achieve higher energy density in lithium-ion batteries, high-capacity positive electrode materials are required. Li-rich disordered rocksalt oxides have attracted much attention as promising positive electrode materials for high-energy lithium-ion batteries. Despite the absence of specific Li diffusion pathways in the disordered rocksalt-type structure, nanosizing strategy provides percolation $Li^+$ conduction pathways, thus resulting in a large reversible capacity. $Li_2MoO_3$ delivers a large reversible capacity exceeding 300 mA h $g^{-1}$ through a two-electron redox reaction of $Mo^{4+}/Mo^{6+}$.[1] In this study, $Li_2MoO_3$ is examined as a positive electrode material. Mechanical milling increases the reversible capacity of $Li_2MoO_3$ from 130 mA h $g^{-1}$ to 215 mA h $g^{-1}$, and subsequent carbon compositing further improves the capacity to approximately 300 mA h $g^{-1}$. However, severe capacity degradation is observed for the nanosized sample. This degradation is attributed to the dissolution of Mo into the electrolyte solution associated with the increases contact area with the electrolyte. The cyclability of nanosized and carbon-composited $Li_2MoO_3$ is greatly improved by using a highly concentrated electrolyte (5.5 M $LiN(SO_2F)_2$ (LiFSA) in dimethyl carbonate (DMC)), in which the presence of free solvent molecules is eliminated[2,3]. For comparison, stoichiometric layrerd-type $LiMoO_2$ and disordered rocksalt-type $Li_{1+x}MoO_2F$ [4] are also synthesized and characterized. Based on these results, the electrochemical properties of molybdenum-based positive electode materilas are systematically compared and discussed.

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# Electrochemical Reversiblity of Li Insertion into Oxide-Based Negative Electrode Materials Containing 4d/5d Transition Metal Ions

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In recent years, lithium-ion batteries have been utilized in a wide range of applications, and further improvements in cycle life and safety have been strongly required. Graphite, which is widely used as a negative electrode material, exhibits a high reversible capacity and operates at a low potential close to that of metallic lithium. However, this low operating potential lies beyond the electrochemical stability window of conventional organic electrolytes, leading to undesirable reductive decomposition of the electrolyte coupled with metallic Li deposition, which shorten battery lifetime and raises safety concerns.

In this study, rutile-type transition-metal oxides, $NbO_2$, $MoO_2$, and $WO_2$, which exhibit relatively high operating potentials compared with graphite, are revisited as negative electrode materials.[1-3] These oxides crystalize into distorted rutile-type structures: $NbO_2$ adopts a tetragonal symmetry, whereas $MoO_2$ and $WO_2$ possess monoclinic symmetry. Upon insertion/exraction of 1 mol of $Li^+$, $NbO_2$ shows a sloping voltage profile characteristic of a single-phase reaction, whereas $MoO_2$ and $WO_2$ show stepwise voltage changes originating from multiphase transitions, with pronounced voltage steps around 1.5 and 0.7 V, respectively. When $Li^+$ insertion/extraction is limited to half of the theoretical capacity, the cyclability of $MoO_2$ and $WO_2$ is significantly improved. Structural evolution during charge/discharge and the electrochemical properties of binary systems will be also discussed.

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# Upcycling Waste PET Bottles into Hard Carbon Anodes for Sodium-Ion Batteries

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The growing demand for sustainable and low-cost energy storage systems has stimulated significant interest in sodium-ion batteries (SIBs) as an alternative to lithium-ion batteries due to the natural abundance and low cost of sodium [1]. Among various anode materials, hard carbon (HC) is considered one of the most promising candidates because of its disordered structure, enlarged interlayer spacing, and ability to effectively store sodium ions [2].
At the same time, the accumulation of polyethylene terephthalate (PET) waste has become a serious environmental problem [3]. Converting PET waste into carbon materials through carbonization offers a sustainable approach for both plastic recycling and the development of advanced electrode materials. The structural properties of PET-derived HC strongly depend on the heat treatment temperature, which influences the degree of graphitization, pore structure, and electrochemical behavior.
In this work, recycled PET was used as a precursor for the preparation of HC through direct carbonization at temperatures ranging from 900 to 1400 °C. The obtained materials were characterized using X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM) to analyze their structural disorder, graphitic domains, and morphology. Electrochemical behavior was evaluated in sodium-ion half-cells using galvanostatic charge–discharge cycling, cyclic voltammetry (CV) measurements and rate capability tests at various C-rates. The obtained results demonstrated that the carbonization temperature strongly affects both the structure and sodium-storage performance of the materials. Among all samples, PET_1000 and PET_1100 exhibited the best electrochemical performance, delivering reversible capacities of 275–280 mAh $g^{-1}$ at a current density of 20 mA $g^{-1}$ in sodium-ion half-cells. These findings confirm that waste PET can be effectively converted into high-performance hard carbon anodes for SIBs while simultaneously providing a promising route for plastic waste valorization.

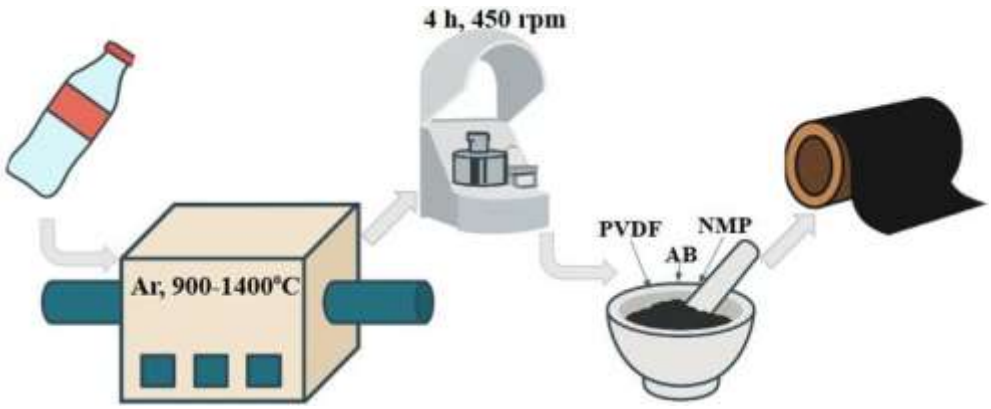



Figure 1. Schematic illustration of the synthesis process of hard carbon (HC) anode materials derived from waste PET bottles

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# Conversion of Waste ABS Plastics into Nanostructured Carbon Anodes for Lithium-Ion Batteries

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The rapid accumulation of plastic waste has become a serious environmental challenge worldwide, encouraging the development of sustainable recycling technologies and environmentally friendly functional materials for energy storage applications. Among various polymer wastes, acrylonitrile butadiene styrene (ABS) has attracted increasing attention due to its extensive use in electronics and 3D printing filaments, as well as its non-biodegradable nature. Simultaneously, the growing demand for portable electronics and renewable energy storage systems has intensified the need for high-performance lithium-ion batteries (LIBs). In this work, waste ABS plastics obtained from discarded 3D printing scraps and failed prints were successfully converted into nanostructured carbon anode materials for LIBs through an acid-assisted carbonization process. Prior to pyrolysis, the ABS precursor was treated with sulfuric acid ($H_2SO_4$), introducing sulfonic functional groups ($-SO_3H$) into the polymer structure. This cross-linking process enhanced structural stability during heat treatment, promoted partial graphitization, and facilitated the formation of a defect-rich porous carbon framework. As a result, the carbon yield reached 30.13 %, which was approximately six times higher than that obtained from untreated ABS. Structural characterization revealed enlarged interlayer spacing (~3.7 Å), nanoscale graphitic domains, and a disordered porous microstructure favorable for lithium-ion intercalation and transport. Electrochemical evaluation demonstrated an initial reversible capacity exceeding 300 mAh $g^{-1}$ with stable cycling performance over 100 cycles and a Coulombic efficiency of approximately 98%. Furthermore, the material maintained excellent electrochemical performance even at low temperatures (-15 °C). The proposed strategy demonstrates an effective and scalable approach for converting waste ABS plastics into value-added carbon anode materials for sustainable lithium-ion battery technologies and circular economy applications.

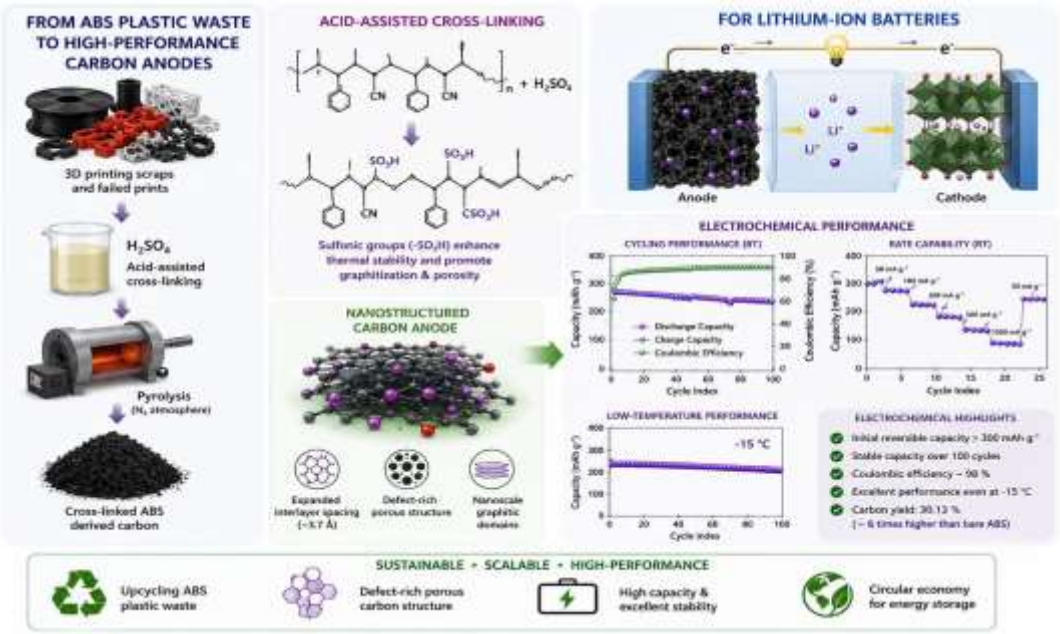



Figure 1. Graphical abstract.

**Acknowledgements**
This research was funded by the research targeted program BR24992766 “Development of methods and technologies for environmentally friendly “green” processing of polymer waste for energy storage” from the Science Committee, Ministry of Science and Higher Education of the Republic of Kazakhstan.

# Entropy Profiling for Battery State Estimation: A Review of Measurement Approaches and Physicochemical Interpretation

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Accurate battery state estimation remains one of the key challenges in the development of advanced battery management systems (BMS). Conventional state estimation techniques are primarily based on electrical parameters and data-driven approaches; however, their accuracy may be affected by battery aging and operating conditions [1]. Among emerging diagnostic techniques, entropy profiling has attracted increasing attention because it provides thermodynamic information directly related to electrochemical processes occurring inside a battery. Entropy measurements can reveal electrode phase transitions, lithium distribution, reaction mechanisms, and degradation phenomena, making them a promising tool for state-of-charge (SOC) and state-of-health (SOH) estimation. This review examines the current state of entropy-based battery diagnostics with particular emphasis on entropy profile measurement methodologies and the physicochemical interpretation of entropy features. Existing entropymetry approaches, including potentiometric methods based on the temperature dependence of open-circuit voltage and recently proposed accelerated measurement techniques, are systematically analyzed. The applicability of entropy-based diagnostics is discussed in the context of battery aging mechanisms, electrolyte evolution, and electrode degradation processes that significantly influence battery performance over time [2]. Furthermore, the review evaluates current interpretations of entropy profiles reported for various lithium-based battery chemistries and examines their relationship with underlying physicochemical phenomena. Particular attention is given to the use of thermodynamic parameters for battery state estimation and to entropy-based SOC assessment concepts derived from Yazami's thermodynamic framework [3]. While entropy features have demonstrated strong sensitivity to battery state, a comprehensive understanding of their physical meaning and their dependence on battery chemistry remains limited. The analysis identifies two major research challenges: (i) the long measurement times required for conventional entropy profiling due to open-circuit voltage relaxation procedures, and (ii) the lack of a unified physicochemical interpretation of entropy-derived indicators. Based on these findings, future research directions are proposed toward the development of accelerated entropy measurement techniques and physically interpretable entropy-based models for battery state estimation. The review provides a foundation for establishing quantitative relationships between battery chemistry, battery state, and entropy profiles, supporting the next generation of thermodynamics-based diagnostic methodologies.

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# Al-Decorated Nitrogen-Doped Graphene Oxide-based Materials for Hydrogen Storage Applications

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Hydrogen is considered one of the most promising clean energy carriers due to its high energy density and environmentally friendly combustion product. However, the development of safe, efficient, and reversible hydrogen storage materials remains a major challenge for practical hydrogen-based energy systems. Carbon-based nanomaterials, particularly graphene oxide and its derivatives, have attracted significant interest for hydrogen storage because of their high surface area, lightweight structure, and tunable surface chemistry.

In this work, aluminum-decorated nitrogen-doped graphene oxide-based materials were prepared with different aluminum ratios and investigated as potential hydrogen storage materials. Nitrogen doping was introduced to modify the electronic structure of graphene oxide and provide additional active sites, while aluminum decoration was applied to enhance the interaction between hydrogen molecules and the carbon-based surface. The combined effect of nitrogen doping and aluminum decoration is expected to improve adsorption behavior by tuning the surface properties and increasing the number of accessible hydrogen interaction sites.

The prepared samples were characterized to study their structural, morphological, and chemical properties, and their hydrogen storage behavior was evaluated. The influence of aluminum content on hydrogen adsorption performance was investigated in order to understand the role of metal decoration in improving the storage properties of nitrogen-doped graphene oxide. The results demonstrate that Al-decorated N-doped graphene oxide is a promising material system for hydrogen storage applications, where controlled surface modification can play an important role in enhancing hydrogen uptake.

This study highlights the potential of metal-decorated heteroatom-doped graphene oxide materials for clean energy storage and provides useful insight into the design of advanced carbon-based hydrogen storage materials.

**Acknowledgments**

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# Influence of Particle Size on Hydrogen Absorption Kinetics and Cyclic Stability of Mg–Ni–Ce System Materials

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This work is devoted to investigating the influence of particle size on the durability and hydrogen storage performance of Mg–Ni–Ce materials. The relevance of the study is associated with the need to develop efficient metal hydride materials that combine rapid hydrogen absorption kinetics, high hydrogen storage capacity, and long-term operational stability [1].

Based on preliminary thermodynamic and diffusion modeling performed using the Thermo-Calc/DICTRA software package, characteristic particle size ranges affecting hydrogen transport processes in the Mg–Ni–Ce system were identified. To experimentally verify the modeling results, three powder fractions of the Mg–Ni–Ce system with average particle sizes of approximately 20, 30, and 40 μm were prepared. The particle size distributions were confirmed by laser granulometry measurements.

To evaluate the influence of particle size on material performance, a comprehensive set of investigations was carried out, including specific surface area measurements using the Brunauer–Emmett–Teller (BET) method, pore structure analysis using the Barrett–Joyner–Halenda (BJH) method, particle morphology characterization by scanning electron microscopy (SEM), phase composition analysis by X-ray diffraction (XRD), and hydrogen sorption measurements using an H-Sorb 2600 PCT system.

The results demonstrated that reducing particle size increases the specific surface area and shortens the diffusion path of hydrogen atoms, leading to enhanced hydrogenation kinetics and more efficient utilization of the active material volume. Prior to cyclic testing, the powder fraction with an average particle size of approximately 20 μm exhibited the highest hydrogen storage performance, reaching a hydrogen capacity of 4.5 wt.% $H_2$. For the 30 μm fraction, the hydrogen capacity was 4.3 wt.% $H_2$, while the 40 μm fraction showed a capacity of 3.9 wt.% $H_2$. Larger particles exhibited somewhat slower hydrogen absorption kinetics due to the reduced active surface area and increased hydrogen diffusion distance.

The cyclic testing results revealed that a higher degree of dispersion does not necessarily ensure superior long-term performance. Although the 20 μm fraction demonstrated the highest initial hydrogen capacity, it exhibited a more pronounced degradation of sorption properties during repeated hydrogenation–dehydrogenation cycles. This degradation is assumed to be associated with particle agglomeration, accumulation of structural defects, and partial oxidation of the highly developed particle surface [2].

The powder fractions with average particle sizes of 30 and 40 μm demonstrated greater stability during cycling. Among the investigated materials, the fraction with an average particle size of approximately 30 μm provided the most favorable combination of hydrogen storage capacity, hydrogen absorption kinetics, and cyclic stability.

The obtained results indicate the existence of an optimal particle size range for Mg–Ni–Ce materials and confirm the importance of balancing hydrogen absorption kinetics and long-term durability when designing metal hydride hydrogen storage systems.

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# The Detrimental Role of $H_2O_2$ in Malonic Acid Leaching of Real Industrial Black Mass: Fenton-like Degradation and Ni–Co Oxalate Re-precipitation

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Hydrometallurgical processing of cathode black mass from spent lithium-ion batteries with organic acids has traditionally relied on the addition of hydrogen peroxide as a reducing agent, converting the sparingly soluble $Co^{3+}$ and $Mn^{4+}$ into their soluble divalent form [1,2]. Malonic acid, HOOC–$CH_2$–COOH, occupies a special place among organic reagents owing to its bidentate chelate coordination and the presence of an active methylene group capable of acting as an intrinsic reducing agent. However, the available literature data have been obtained almost exclusively on first-generation model cathodes (NMC-111, LCO) and overlook the phase heterogeneity of real industrial black mass and the fundamentally different electronic structure of high-nickel compositions [3]. The aim of the present work was a systematic study of the role of $H_2O_2$ in the leaching of real industrial high-nickel black mass (NCA with a minor NMC admixture) with malonic acid, and the elucidation of the mechanism of the observed effects by a combination of independent methods.

The black mass (Ni 22.5; Co 4.3; Mn 0.4; Li 3.0 wt.%; impurities Cu ~1.2 and Fe ~0.9 wt.%), donated from local battery recycling company, was leached with 2.0 M malonic acid (70 °C, 2 h, S:L = 1:30) while varying the $H_2O_2$ fraction from 0 to 8 vol.%; the solutions were analyzed by AAS, and the solid residues by XRD, SEM-EDS, and FT-IR spectroscopy. Without any external reducing agent, owing to the intrinsic reductive activity of its active methylene group, malonic acid achieved recoveries of Ni 90%, Mn 98%, Li 100%, and Co 69%. Contrary to the classical recommendations, the addition of $H_2O_2$ did not increase but monotonically lowered the recovery of the transition metals (Ni from 90 to 51%, Co from 69 to 46% at 8 vol.%), whereas the lithium recovery remained unchanged (100%) over the entire concentration range. A combination of independent methods showed that this decrease arises not from cathode passivation but from Fenton-like oxidative degradation of malonic acid to oxalic acid, initiated by the impurity metals Cu and Fe [4]. The oxalate ion generated in situ binds the $Ni^{2+}$ and $Co^{2+}$ already released into solution as the sparingly soluble mixed dihydrate (Ni,Co)$C_2O_4 \cdot 2H_2O$: according to XRD and SEM, the cathode phase is completely absent from the residue (only oxalate and graphite), while the FT-IR spectrum ($\Delta\nu(COO^-)$ = 258 $cm^{-1}$) confirms the bridging-chelating coordination of the oxalate. The radical nature of the process is proven by the complete suppression of the effect upon addition of methanol as an $HO^{\bullet}$ scavenger (Ni 94%, Co 100%) and by its absence when $H_2O_2$ is replaced with mild reducing agents — ascorbic acid and glucose — which afford nearly quantitative recoveries of Ni (≈99.5%) and Co (100%) [5].

Thus, the classical recommendation to use $H_2O_2$ as a "universal reducing agent" is not applicable to industrial compositions in systems with organic chelating acids prone to radical degradation; for these, ascorbic acid or glucose are preferable.

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# Electrodeposıtıon of Nı–TıO$_2$ and Cu–TıO$_2$ Composıte Coatıngs and Theır Corrosıon Behavıor

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Composite electrochemical coatings (CECs) are metallic coatings whose matrix incorporates dispersed particles of oxides, carbides, or other compounds by electrodeposition [1]. Such systems combine the mechanical strength and electrical conductivity of the metal with the chemical inertness and barrier properties of the dispersed phase, which leads to reduced porosity, grain refinement, and a significant increase in corrosion resistance compared to single-component nickel and copper electrodeposits [2]. Titanium dioxide ($TiO_2$) was chosen as the dispersed phase for nickel- and copper-based CECs due to its high chemical inertness over a wide pH range, thermal and corrosion stability, as well as low toxicity and availability. $TiO_2$ particles incorporated into the Ni and Cu matrix form a physical barrier to the diffusion of aggressive $Cl^-$ ions, act as additional nucleation sites, promote the formation of a dense fine-grained structure and the filling of pores and microcracks, which directly results in a decrease in corrosion current and an increase in the corrosion resistance of the coatings [3].The aim of this work is to develop and study Ni–$TiO_2$ and Cu–$TiO_2$ composite electrochemical coatings on nickel and copper, to establish the regularities of the influence of electrodeposition conditions on $TiO_2$ incorporation, microstructure, and corrosion resistance of the coatings, and to substantiate a unified principle of their barrier action in chloride media. To achieve this aim, electrodeposition of the coatings was carried out from sulfate and sulfuric acid electrolytes while varying current density and current mode, $TiO_2$ concentration, and hydrodynamic conditions. The coatings were obtained by electrodeposition; their morphology and elemental distribution were examined by SEM and EDS, which confirmed the presence of Ti and O in the composite layer and revealed microstructural changes of the deposits upon variation of the deposition parameters. The phase composition was evaluated by X-ray diffraction (XRD) followed by diffractogram analysis. In addition, accelerated assessment of corrosion resistance was performed using a corrosion paste method, while electrochemical corrosion tests were carried out on a BioLogic galvanostat–potentiostat in a glass–graphite electrochemical cell with 3% NaCl solution and an Ag/AgCl reference electrode, analyzing potentiodynamic polarization data (Tafel method), cyclic voltammetry, and gravimetric measurements.

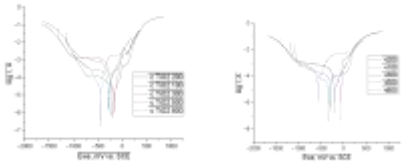


Fig. 1. Tafel curves for Ni (a) and Ni–TiO~2~ (b) at different deposition current densities

Table 1. Effect of $TiO_2$ concentration in the electrolyte on the content of the dispersed phase in the coating ($H_2SO_4$ – 100 g/L, $Cu^{2+}$ – 40 g/L, i = 200 A/m$^2$, τ = 1 h)

| TiO2, g/l | 0 | 5 | 10 | 20 |
|---|---|---|---|---|
| W, % | 100,0 | 100,7 | 101,1 | 101,3 |
| TiO2 coat., % | - | 0,7 | 1,1 | 1,3 |

According to Table 1, an increase in $TiO_2$ concentration in the electrolyte and the use of a pulse current mode promote higher incorporation of the oxide phase into the coating and the formation of a more compact fine-grained Ni–$TiO_2$ structure with reduced porosity; at the same time, the corrosion current decreases significantly compared to pure nickel, and the corrosion potential shifts towards more noble values [4]. For Cu–$TiO_2$ coatings, a decrease in roughness and smoothing of the microrelief were established in comparison with pure copper, which, together with the barrier role of $TiO_2$ particles, provides enhanced corrosion resistance in chloride media and confirms the feasibility of a unified barrier protection principle for nickel- and copper-based CECs [5]. The combination of structural data (SEM/EDS, XRD and particle size analysis) and corrosion test results in 3 % NaCl, as well as the action of the corrosion paste, makes it possible to compare the protective properties of Ni–$TiO_2$ and Cu–$TiO_2$ coatings and to substantiate the role of chemically inert oxide particles embedded in the metallic matrix, which form a dispersed physical barrier, densify the deposit structure, and reduce the corrosion rate in aggressive aqueous media. It is shown that by optimizing the matrix nature, electrodeposition mode, and dispersed phase content, it is possible to significantly increase the $TiO_2$ fraction in the coating, reduce porosity and corrosion rate (by up to 1.87 times for Ni–$TiO_2$), and thus achieve effective anticorrosion protection of metallic surfaces.

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# $TiO_2$ - Decorated AgCl Visible-Light-Responsive Photocatalyst for Microplastic Degradation

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Microplastic (MP) pollution has emerged as one of the most pressing environmental challenges of our time. Conventional wastewater treatment systems are insufficient for complete MP removal, achieving only ~70% efficiency, necessitating the development of advanced treatment strategies [1]. Photocatalysis, leveraging reactive oxygen species (ROS) generated under solar or simulated light, represents a promising approach for MP degradation. Among candidate materials, $TiO_2$-based photocatalysts have been extensively studied; however, their wide bandgap (~3.2 eV) severely limits visible-light utilization. AgCl is known for its strong visible-light activity and plasmonic enhancement via in-situ generated $Ag^0$ nanoparticles, yet AgCl/ $TiO_2$ heterostructures have not been explored for MP degradation to date.

In this work, a series of AgCl/ $TiO_2$ heterostructure photocatalysts were synthesized via a facile mechanochemical method using a planetary ball mill. The synthesis is based on an ion-exchange reaction between $AgNO_3$ and $NH_4Cl$ in the presence of $TiO_2$ (P25), yielding AgCl/$TiO_2$ composites with mass ratios of 95/5, 85/15, 75/25, and 50/50.

Structural and surface analyses confirmed the successful formation of phase-pure AgCl/$TiO_2$ composites with intimate interfacial contact between the two phases. Optical characterization revealed progressively enhanced visible-light absorption relative to bare $TiO_2$, consistent with the bandgap narrowing arising from heterostructure formation.

The 95/5 AgCl/$TiO_2$ composite showed the highest photocatalytic activity toward LDPE microplastic degradation under visible-light irradiation, outperforming both bare $TiO_2$ and all other composite ratios. Product analysis confirmed extensive oxidative chain fragmentation of the LDPE backbone, providing direct mechanistic evidence of photocatalytic degradation.

This study presents the first application of AgCl/$TiO_2$ heterostructures for visible-light-driven MP degradation. The mechanochemical synthesis offers a scalable, solvent-free route, while the plasmonic enhancement from in-situ $Ag^0$ formation and favorable band alignment in the heterostructure enable superior photocatalytic activity under solar irradiation. These results highlight the strong potential of AgCl/$TiO_2$ composites as efficient and practical photocatalysts for environmental remediation of MP pollution.

**Keywords:** microplastics; photocatalysis; $TiO_2$; AgCl; visible light; LDPE degradation; heterostructure; mechanochemical synthesis

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# DFT research $BaTiO_3$/g-$C_3N_4$ Heterojunction for Photocatalysts

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Graphitic carbon nitride (g-$C_3N_4$), one-atom-thick single layer of carbon and nitrogen atoms in packed honeycomb lattice have shown exceptional physical, chemical, optical and mechanical properties. Over past decade, low dimensional nanocomposite materials as graphene, boron nitride and graphitic carbon nitride had a remarkable increase on the study of the degradation of pollutants, and water splitting as well as artificial photosynthesis [1,2]. The close contact or the covalent bonds between the 2D nanocomposite materials and the semiconductor nanoparticles was crucial for achieving the improved photocatalytic performance. Recently, due to the merits of the excellent dielectric, ferroelectric, and piezoelectric properties, barium titanate ($BaTiO_3$) is recognized as the great potential materials used in optoelectronic devices. As a ferroelectric material, the spontaneous polarization exists in $BaTiO_3$ owing to the asymmetry in the crystal lattice which would reveal special properties in photochemistry. It has been proposed that the dipole moment of a polar molecule would interact with the polarization of ferroelectric domains, thereby reducing the energy that required for the bond rupture. However, $BaTiO_3$ with 3.0-3.3 eV band gap notoriously suffered from a weak light response range, which inhibited its promising applications in photo-catalysis. All of researches are focused on the modification of the energy band structure, which is to promote an obvious red shift toward the visible light range. However, there are only few reports about the synthesis and application of (100) $BaTiO_3$/ g-$C_3N_4$ nanocomposites.

In this study considered cubic and tetragonal phase barium titanate (100) planes. For both phases of perovskite (100) planes revealed that the more thermodynamic favorable termination are $TiO_2$ – termination. Thus the thermodynamic favorable structure g-$C_3N_4$/$BaTiO_3$-$TiO_2$-terminated (100) surface is chosen as the ideal model for further investigations. The theoretical analysis revealed enhanced photocatalytic activity of the (100) $BaTiO_3$/g-$C_3N_4$ composite, which could be attributed to the interaction of $BaTiO_3$ nanoparticles with g-$C_3N_4$ via Ti-N bond, reduced band gap due to the introduction of hybridized states leading to increased absorption in visible range and large surface area which provides more active sites for the efficient adsorption of light. The formation of Ti-N bond proved to be highly advantageous for the efficient transport of photogenerated charge carriers, thereby suppressing the recombination of charge carriers. The simulated nanocomposite showed higher catalytic efficiency compared to pure $BaTiO_3$.

**Keywords**: g-$C_3N_4$, photocatalysis, heterostructure, nanocomposite .

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# Plasma-Catalytic Conversion of Methane in Microwave Discharge

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Hydrogen today plays a key role among the promising energy sources of the future and is regarded as a crucial instrument in the fight against climate change. Various countries are actively developing approaches to its production aimed at overcoming existing technical, economic, and environmental barriers. In 2024, Kazakhstan approved an order of the Minister of Energy defining the Concept for the Development of Hydrogen Energy until 2030 [1]. The central idea of this concept is to advance hydrogen energy in Kazakhstan with the goal of reducing carbon emissions and stimulating economic growth.

Water, coal, oil, biomass, and natural gas are traditionally used as feedstocks for hydrogen production. Among the promising directions, methane conversion is of particular interest [2]. However, methane decomposition is a complex process requiring significant energy input ($\Delta H$ = +74.9 kJ/mol) [2]. An effective solution in this case is the use of microwave (MW) discharge for plasma generation, which is notable for its accessibility and relatively low cost [3]. This work investigates the application of microwave discharge in combination with a catalyst for the efficient decomposition of methane. A steel cylinder (length 20 mm, diameter 25.5 mm) with the elemental composition of 30 at.% C, 26 at.% Fe, 22 at.% O, 8 at.% Cr, 5 at.% Al, and 8 at.% Ni was used as the catalyst.

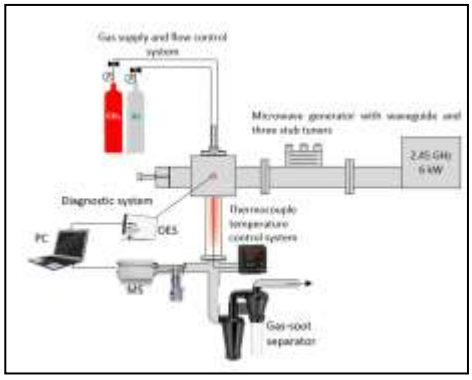



Figure 1. PM-6 applied research installation

The experiments were carried out using a PM-6 setup (Figure 1), equipped with a microwave generator with a power of up to 6 kW (frequency 2.45 GHz). The reaction chamber consisted of a quartz tube with a diameter of 30 mm fitted with a perpendicularly mounted rectangular waveguide. The working gas mixture was supplied in a swirling flow to the central part of the tube, where the plasma discharge was initiated. Analysis of the decomposition products was performed using a mass spectrometer. As a result, a technology for hydrogen production using a catalyst and microwave discharge was developed: the maximum methane conversion rate reached 31%, with hydrogen selectivity of 85% at a power of 0.6 kW.

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# The Role of Structural Research Methods in The Design of Advanced Electrocatalysts with Enhanced Activity and Durability

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The challenge of developing and synthesizing advanced electrocatalytic materials with enhanced efficiency and durability remains one of the central issues in the commercialization of proton exchange membrane fuel cells (PEMFCs), with the focus in recent years shifting towards improving the durability of electrocatalysts and the electrodes based on them [1]. To determine the effect of the impact of components in a multicomponent electrocatalyst on its durability, as well as the role of the nature of the modifier, it is important to understand the interrelationships between the composition, structure, arrangement of particles, and the nature of their interaction: both between the modifier and the support, and between the modifier and the active sites component [2].

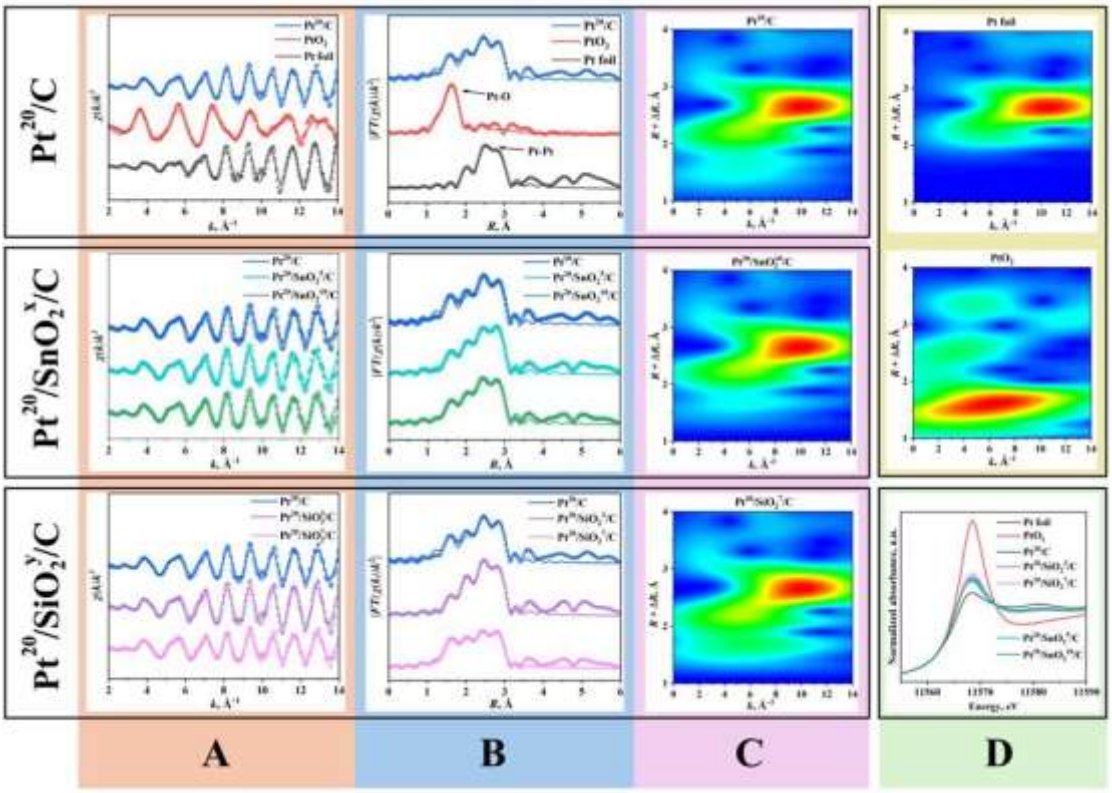



Figure 1. EXAFS spectrum (A) and Fourier transform modulus (B) for $Pt^{20}$/Mod/C (Mod = $SnO_x$, $SiO_y$), $Pt^{20}$/C, $PtO_2$ and Pt-foil (Pt L3-edge). Round symbols represent theoretical data. (C) Wavelet transform of EXAFS spectra for $Pt^{20}$/Mod/C (Mod = $SnO_x$, $SiO_y$), Pt-foil and $PtO_2$. (D) XANES spectra of the L3- absorption edge of Pt electrocatalysts.

The interaction between the particles within the cluster and the support material was described based on XRD, XPS, XANES, and EXAFS data of the particles' fine structure (see Fifure 1). As a result of the comprehensive analysis of the structure of the modified samples, regardless of the nature of the modifying oxide (metal/non-metal oxide), the formation of hetero-clusters of individual platinum and modifier particles with a **Janus structure** on the surface of the carbon support has been established, with the interaction of particles within the cluster occurring via the **–Pt–O–Mod–O–** bond (Mod = Sn or Si).

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# Initial Investigation of $Ag_3PO_4$ Deposited on PAN-Derived Carbon Fibers for Photocatalytic Degradation of Polystyrene

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The accumulation of microplastics in aquatic environments poses a significant environmental challenge due to their chemical stability and resistance to natural degradation [1]. In this work, a hybrid photocatalytic material consisting of silver phosphate (Ag3PO4) deposited on polyacrylonitrile-derived carbon fibers (C/Ag3PO4) was developed for the degradation of polystyrene (PS) under simulated sunlight irradiation.

PAN fibers were fabricated via electrospinning and subsequently carbonized at 700°C under argon atmosphere to obtain a conductive carbon framework. Ag3PO4 nanoparticles were incorporated into the PAN matrix through a two-step ion-exchange process using $AgNO_3$ and $Na_3PO_4$ solutions.

SEM results demonstrated the formation of a uniform fibrous network with fiber diameters in the range of 0.3-0.5 μm, while the deposition of Ag3PO4 nanoparticles (100-300 nm) on the fiber surface was confirmed. EDS mapping verified the homogeneous distribution of Ag, P, and O elements, indicating successful decoration of the C fibers surface. XRD analysis confirmed the presence of crystalline Ag3PO4 with the amorphous C matrix.

The photocatalytic performance of the C/Ag3PO4 was evaluated through the degradation of PS in aqueous medium under simulated sunlight irradiation. FTIR analysis revealed the formation of oxygen-containing functional groups (–OH, C=O), indicating oxidative degradation of the polymer. SEM observations showed surface damage, including pore formation and fragmentation, in contrast to minimal changes observed under photolysis without catalyst.

The results demonstrate that C/Ag3PO4 is a promising material for the photocatalytic degradation of PS microplastics under sunlight.

**Keywords:**
Ag3PO4, carbon fibers, photocatalysis, microplastics, polystyrene, PAN-derived carbon, electrospinning

**Acknowledgments**

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# Preliminary Study on The Photocatalytic Degradation of Polystyrene Microplastics Using an AgBr/G-$C_3N_4$ Composite under Simulated Solar Light

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Polystyrene (PS) is among the most widely produced synthetic polymers globally, extensively used in disposable packaging and insulation [1]. Its high hydrophobicity and structural rigidity make it exceptionally resistant to biodegradation, causing it to persist in the environment for centuries and fragment into microplastics (MPs) that infiltrate aquatic ecosystems and food chains [1, 2]. Photocatalysis has emerged as a promising advanced oxidation process for MPs degradation due to its low operational cost, environmentally friendly by-products, and ability to harness solar energy as a renewable light source [3].

Silver bromide (AgBr) is recognized for its high photocatalytic activity in the visible light region; however, its practical application is limited by rapid aggregation and photodecomposition under prolonged irradiation [4, 5]. To address these drawbacks, AgBr nanoparticles were combined with graphitic carbon nitride (g-$C_3N_4$) to form a composite, which can potentially improve AgBr dispersibility and long-term stability [6, 7].

The present study investigates the synthesis, characterization, and photocatalytic performance of AgBr/g-$C_3N_4$ composites (75:25, 50:50, and 25:75 ratios) for the degradation of PS microplastics under simulated solar light. The phase composition and morphology were characterized by XRD and SEM. XRD analysis proved the formation of g-$C_3N_4$ and the cubic phase of AgBr; SEM revealed that the composites consisted of microsized grains of AgBr and layered g-$C_3N_4$. Degradation efficiency of PS MPs was evaluated by FTIR spectroscopy, and changes in MPs' surface morphology were monitored by SEM. FTIR analysis confirmed chain scission and oxidation of PS MPs across all tested conditions, including photolysis, bare AgBr and g-$C_3N_4$, and AgBr/g-$C_3N_4$ composites. The AgBr/g-$C_3N_4$ (75:25) composite retained degradation performance comparable to pure AgBr while exhibiting improved photostability. SEM analysis showed that PS microplastics treated with the 75:25 composite displayed more pronounced surface roughening than those subjected to photolysis or individual components, indicating enhanced surface degradation.

This work demonstrates that AgBr/g-$C_3N_4$ is a promising composite photocatalyst for PS MPs degradation, contributing to the understanding of stable, efficient systems for environmental applications.

**Keywords:** microplastics, polystyrene, photocatalytic degradation, silver bromide, graphitic carbon nitride

**Acknowledgments**

This research was funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan, grant number AP22788706.

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# Modern Catalysts for Proton-Exchange Membrane Fuel Cells: Problems and Prospects

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Hydrogen energy is considered a key area for the development of a low-carbon economy. Proton-exchange membrane fuel cells (PEMFCs), which efficiently convert the chemical energy of hydrogen into electrical energy without carbon dioxide emissions, occupy a special place in this field. The efficiency and durability of PEMFCs are largely determined by the characteristics of the electrocatalysts used in the electrode processes. The most common catalysts for PEMFCs are platinum-based materials, which exhibit high catalytic activity in hydrogen oxidation and oxygen reduction reactions. However, the high cost of platinum and its limited global reserves significantly increase the cost of fuel cells and limit their widespread commercial application. Currently, much attention is being paid to the development of bimetallic catalysts containing platinum and other metals such as ruthenium, nickel, cobalt, and copper. Of particular interest are Pt–Ru/C catalysts, which demonstrate high resistance to carbon monoxide poisoning and improved electrochemical performance compared to traditional platinum systems. The use of carbon supports ensures high dispersion of catalytically active particles and an increase in the electrochemically active surface area. A promising area of research is the creation of catalysts with ultra-low platinum content, as well as the development of platinum-free materials based on transition metals. At the same time, work is underway to improve the durability of catalysts and the stability of membrane-electrode assemblies (MEAs) under long-term operation. Thus, improving catalytic materials remains a critical challenge in the development of PEMFCs. The development of efficient and affordable catalysts will accelerate the adoption of hydrogen technologies in the transportation, energy, and industrial sectors.

**Keywords:** hydrogen energy, PEMFC, catalyst, platinum, ruthenium, Pt–Ru/C, membrane electrode assembly.

# Corrosion Protection of Si Photocathode via Hybrid Island-and-Sea Strategy for Neutral-pH Water Splitting

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Solar energy is converted to green hydrogen via photoelectrochemical (PEC) water splitting, which is considered a promising approach, but photoelectrodes' long-term stability remains a pressing challenge. To overcome this problem, corrosion protection of photoelectrode materials is a feasible strategy which has been attracting attention. In this work, an "island-and-sea" strategy is presented to ameliorate the long-term stability of silicon-based photocathodes in neutral media water splitting. Si photocathode is a seabed which is covered with a hydrophobic 1-octadecyl (OD) self-assembled monolayer ("sea") behaving as a corrosion-resistant barrier. However, the sea has lots of "islands" in the form of platinum nanoparticles deposited on Si to enhance the charge transfer. This simple yet effective strategy resulted in a durable PEC operation not affecting the band structure of the semiconductor and avoiding complex fabrication routes. Unprotected Si/Pt photocathode degrades after 3 h of operation, showing a 50% decrease in photocurrent, while the Si/Pt+OD structure exhibits a stable performance over 6h. Additionally, this work is crucial for real-world applications due to the availability of neutral electrolytes such as seawater on the planet.

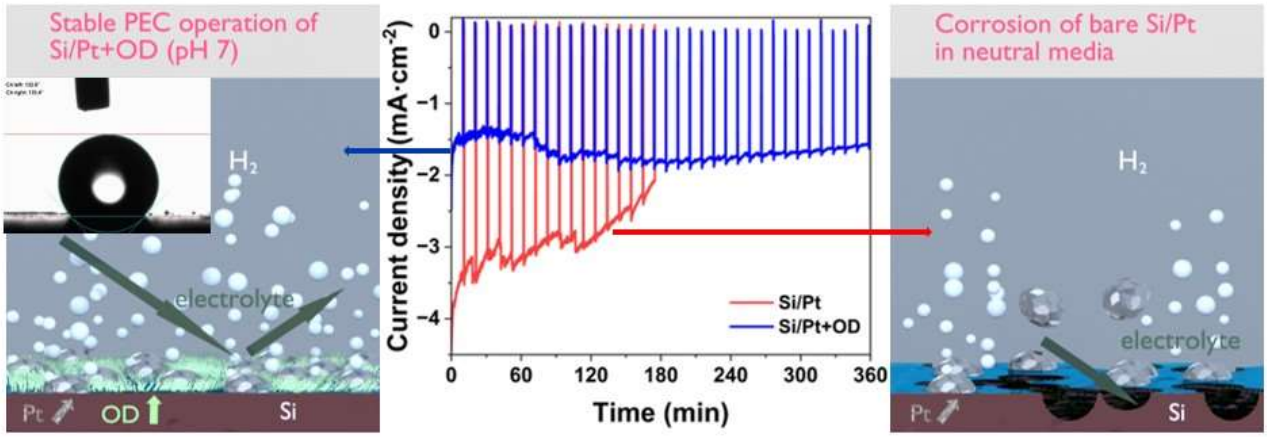



Figure 1. A graphical abstract to present the "island-and-sea" approach and its effect on photoelectrochemical neutral media water splitting.

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# Synthesis of ZnO@NiO Nanofibers Using Electrospinning and SILAR Methods for Gas Sensor Applications

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Air pollution remains a critical global issue, necessitating the development of efficient gas sensing technologies for environmental monitoring. Metal oxide semiconductor (MOS) sensors are widely studied due to their strong sensing capabilities; however, their high operating temperatures limit practical applications [1].
In this work, ZnO@NiO@C core–shell nanofibers are proposed as an advanced sensing material, combining high surface area, enhanced charge transfer via p–n heterojunctions, and improved conductivity from the carbon layer. These features enable sensitive and selective gas detection at room temperature, reducing energy consumption and improving safety [2,3].
The nanofibers were synthesized using a combination of electrospinning and the Successive Ionic Layer Adsorption and Reaction (SILAR) method, allowing precise control over morphology and structure. The fabricated sensors demonstrate high gas response, fast recovery, and stable low-temperature operation, indicating strong potential for next-generation gas sensing applications [4].

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# Aptamer and DNA-Based Biosensors Amplified with Mxene Nanomaterials

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Accurate and sensitive monitoring of disease biomarkers and anticancer drugs is essential for early diagnosis, personalized treatment, and effective clinical management. In recent years, aptamer- and DNA-based biosensors have attracted considerable attention owing to their exceptional molecular recognition capability, high selectivity, and adaptability to various sensing platforms. Among the emerging nanomaterials, MXenes have demonstrated remarkable potential as signal-amplifying components due to their high electrical conductivity, large surface area, tunable surface chemistry, and excellent biocompatibility. In this presentation, recent advances in MXene-amplified DNA and aptamer biosensors will be discussed, with a particular focus on their design, fabrication, and analytical performance for the detection of clinically important biomarkers and anticancer drugs. Various signal enhancement strategies based on MXene nanostructures, surface engineering, hybrid nanocomposites, and electrochemical transduction mechanisms will be highlighted. The role of MXenes in improving sensitivity, selectivity, electron-transfer efficiency, and long-term stability of biosensing platforms will also be addressed. Furthermore, practical applications of these biosensors in biological fluids and pharmaceutical samples will be presented, demonstrating their potential for real-world clinical analysis, point-of-care diagnostics, and precision medicine. Finally, future perspectives on the integration of MXene-based nanomaterials with next-generation biosensing technologies will be explored, emphasizing their promise in bridging advanced nanotechnology with healthcare applications.

# Computationally Intelligent Calibration Framework for Durable Soft Strain Sensors

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The ever-growing demand of soft strain sensors in ubiquitous electronics poses urgent need of device durability innovations to reduce resource waste. As most soft sensors use non-degradable materials, it is important to ensure durable sensor performance with reliable sensing signals over its lifecycle to reduce device waste, yet facing pervasive signal predicaments of nonlinearity, hysteresis, cycling attenuation, and batch inconsistency.

Herein, instead of empirical experiments via material or structural engineering, we propose an efficient computational calibration framework to comprehensively address these signal predicaments by utilizing hierarchical physics-guided machine learning (ML) models. Using an eco-friendly carbon waste-based strain sensor as a case study, physics-guided ML models are developed and show both high computation efficiency and learning accuracy in terms of real-time sensing signal calibration of the developed sensor, which automatically calibrates its unsatisfied sensing performance to equivalently linear, non-hysteresis, long-term stable, and batch consistent one without trial-and-error experiments. As final demonstrations, the ML-driven calibration models are capable of expanding sensor's reliable working lifetime for >3,000 times than its own counterpart for multiple robotic tasks, facilitating their long-term usages during practical applications.

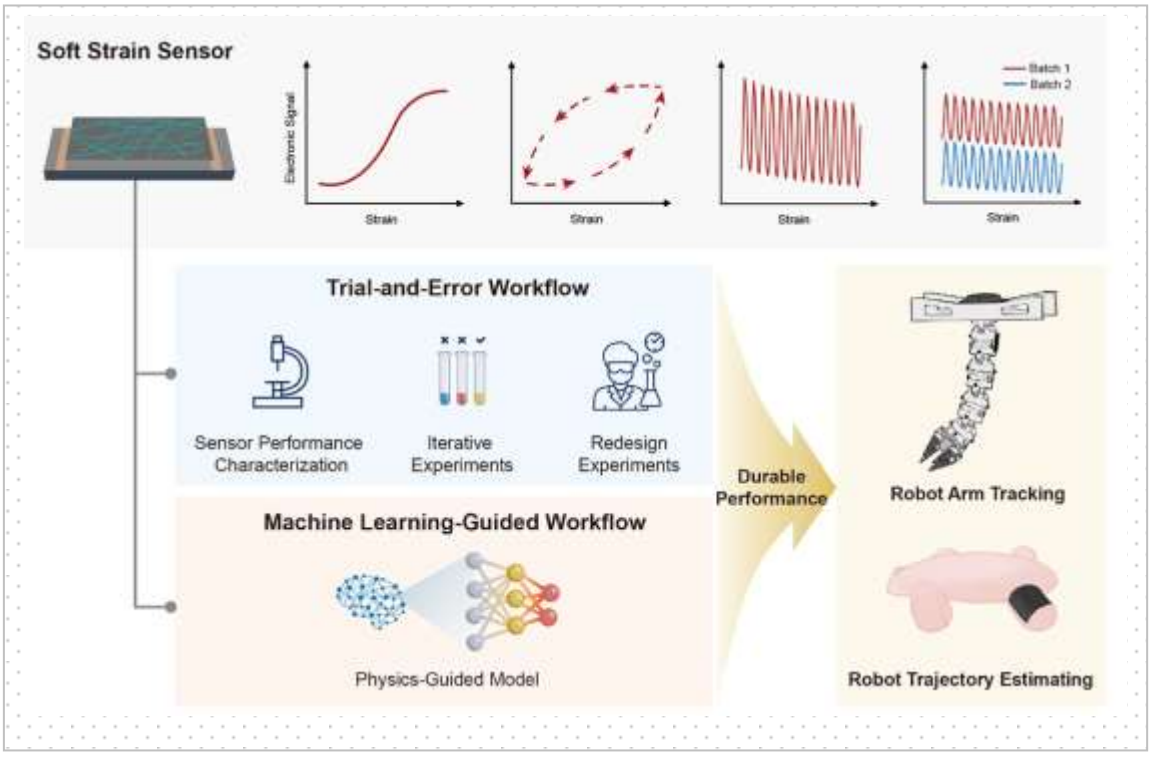



Figure 1. A computational calibration approach to enhance the performance durability of soft strain sensor.

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# Efficient and Low-Power Consumption Organic Light-Emitting Transistors

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The organic field-effect light-emitting transistors (OFE-LETs) combine the switching function of transistors with the function of light-emitting diodes, and have attracted attention due to their low leakage current and ease of integration. However, it has problems such as imbalance in electron and hole transport and insufficient energy transfer, resulting in low utilization of excitons and device efficiency. We proposed strategies such as improving the material morphology and the sensitization strategy of the light-emitting layer, among which the most representative one is the new device concept of spatially separating the carrier transport and exciton emission functions. Using a bipolar host material composed of a carbazole/oxadiazole hybrid molecule combined with a cyano group, we achieved balanced transport and broadened the exciton recombination region. Ultimately, OFE-LETs achieved high external quantum efficiency, current efficiency and brightness, and its performance reached the highest level of OLETs and met the requirements of future display application.

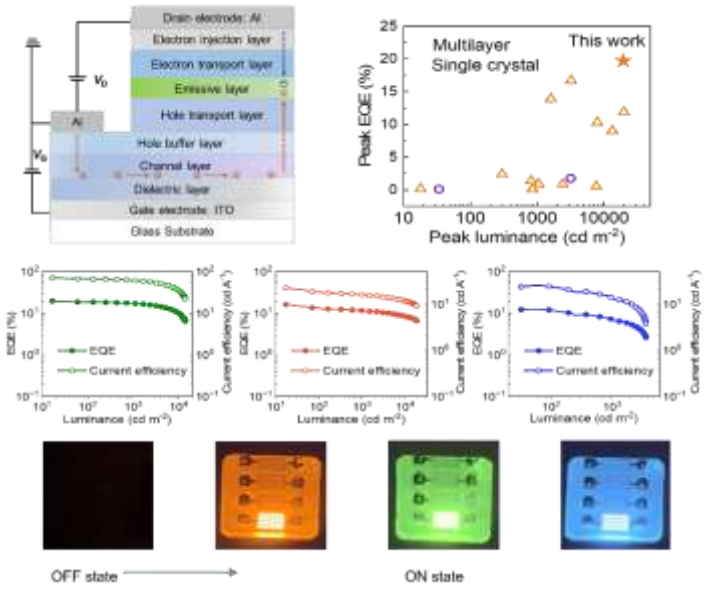



Figure 1. The device structure and performance of OFE-LETs

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# Perovskite Photovoltaics, Light-emitting Diodes, and X-ray Detectors for Flexible Electronics

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ABSTRACT: Organic–inorganic hybrid perovskites, with exceptional photophysical properties including long carrier lifetimes, low recombination rates, adjustable bandgaps, and high defect tolerance, have emerged as revolutionary candidates for optoelectronic devices. Despite their promise, critical challenges such as long-term stability, power conversion efficiency limits and scalable fabrication methods must be overcome to enable widespread commercialization. In this presentation, I will share our group's latest breakthroughs in perovskite solar cells (PSCs), perovskite light emitting diodes (PeLEDs) and perovskite X-ray detectors. Key highlights include stabilizing black-phase formamidinium perovskite formation at room temperature and high humidity through design and synthesis of novel protic ionic liquid solvents, as well as regulating the rheological behavior of the perovskite inks for screen-printing perovskites. Additionally, we have explored strategies to accelerate radiative recombination through additive treatments for efficient perovskite light-emitting diodes (LED), and developed spin-coated epitaxial heterodimensional tin perovskites for LED applications. Finally, we have developed perovskite nanocrystal scintillators for improved performance in X-ray detection. These innovations help address longstanding bottlenecks in the field while unlocking new opportunities for industrialization.

# Flexible Temperature Sensing Systems for Thermal Field Perception

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Flexible sensors exhibit tremendous application potential in various fields, including human-computer interaction, smart medical systems, and electronic skin. Among them, flexible temperature sensors and systems play a crucial role. They can replicate and transmit thermal sensations, thereby reflecting important temperature information of the human body, environment, and objects. However, current materials and devices still face critical challenges in practical applications: poor mechanical flexibility, limited sensitivity, complex device fabrication processes, and poor carrier transport and thermal conductivity. Based on the above, we have been proposed a facile, efficient, and low-cost in situ fabrication strategy to controllably design nickel oxide -based heterostructure devices, and the self-gated carrier devices with metal-semiconductor-metal structure were constructed, exhibiting excellent carrier transport properties and sensing performance. To further promote the flexibility of the device, we obtained flexible fiber and film-based temperature sensors through facile material synthesis and device fabrication methods, which presented excellent deformability and temperature sensing properties. Based on the flexible temperature sensors, the sensor arrays were fabricated and the sensing systems for thermal field perception were designed and used in signal monitoring and temperature warning systems, especially in the field of battery safety monitoring

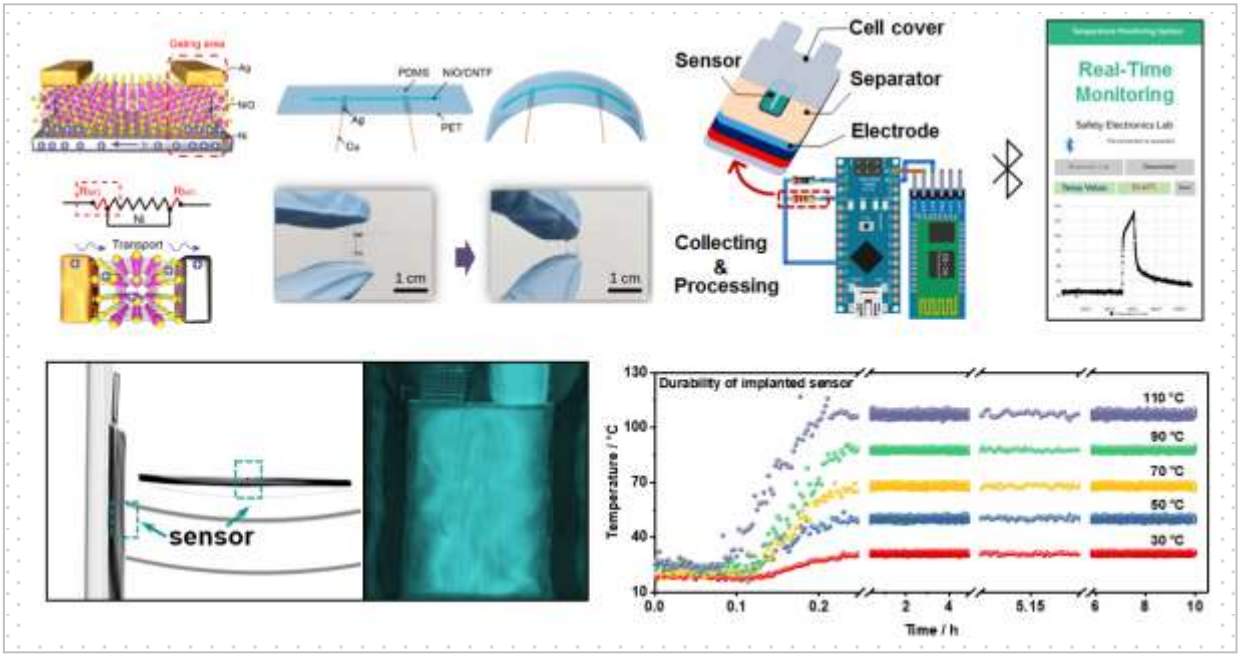



Figure 1. Flexible Temperature Sensors and Battery Safety Monitoring.

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# ZnO-Decorated Carbon Nanofibers for Energy-Efficient Room-Temperature $CO_2$ Sensing Toward Sustainable Environmental Monitoring

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In this work, carbon nanofibers decorated with zinc oxide nanoparticles (ZnO/CNF) were successfully fabricated with the unique morphology via a coaxial electrospinning method followed by controlled stabilization and carbonization processes for CO2 sensing. Unlike conventional ZnO-based gas sensors that that typically operate at elevated temperatures (200–400 °C), the fabricated ZnO/CNF sensor exhibited stable and reversible $CO_2$ sensing at room temperature over a concentration range of 1-1000 ppm. Compared with pristine CNF, the ZnO/CNF composite demonstrated significantly enhanced sensing response of 2.5% for 50 ppm CO2 at RT and for pristine CNF is 0.3% at the same gas sensing parameters, highlighting the effectiveness of the proposed architecture in enabling energy-efficient sensing. Observed improved signal stability, and lower detection limit owing to the synergistic interaction between the conductive carbon nanofiber network and surface-active ZnO nanoparticles. The enhancement is attributed to increased oxygen-vacancy-mediated adsorption, efficient electron transport pathways, and improved interfacial charge transfer within the hybrid architecture. Furthermore, the sensor showed repeatable response-recovery characteristics during cyclic measurements. Notably, the obtained sensing material is freestanding, lightweight, and mechanically adaptable, offering strong potential for flexible and wearable gas-sensing platforms. More importantly, room-temperature operation eliminates the need for an external heating element, substantially reducing energy consumption while simplifying device architecture. These advantages make the developed ZnO/CNF material a promising low-power sensing platform for battery-powered, portable, and wireless environmental monitoring systems, contributing to the development of energy-efficient and sustainable sensing technologies.

# Strategic Vigilance Molybdenum Nanotechnology Sensors in Early Warning Systems for Public Safety

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Heavy metal ions threaten ecosystems and human health due to their carcinogenicity, bioaccumulativity, and persistence, demanding highly sensitive, low-cost real-time detection. Electrochemical sensing technology has gained significant attention owing to its rapid response, high sensitivity, and low cost. Molybdenum disulfide (MoS2), with its layered structure, tunable bandgap, and abundant edge active sites, demonstrates significant potential in the electrochemical detection of heavy metals. This review systematically summarizes the crystal structure characteristics of MoS2, various preparation strategies and their mechanisms for regulating electrochemical sensing performance. It particularly explores the cooperative effects of MoS2 composites with other materials, which effectively enhance the sensitivity, selectivity, and detection limits of electrochemical sensors.

Heavy metals are naturally present in the Earth's crust. In recent years, with the continuous growth of the population, excessive exploitation of heavy metals, expansion of the metal smelting industry, and the discharge of agricultural and domestic waste, the content of heavy metals in the environment has significantly increased [1]. Heavy metal pollution primarily originates from wastewater generated by industrial and domestic pollution. Industrial pollution: Most industrial production activities are accompanied by the generation of heavy metal pollutants, with mining and smelting being the main sources of heavy metal pollution. During the mining process, scattered open-pit tailings can be washed away by wind and rain, infiltrating groundwater and subsequently contaminating water sources [2].

Despite the demonstrated advantages of MoS2-based compositions in the electrochemical detection of heavy metals, their practical implementation faces numerous difficulties.

1. While top-down strategies yield structurally homogeneous MoS2 with minimal defects, they struggle with layer uniformity and scalability. Conversely, bottom-up approaches enable mass production but require stringent control to prevent sulfur deficiencies and lattice defects that impair conductivity and catalytic activity.
2. Compromises in the design of materials: Balanced competitive properties are necessary in the design of engineering structures. Noble metal nanoparticles offer an exceptional choice of troactivity, however, requires high inhibition costs. The conductive polymer has limited electrochemical stability. Carbon matrices require complex surface functionalization. Metal oxides have low electrical conductivity. Biomaterials have insufficient long-term stability. Systematic optimization of electrical activity, electrical conductivity, durability and biocompatibility remains a prerequisite.
3. Obstacles to real-world applications: Complex matrices (for example, highly saline wastewater, biofluids) contain interfering substances that reduce selectivity and accuracy [3,4].

Future research must prioritize low-cost, eco-friendly synthesis of MoS2 electrode materials, utilizing continuous microreactor methods to replace traditional toxic chemical vapor deposition. This shift toward scalable and well-controlled production is essential to overcome the limitations of hydrothermal synthesis and enable the broad practical application of electrochemical heavy metal detection. Current analytical methods for heavy metal ions are diverse and can be primarily classified by detection principles into the following categories: atomic spectroscopy [5], mass spectrometry [6], inductively coupled plasma mass spectrometry [7], spectrophotometry [8].

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# Polyaniline/Carbon Nanotubes (PANi/CNT) Chemiresistive Gas Sensors for Selective Methane Detection at Room Temperature

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The development of efficient gas sensors for methane ($CH_4$) detection at room temperature remains a significant challenge due to its chemical inertness and low adsorption activity on conventional sensing materials. Most metal oxide-based sensors require elevated operating temperatures, leading to increased energy consumption and limiting their applicability in flexible and low-power systems. Therefore, the design of alternative sensing materials capable of selective $CH_4$ detection under ambient conditions is of considerable interest.

In this study, the synthesis and systematic investigation of a polyaniline (PANi)/carbon nanotube (CNT) composite as a chemiresistive sensing material are presented. PANi serves as the functional matrix due to its tunable electrical conductivity and reversible protonation–deprotonation mechanism; however, pristine PANi typically exhibits limited sensitivity and inefficient charge transport.

The incorporation of CNTs into the PANi matrix results in the formation of hierarchical conductive networks with high aspect ratio pathways, significantly enhancing electron mobility and interfacial charge transfer. The developed PANi/CNT composite demonstrates a pronounced and selective response toward $CH_4$ at room temperature, with a maximum response of 3.08%, a limit of detection of ~100 ppm, and fast response characteristics.

Morphological and structural analyses (SEM and Raman spectroscopy) confirm the uniform dispersion of CNTs and strong interfacial interaction within the composite, leading to an increased effective surface area and improved gas diffusion pathways. This architecture enables enhanced accessibility of active sites and efficient modulation of electrical properties upon gas exposure.

The sensing mechanism is governed by changes in charge carrier density in PANi induced by $CH_4$ adsorption, which affects the protonation state of the polymer chains and leads to measurable resistance variations. CNTs act as conductive bridges and electron transport facilitators, amplifying the sensing signal and stabilizing charge carriers at the PANi/CNT interface.

This work highlights the critical role of carbon nanostructures in engineering conductive polymer networks and provides a rational strategy for developing low-temperature, selective gas sensors based on hybrid nanocomposites.

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# ZnO-Doped Green Carbon-Based Electrode for pH Sensing in Aqueous Acid-Base Systems

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Carbon paste electrodes (CPEs) have been widely used in electrochemical measurements, particularly attractive for potentiometric applications due to their easily adjustable composition, simple surface renewal, and the ability to incorporate functional modifiers without complex fabrication procedures [1,2]. In this context, sustainable, low-cost potentiometric pH sensors were developed based on a carbon paste containing ZnO-doped activated biocarbon. The incorporation of ZnO most likely enhances electroanalytical performance and improves pH detection sensitivity. The developed ZnO–AC-based carbon-paste electrode exhibited sub-Nernstian response with a slope of –45.5 $mV \cdot pH^{-1}$, respectively, along with good linearity and fast response time. In potentiometric titration, the electrode demonstrated high performance toward mono- and polyprotic carboxylic acids. Testing CPE as a pH sensor on industrial water samples showed good ageement with a conventional glass electrode (accuracy: 92.90–99.86%). The sensing mechanism is attributed to proton-exchange reactions at surface hydroxyl groups (≡Me–OH) and to the formation of an electrical double layer at the electrode–solution interface [3]. Cyclic voltammetry revealed quasi-rectangular curves without redox peaks, indicating a predominantly non-faradaic mechanism [4]. Structural and compositional analysis confirmed the electrode material's stability after electroanalytical measurements. These results highlight the potential of metal oxide-doped biocarbon as an environmentally friendly, efficient material for solid-state pH sensing.

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# Carbon Nanotube-Integrated Smart Sensing Platforms for Extreme Environment Monitoring: from Space Applications to Advanced Energy Systems

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The development of smart sensing platforms capable of operating reliably in extreme environments represents a critical challenge at the intersection of advanced materials science, nanotechnology, and integrated sensor design. Both space exploration systems — particularly extravehicular activity (EVA) suits — and advanced energy storage and conversion systems share a fundamental materials challenge: sensor interfaces must maintain high sensitivity and structural integrity under conditions of intense radiation, extreme thermal cycling, mechanical stress, and chemically aggressive atmospheres. Bridging nano-engineered sensing elements with robust protective architectures is therefore essential for the next generation of resilient sensor platforms capable of functioning across these demanding application domains.

This study investigates carbon nanotube (CNT)-based nanocomposites and carbon-based electrochemical interfaces as multifunctional sensor substrate materials suitable for both space-grade and advanced energy system monitoring applications. Multi-walled CNT-reinforced polymer matrices are evaluated for their combined mechanical toughness, electrical conductivity, and magnetic permeability

— properties essential for biomagnetic sensing in EVA suits as well as electrochemical signal transduction in battery and fuel cell monitoring platforms. Stimuli-responsive polymer coatings are additionally explored as protective yet flexible interfaces that preserve sensor sensitivity under sustained thermomechanical loading, a requirement shared by both space and industrial energy environments.

The characterization methodology integrates cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) to evaluate the electrochemical stability and signal-to-noise ratio of CNT-modified electrode surfaces under simulated extreme stress conditions, including radiation-induced lattice defect accumulation and thermal fatigue cycling. Surface morphology and conductivity evolution are assessed through scanning electron microscopy (SEM) and four-probe electrical measurements. Structural integrity under cyclic thermal loading representative of low Earth orbit thermal environments is further modeled through finite element analysis, enabling systematic correlation between nanoscale material degradation mechanisms and macroscale sensor performance loss.

Preliminary analysis indicates that multi-walled CNT composites embedded in biocompatible polymer matrices maintain over 85% of their initial electrochemical activity after simulated radiation exposure equivalent to a 6-month low Earth orbit mission profile. Stimuli-responsive hydrogel coatings demonstrate reversible swelling behavior that accommodates thermal expansion mismatch between CNT sensor substrates and surrounding structural layers, reducing delamination risk under repeated thermal cycling. These findings collectively suggest that CNT-integrated sensing architectures represent viable candidates for resilient sensor platforms in both space exploration and advanced energy storage monitoring contexts.

The convergence of space-grade sensor resilience requirements and the operational demands of next-generation energy storage monitoring defines a productive research direction for integrated smart sensing platform design. By developing CNT-based nanocomposite interfaces that simultaneously satisfy mechanical robustness, electrochemical stability, and magnetic sensitivity criteria, this work contributes to the emerging field of integrated smart sensing skins applicable to EVA suit health monitoring, nuclear material diagnostics, and real-time electrochemical sensing in advanced energy systems. This research is conducted by an early-stage undergraduate researcher as part of a broader interdisciplinary framework bridging nuclear engineering, space materials science, and biomagnetic sensing technologies.

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# Sustainable Electrochemical Sensor: Utilising Agricultural Waste-Derived Activated Carbon for Metal Oxide-Modified Electrode

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The paradigm of green electroanalysis requires a shift towards ecologically benign carbon matrices derived from renewable biomass [1]. The activated carbon matrix yields an expanded electrochemically active surface area, while the graphite phase minimises ohmic overpotential and accelerates charge transfer [2]. This composition effectively suppresses surface passivation by interferents, ensuring enhanced potential stability and reproducibility [3]. Consequently, the developed composite electrode provides a highly efficient and sustainable platform for robust ion-selective potentiometric analysis [4]. The present study focuses on the fabrication and characterisation of a nickel-modified carbon paste electrode (Ni-CPE), in which a two-step thermocarbonisation process was employed to transform the biomass into activated carbon. This treatment increased the carbon content to 58.17% and reduced the H/C atomic ratio to 0.01, as confirmed by CHNS analysis, underscoring a high degree of aromatisation and enhanced hydrophobicity, which are crucial for electrode stability. Raman spectroscopy revealed an $I_D/I_G$ ratio of approximately 1.137, indicating an optimal balance between structural defects and partially graphitised phases, while XRD and SEM-EDX analyses confirmed the homogeneous distribution of graphite, graphene oxide, and nickel crystalline phases, ensuring electrochemical activity. Morphological evaluation via BET analysis yielded a specific surface area of 91.23 $m^2/g$, and BJH analysis identified a mesoporous structure (total pore volume of 0.0542 $cm^3/g$), providing an ideal architecture for ion diffusion

Further, Ni-modified activated carbon has been used as an electrode-active material in manufacturing carbon-paste electrode, with polyvinylidene fluoride (PVDF) in N-methyl-2-pyrrolidone (NMP) used as a binder. The electrochemical performance of the Ni-CPE was systematically evaluated through potentiometric titration and analysis of redox and acid-base systems. In both permanganatometric and acid-base titrations, the electrode shows high accuracy and precision in detecting the endpoint and the analyte concentration. The enhanced electrochemical performance of the Ni-CPE is attributed to improved electron-transfer processes, the electrocatalytic activity of nickel species supported on the biochar surface, and the binder role, suggesting its potential utility in analytical applications.

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# Formation of Molybdenum-Containing Structures on the Surface of a Glassy Carbon Electrode for Biosensor Applications

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The development of functional nanostructured materials for electrochemical and biosensor systems remains one of the important directions of modern analytical chemistry and materials science. Among various modifier materials, molybdenum-containing structures attract considerable attention due to their high electrocatalytic activity, chemical stability, developed surface morphology, and ability to enhance interfacial charge-transfer processes [1]. Surface modification of electrodes with such materials significantly improves the electrochemical characteristics of sensor platforms and broadens their applicability in bioanalytical systems [2,3].

The present work is devoted to the formation of molybdenum-containing structures on the surface of a glassy carbon electrode (GCE) and investigation of their electrochemical behavior. The modifier was synthesized via a chemical route based on sodium molybdate precursor solution followed by deposition onto the GCE surface. The formation process of the modified platform is schematically illustrated in Figure 1. Electrochemical characterization of the obtained systems was carried out using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and differential pulse voltammetry (DPV) in the presence of the $Fe(CN)_6]^{3-}/[Fe(CN)_6]^{4-}$ redox probe.




Figure 1. Schematic illustration of the formation of molybdenum-containing structures on the surface of a glassy carbon electrode.

The obtained results demonstrated that the formation of molybdenum-containing structures on the electrode surface contributes to improved charge-transfer characteristics and enhanced electrochemical activity of the modified electrode. Compared with bare GCE, the modified platform exhibited a more pronounced electrochemical response and lower charge-transfer resistance, indicating improved conductivity of the formed surface layer. The obtained findings confirm the potential applicability of the developed molybdenum-containing platform for further fabrication of electrochemical biosensors and bioanalytical devices.

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# Al-Decorated Nitrogen-Doped Graphene Oxide-Based Materials for Gas Sensing Applications

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The detection of hazardous gases and volatile organic compounds is important for environmental monitoring, industrial safety, and human health protection. Acetone is a common volatile organic compound that can be harmful at elevated concentrations and is also highly flammable, while hydrogen requires careful monitoring due to its low ignition energy and wide flammability range. Therefore, the development of sensitive and reliable sensing materials for detecting these gases is of great practical importance.

In this study, aluminum-decorated nitrogen-doped graphene oxide-based materials were prepared with different aluminum ratios and investigated as active sensing layers for acetone and hydrogen detection. Graphene oxide was selected due to its high surface area and abundant functional groups, while nitrogen doping was introduced to modify the electronic structure and create additional active sites. Aluminum decoration was further applied to enhance surface interaction with gas molecules and improve the sensing response.

Gas sensing measurements were carried out at a concentration of 40 ppm, starting from room temperature and continuing to higher operating temperatures. The influence of aluminum content and operating temperature on the sensing behavior was evaluated. The results show that the combination of nitrogen doping and aluminum decoration enhances the gas sensing performance of graphene oxide-based materials. The improved response may be attributed to modified surface chemistry, increased active sites, and enhanced charge-transfer interactions between the sensing layer and target gas molecules.

This work demonstrates the potential of Al-decorated N-doped graphene oxide-based materials for acetone and hydrogen gas sensing applications and provides insight into the role of aluminum decoration in improving the sensing properties of graphene oxide-derived materials.

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# PANI coated with PAN/Mxene for Gas Sensing Applications

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Electrospun nanofiber based chemoresistive gas sensors have gained increasing attention for use in environmental and industrial monitoring because of their large surface to volume ratio, flexibility, and ability to interact efficiently with gas molecules. Electrospinning is a convenient and adaptable technique that enables the fabrication of continuous nanofibrous structures with controlled morphology. Integrating diverse nanomaterials such as carbon-derived structures and conductive polymers into electrospun nanofibrous mats can markedly enhance the performance characteristics of gas sensors.
In this work, nanofibrous membranes were produced by electrospinning with polyacrylonitrile (PAN) serving as the base polymer due to its reliable fiber-forming ability and mechanical robustness. Key electrospinning parameters and the composition of the precursor solution were adjusted to obtain uniform, bead-free fibers. After fabrication, the PAN nanofibers were coated with a thin polyaniline (PANI) layer using an in situ polymerization approach. This conductive coating was intended to promote more efficient charge transport and strengthen interactions between the sensing material and gas molecules. Moreover, to improve sensing performance MXene nanosheets were introduced into the solution during polymerization of PANI, which enhanced electrical conductivity while also increasing the available surface area and creating additional active sites for gas adsorption. The sensing behavior of the resulting composite was then examined by tracking resistance variations when exposed to different gases under a range of concentrations and operating conditions.

The hybrid architecture formed by PAN, MXene, and the PANI coating creates a large accessible surface along with efficient charge transport pathways and strong affinity for gas molecules. MXene contributes to faster electron movement, while the PANI layer enhances interactions with target gases through reversible doping processes. Owing to this combined effect, the PANI-coated PAN/MXene nanofibers show noticeably improved sensing behavior, including increased sensitivity and quicker response and recovery times.

**Acknowledgments**

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# Functionalized Nanoparticle-Modified Electrochemical Sensor for Simultaneous Cr(III) and Cr(VI) Determination

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Airborne particulate matter (PM) has emerged as a significant global environmental issue, impacting atmospheric processes, public health, and global climate patterns. In the context of Kazakhstan's expanding industrialization and urban development, this endeavor carries exceptional scientific importance.
The proposed project holds great promise in tackling pressing environmental and public health challenges specific to Kazakhstan. One such challenge is the contamination of ambient PM with chromium, which poses potential health risks to the population. Kazakhstan hosts multiple trace element mines and mineral processing facilities, yet there is a lack of ambient concentration data for both Cr(III) and Cr(VI), particularly in the Central Asian region. This scarcity of information hampers the formulation of effective control strategies necessary to combat Cr(VI) pollution, especially in industrial cities such as Aktobe.
This study involves conducting fundamental research, design and fabrication of inexpensive, robust and promising electrochemical sensor using functionalized nanoparticles that can simultaneously detect Cr(III) and Cr(VI) in ambient PM in Kazakhstan. The development of an advanced sensor array capable of simultaneously detecting Cr(III) and Cr(VI) not only addresses Kazakhstan's air quality concerns but also represents a significant advancement in technology and knowledge. This project promises to provide critical insights into a specific and urgent environmental issue, offering valuable data to inform policies and measures aimed at improving air quality and protecting public health in Kazakhstan.

# Fully Vacuum-Deposited Perovskite Optoelectronic Devices

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Metal halide perovskites have emerged as promising materials for optoelectronic applications such as solar cells and light-emitting diodes. While solution-processed devices have achieved near–theoretical-limit efficiencies, challenges in scalability and long-term stability remain. Thermal evaporation, a mature semiconductor manufacturing technique, offers a viable pathway toward large-area, uniform, and reproducible perovskite devices. In this work, we present our recent advances in fully vacuum-deposited perovskite photovoltaics and light-emitting devices. To address the limited efficiency and unclear solid-state crystallization in evaporated perovskites, we develop a reverse sequential deposition strategy, enabling efficient precursor diffusion and reaction during annealing. Combined with in situ characterization and molecular dynamics simulations, we elucidate the crystallization mechanism and achieve state-of-the-art device performance. Furthermore, by introducing seed-layer-assisted growth and reducing solid-state reaction barriers, we significantly improve film quality, leading to record efficiencies in fully evaporated perovskite solar cells. This strategy is also extended to high-performance perovskite LEDs, enabling bright, efficient, large-area, and patterned emission. These results provide insights into solid-state crystallization and advance the scalable fabrication of high-performance perovskite optoelectronic devices.

# Upcycling of Plastic Mixtures into Carbon Anode Materials for Lithium-Ion Batteries

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Exploring advanced approaches for recycling mixed plastic waste has become an important direction in modern materials science and sustainable energy research. Among the promising strategies for polymer waste utilization, upcycling attracts significant attention, as it enables the transformation of low-value plastic waste into high-value functional carbon materials [1]. In this study, particular emphasis is placed on mixed plastic systems consisting of Polyethylene terephthalate (PET) and Polymethyl methacrylate (PMMA), which are widely used in packaging, consumer products, and industrial applications. The research focuses on the synthesis of carbon materials from PET/PMMA mixtures through controlled thermal treatment and template-assisted pyrolysis methods [2-3]. Special attention is devoted to investigating the influence of polymer composition, processing conditions, and solvent-assisted preparation techniques on the structural, physicochemical, and electrochemical properties of the obtained carbon materials for potential application in lithium-ion battery systems. To obtain carbon anodes, PET bottles of the Coca-Cola Classic brand drink were used. The bottles were washed with water and ethanol, air dried and cut into small pieces of 3-4 mm square prior to dissolution.

During the heat treatment process, PET and PMMA undergo complex thermo-destructive transformations. PET predominantly forms aromatic carbon structures due to the presence of terephthalate fragments in its molecular backbone, whereas PMMA acts mainly as a sacrificial and pore-forming component because of its relatively high depolymerization tendency and volatile decomposition products. The simultaneous pyrolysis of these polymers under inert atmosphere conditions (Ar or $N_2$) at temperatures ranging from 600 to 1000 °C promotes the formation of porous carbon matrices with developed surface area and partially graphitized domains.The resulting carbon materials were used as an anode material for Li-ion half-cells. The electrochemical properties of the batteries were measured using CV and galvanostatic charge/discharge methods.

The presented EDS analysis of the carbonized (Figure 1) PET/PMMA-derived material demonstrates the formation of a predominantly carbon-rich structure after thermal treatment. The SEM micrographs reveal a heterogeneous layered morphology with compact carbon domains, folded surface regions, and partially developed microstructural defects, indicating successful carbonization and structural reorganization during pyrolysis. Elemental mapping confirms the uniform distribution of carbon and oxygen throughout the analyzed area, while the EDS spectrum shows that the sample mainly consists of carbon (80.4 wt.%) and oxygen (19.6 wt.%).

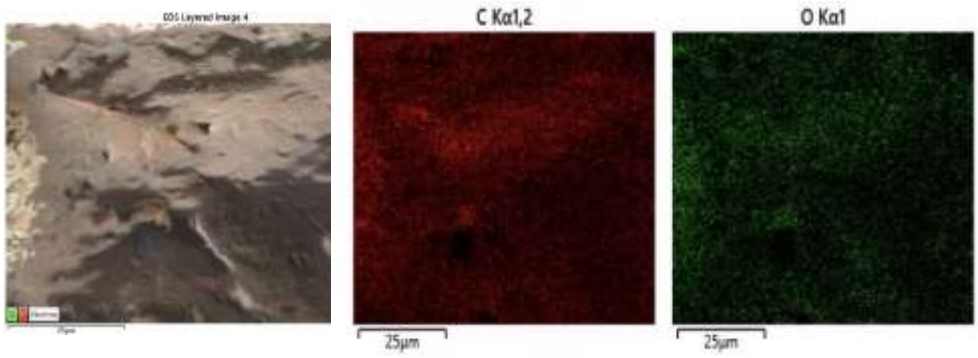



Figure 1. EDS analysis of the carbonized PET/PMMA

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# Upcycling PET Waste into Structurally Ordered Carbon for Lithium-Ion Batteries

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The rapid increase in plastic waste generation has created significant environmental concerns, driving the development of sustainable strategies for converting waste polymers into value-added functional materials. Among various waste plastics, polyethylene terephthalate (PET) is one of the most widely used materials in beverage bottles and packaging applications. In this study, structurally ordered carbon was synthesized from waste PET bottles through a catalyst-assisted carbonization process and evaluated as a promising carbon material for lithium-ion battery (LIB) applications [1].

For the synthesis, waste PET and nickel acetylacetonate (Ni(acac)2) were dissolved in hexafluoroisopropanol (HFIP) to obtain a homogeneous precursor solution (Figure 1). The solution was subjected to casting and solvent evaporation to form a solid precursor film. Subsequently, the precursor was heat-treated under an argon atmosphere at temperatures ranging from 900 to 1500 $^{o}$C. During thermal treatment, the Ni catalyst promoted catalytic graphitization and structural rearrangement of the carbon framework, resulting in the formation of structurally ordered structure. The final product was mechanically milled to obtain fine carbon powder suitable for electrode fabrication [2].

The effect of carbonization temperature on the structural evolution and ordering behavior of the carbon materials was systematically investigated. Increasing heat-treatment temperature led to improved graphitic ordering and enhanced crystallinity due to the catalytic effect of Ni. The obtained ordered carbon exhibited favorable electrical conductivity and structural stability, which are essential properties for high-performance LIB electrode materials. The synthesized carbon can potentially serve as a conductive additive or anode material in LIBs, contributing to improved electron transport and electrochemical performance [3].

This work demonstrates a simple and scalable route for transforming waste PET into high-value structurally ordered carbon materials through catalyst-assisted thermal conversion. The proposed approach not only provides an effective recycling pathway for plastic waste but also offers a sustainable strategy for developing advanced carbon materials for next-generation energy-storage systems.




Figure 1. Synthesis process.

**Acknowledgements.**

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# Interface Engineering of $MoO_X/SiO_X$ Hole-Selective Contacts: Effect of $SiO_X$ Preparation and Comparison with a-Si:H

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Silicon (Si)-based solar panels account for over 90% of the current photovoltaics market, driving strong demand for higher efficiency. Moreover, achieving this goal on an industrial scale through safe manufacturing processes is of utmost importance. Currently, high power conversion efficiencies (PCEs) approaching 25% are achieved primarily in laboratory settings and often rely on toxic and/or flammable gases such as hydrogen ($H_2$), silane ($SiH_4$), diborane ($B_2H_6$), phosphane ($PH_3$), and ammonia ($NH_3$). The use of these gases on an industrial scale requires substantial investment in safety infrastructure and handling procedures. Therefore, reducing production costs by decreasing the use of such gases, while maintaining a similar rate of PCE, is essential. In response, many research groups are investigating alternative materials that can be synthesized safely [1]. Among these, transition metal oxides (TMOs) have attracted considerable attention in recent years because of their ease of deposition, potential for industrial scalability, and the absence of toxic gases during processing. In addition, the high transparency of thin-film TMOs, which minimizes parasitic absorption, makes them promising for application in Si/perovskite tandem solar cells. Consequently, several TMOs, including $VO_X$, $TiO_X$, $WO_X$, and $MoO_X$, have been widely investigated [2]. Among them, molybdenum oxide ($MoO_X$) has attracted particular interest because of its high work function and low deposition temperature.

In Si solar cells, $MoO_X$ serves as a hole-selective layer that enables efficient hole transport while blocking electrons, thereby improving charge collection efficiency. In addition to its carrier-selective properties, $MoO_X$ has also been reported to provide a certain degree of surface passivation. However, this passivation alone is generally insufficient to effectively suppress interface recombination, necessitating an additional chemical passivation layer. Among the various passivation materials, hydrogenated amorphous silicon (a-Si:H) is one of the most widely used. The record PCE for $MoO_X$/a-Si:H-based solar cells currently stands at 23.5%. However, a-Si:H is typically deposited using chemical vapor deposition (CVD) processes involving flammable and toxic $H_2$ and $SiH_4$ gases. Consequently, an alternative passivation material is needed, and one such candidate is ultrathin $SiO_X$. $SiO_X$ has already been successfully employed as a passivation layer in structures such as TOPCon, where it plays a critical role [1]. Research on $MoO_X/SiO_X$ structures for solar-cell applications is ongoing but remains limited. Therefore, optimizing the $SiO_X$ interfacial passivation layer in combination with $MoO_X$ to achieve both low recombination rates and efficient carrier transport remains an important challenge.

This work investigates $MoO_X/SiO_X$/Si structures in comparison with the reference $MoO_X$/a-Si:H/Si structure, with particular emphasis on the influence of $SiO_X$ deposition conditions and post-deposition forming-gas annealing (FGA) on structural and electrical properties. For the $MoO_X/SiO_X$/Si structures, interlayers prepared by UV/$O_3$ oxidation and nitric-acid oxidation of silicon (NAOS) were studied both with and without FGA treatment and compared with naturally oxidized Si reference samples. X-ray reflectometry (XRR) revealed significant differences in interlayer thickness, density grading, and $MoO_X$ growth depending on the oxidation route and annealing conditions. The samples were characterized in terms of minority-carrier lifetime and contact resistivity using the μ-PCD and TLM methods, respectively.

Within this work, different Si surface oxidation methods were compared with each other and with the reference $MoO_X$/Si structure. NAOS combined with FGA produced the most compact interlayer structure and yielded the highest minority-carrier lifetime, reaching up to 250 μs. In contrast, the $MoO_X$/Si structure exhibited lower contact resistance but reduced passivation quality, with a minority-carrier lifetime of 156 μs. The UV/$O_3$ method resulted in lower lifetime values and non-ohmic contacts despite the long processing time. These results indicate that achieving an appropriate balance between $SiO_X$ growth and post-deposition treatment conditions is crucial for successful implementation in solar cells. The obtained parameters were additionally compared with those of the $MoO_X$/a-Si:H/Si structure and evaluated through simulations based on the measured values.

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# Proximity Rapid Thermal Diffusion for Simultaneous Phosphorus and Boron Doping of Silicon

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Controlled phosphorus and boron diffusion are essential for the fabrication of advanced photovoltaic and electronic devices, including TOPCon solar cells, photodiodes, and bipolar semiconductor structures. Conventional industrial diffusion methods, such as $POCl_3$ and $BBr_3$ diffusion, provide uniform and reliable doping but involve toxic and corrosive gases, increasing fabrication complexity and safety requirements. As an alternative, spin-on doping (SOD) combined with rapid thermal diffusion (RTD) has attracted considerable attention due to its low cost, simplicity, and compatibility with scalable deposition techniques. Previous studies demonstrated successful fabrication of TOPCon solar cells using commercial SOD solutions, achieving power conversion efficiencies above 17 % and open-circuit voltages close to 700 mV [1]. Nevertheless, conventional RTD processes can introduce metallic impurities and defects into the Si wafer. In particular, boron diffusion may lead to the formation of a boron-rich layer (BRL), which degrades minority-carrier lifetime and reduces device performance [2]. To overcome these limitations, Proximity Rapid Thermal Diffusion (PRTD) has been proposed as an effective alternative diffusion strategy. Unlike conventional RTD, PRTD transfers dopants through the gas phase from a nearby dopant source wafer without direct contact with the processed Si wafer. Currently, PRTD method is typically performed either as a one-sided diffusion process (referred to as two-layer PRTD in this study) to form $n^+$ or $p^+$ region, or as two separate diffusion steps for creation of $n^+pp^+$ structures. To reduce process complexity, a simultaneous phosphorus and boron co-diffusion is introduced in this study to form an $n^+pp^+$ structure through single-step thermal annealing. This is achieved using a three-layer PRTD configuration, in which phosphorus and boron SOD sources are placed on opposite sides of the processed wafer. After optimization of relevant parameters, three-layer PRTD, two-layer PRTD and conventional RTD samples were compared to demonstrate the effect of PRTD method on performance of Si solar cell.

A systematic investigation was conducted to examine the effects of annealing temperature and duration, pre-baking temperature, and $O_2$ concentration on dopant incorporation and sheet resistance (*Rs*). Optimal diffusion conditions were identified at 925 °C for 180 s with a pre-baking temperature of 300 °C under O2-free ambient conditions. To characterize the chemical composition of PSG and BSG thin films Fourier transform infrared spectroscopy (FTIR) analysis was performed. FTIR analysis revealed that pre-baking and annealing promote hydroxyl removal, network polymerization, and densification of PSG and BSG films, accompanied by the formation of Si–O–P and B–O–Si bonds. These structural modifications provide a consistent explanation for the observed *Rs* behaviour, highlighting the strong correlation between SOD film chemistry and dopant diffusion during PRTD. Comparative device characterization indicated that both two-layer and three-layer PRTD configurations outperform conventional RTD in terms of photovoltaic performance. External Quantum Efficiency (EQE) analysis confirmed improved carrier collection efficiency in PRTD-based solar cells. In particular, the three-layer PRTD configuration enabled uniform and effective co-diffusion of phosphorus and boron, resulting in enhanced device performance and reduced defect formation. The obtained results demonstrated that three-layer PRTD is an effective noncontact diffusion technique capable of reducing contamination and improving the electrical and photovoltaic characteristics of silicon solar cells. Comparative analysis showed that both two-layer and three-layer PRTD configurations outperform conventional RTD structures, while the three-layer configuration provided the best overall device performance.

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# FTS Magnetron Sputtered TiNx Electron Selective Contacts: Influence of Sputtering Parameters on Structural and Electrical Properties

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Titanium nitride ($TiN_x$) thin films are promising materials for advanced microelectronic, optoelectronic, and photovoltaic applications due to their high electrical conductivity, chemical stability, mechanical hardness, thermal stability, and compatibility with semiconductor processing technologies. Recently, TiN has attracted significant attention as an electron-selective contact material for silicon solar cells and other semiconductor devices because of its low contact resistivity, metallic conductivity, and stability. $TiN_x$ thin films can be fabricated using various deposition techniques, including reactive sputtering, chemical vapor deposition (CVD), atomic layer deposition (ALD), pulsed laser deposition (PLD), cathodic arc deposition, and ion-assisted deposition. Among these, magnetron sputtering techniques such as DC and RF sputtering remain the most widely used because they offer simplicity, uniformity, and scalability. However, conventional sputtering techniques may introduce several limitations, including energetic particle bombardment, substrate overheating, plasma-induced defects, and structural damage to sensitive semiconductor surfaces. Facing Target Sputtering (FTS) is an alternative sputtering configuration capable of overcoming many of these limitations. In the FTS geometry, the plasma is primarily confined between opposing targets, significantly reducing direct plasma exposure and energetic particle bombardment of the substrate surface.[1,2]. In this work, $TiN_x$ thin films were deposited by FTS magnetron sputtering under different deposition conditions and then compard to films obtained by RF and DC sputtering. Film thickness and density were determined from X-ray reflectometry (XRR) measurements using a ComplexRay C6 system, while electrical resistivity was measured by the four-probe method using a Keithley measurement system. Contact resistivity was evaluated using the Cox–Strack method, also employing a Keithley setup. The obtained TiNx films were additionally integrated into silicon solar cell structures to evaluate their suitability as electron-selective contact layers.

The influence of deposition parameters, including magnetron power, argon flow rate, and distance between the targets, on the structural and electrical properties of $TiN_x$ films was investigated. The results demonstrated that increasing magnetron power generally decreased film resistivity while increasing the deposition rate. Lower resistivity and higher density values were observed at smaller distance between the targets due to improved plasma confinement. Among the investigated parameters, argon flow rate had the strongest influence on film quality: increasing the flow rate resulted in significantly higher resistivity and lower density, likely due to enhanced oxygen incorporation from residual gases in the chamber [3]. Films deposited at magnetron distances of 9.75 cm and 11 cm demonstrated resistivity values on the order of $10^{-5}$ Ω·cm, corresponding to high-quality TiNx coatings. Contact resistivity measurements showed behavior consistent with bulk resistivity trends, with the lowest value reaching approximately 14 mΩ·cm$^2$.

X-ray diffraction analysis confirmed the formation of a TiN face-centered cubic (FCC) structure with diffraction peaks corresponding to the (111), (200), and (220) crystallographic planes. Films deposited using the FTS method exhibited the clearest crystalline structure and the lowest resistivity value of $9.90 \times 10^{-5}$ Ω·cm. The diffraction peak shifts toward lower diffraction angles observed for both FTS- and RF-deposited films indicate lattice expansion associated with oxygen incorporation into the TiNx lattice. For RF-sputtered films, this effect is likely associated with the relatively low deposition rate, which increases exposure of the growing film surface to residual gases. In contrast, for FTS-deposited films, the peak shift may be related to chamber geometry and plasma distribution rather than deposition rate effects alone.

The obtained results demonstrate that optimization of FTS sputtering parameters plays a critical role in achieving high-quality $TiN_x$ thin films with improved electrical and structural characteristics. In particular, argon flow rate and magnetron configuration strongly influenced film resistivity, density, and crystallinity. The FTS configuration enabled the deposition of conductive $TiN_x$ coatings with resistivity values on the order of $10^{-5}$ Ω·cm while reducing plasma-induced substrate damage. Integration of the deposited $TiN_x$ films into silicon solar cell fabrication additionally confirmed their potential applicability as electron-selective contacts for photovoltaic devices.

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# Interface Engineering via Spin-Coated Oxide Interlayers and Low-Damage Facing Target Sputtering for Semitransparent Inverted Perovskite Solar Cells

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Inverted perovskite solar cells (PSCs) have emerged as one of the most promising photovoltaic (PV) technologies due to their high power conversion efficiency, low-temperature fabrication, reduced hysteresis, and compatibility with scalable device processing. In particular, inverted p-i-n architectures have attracted significant attention owing to their favorable compatibility with multilayer device integration, making them particularly attractive for tandem PV applications. In tandem architectures, semitransparent top cells are required to efficiently transmit a portion of the incident spectrum to underlying subcells, leading to increasing interest in semitransparent inverted PSCs. Such device architectures require transparent conductive electrodes (TCEs) as top contacts that combine high optical transparency with efficient charge collection.

Among various TCE materials, indium-based electrodes are widely employed due to their favorable combination of optical transparency and electrical conductivity. However, sputter deposition of these TCEs introduces plasma-related and particle-induced damage to the underlying organic transport and perovskite layers, resulting in interfacial degradation and performance losses. To suppress sputtering-induced damage, protective oxide interlayers can be introduced between the electron transport layer and the top transparent electrode [1]. In many studies, these protective interlayers are commonly fabricated using atomic layer deposition (ALD), which provides excellent film conformity and interface protection but remains relatively complex, expensive, and less compatible with industrial-scale fabrication [2]. Therefore, the development of cost-effective and scalable interfacial protection strategies that avoid complex deposition approaches remains an important challenge for semitransparent PSCs.

In this work, spin-coating and low-damage vacuum deposition method via Facing Target Sputtering (FTS) were explored as alternative fabrication approaches. Semitransparent inverted PSCs with the architecture: glass/ITO/$NiO_x$/SAM/$Cs_{0.05}(MA_{0.23}FA_{0.77})$ (0.95) $Pb(I_{0.77}Br_{0.23})_3$/PCBM/AZO or $SnO_2$/ITO were fabricated and investigated. Spin-coated AZO and SnO2 interlayers were employed as protective buffer layers prior to top ITO magnetron sputtering. In addition, FTS was investigated as a softer deposition approach for TCE fabrication compared to conventional sputtering. The influence of the oxide interlayers and deposition methods on the PV and interfacial properties of the devices was systematically studied. The incorporation of AZO and $SnO_2$ interlayers and implementation of FTS demonstrated the potential of low-cost deposition approaches as alternatives to ALD-based interface engineering strategies. Electrical characterization parameters including open-circuit voltage, fill factor, and hysteresis behavior were analyzed and compared to reference devices without protective interlayers.

To elucidate the charge recombination kinetics and evaluate the extent of sputtering-induced damage, electrochemical impedance spectroscopy (IS) was systematically performed under open-circuit conditions at different illumination intensities. Key parameters, including recombination resistance (*Rrec*) and charge carrier relaxation time (τ), were extracted from the impedance spectra. To precisely identify the dominant recombination mechanisms, the diode ideality factor ($n_{id}$) was determined and cross-examined using two independent approaches: the light-intensity dependence of the open-circuit voltage (*Voc* vs. intensity) and the intensity-dependent behavior of the high-frequency recombination resistance (*Rrec* vs. intensity) [3]. The devices with protective interlayers demonstrated increased *Rrec* and prolonged τ, accompanied by a reduction in the $n_{id}$ compared to the reference cells, identifying that the introduced oxide interlayers indeed suppress trap-assisted recombination at the sputtered TCE interface.

The obtained results highlight the feasibility of semitransparent inverted PSCs employing sputtered indium-based TCEs for tandem photovoltaic applications. Furthermore, the introduction of AZO and $SnO_2$ protective interlayers fabricated via spin coating and softer TCEs deposition methods such as FTS represents a promising alternative to more complex ALD-based processing, providing an effective strategy for the development of efficient, scalable, and tandem-compatible semitransparent PSCs.

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# Role of Target-to-Target Distance in Controlling the Optoelectronic Properties of ITO Films Deposited by Facing-Target Sputtering

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Indium tin oxide (ITO) is a transparent conducting oxide widely used as a transparent electrode in optoelectronic and photovoltaic devices due to its combination of high optical transparency in the visible range and low electrical resistivity. It is typically deposited by conventional magnetron sputtering or pulsed DC sputtering, which enable scalable thin-film fabrication but inherently involve energetic ion bombardment of the growing film. This can lead to increased defect density, reduced carrier mobility, and degradation of underlying functional layers in multilayer device structures, while also limiting precise control over the balance between optical transparency and electrical conductivity.

Facing-target sputtering (FTS) offers an alternative configuration in which two targets are arranged face-to-face, and the substrate is positioned outside the direct plasma zone. This geometry significantly reduces energetic particle bombardment and minimizes damage to the growing film, making FTS particularly attractive for sensitive optoelectronic applications[1-3] such as photovoltaic devices and thin-film stacks. Moreover, the confined plasma between the targets introduces additional degrees of freedom for tuning deposition conditions, which are not present in conventional sputtering systems.

In this work, a custom-built FTS system with adjustable TT distance was employed to investigate the relationship between plasma confinement and the optoelectronic properties of ITO thin films. The TT distance was varied from 9 to 13.5 cm, while additional optimization was performed through variations in sputtering power and oxygen flow rate. Structural, electrical, and optical properties were evaluated using X-ray reflectometry, Hall-effect measurements, four-point probe characterization, and UV–Vis spectroscopy.

The obtained results demonstrate that TT distance plays a critical role in determining charge transport properties. Increasing TT distance reduced the magnetic field strength in the inter-target region from approximately 104 to 55 mT, resulting in weaker plasma confinement and enhanced energy relaxation of sputtered species during transport toward the substrate. Consequently, carrier mobility increased from approximately 4 to 15 $cm^2/V \cdot s$, while resistivity decreased from $2.8\times10^{-3}$ to $0.9\times10^{-3}$ $\Omega \cdot cm$. These improvements occurred despite only minor changes in film density, indicating that reduced defect-related carrier scattering rather than densification is responsible for the enhanced electrical performance. Simultaneously, optical transmittance improved across the visible spectral range, leading to a continuous increase in the Haacke figure of merit with increasing TT distance.

Under optimized deposition conditions (TT distance of 13.5 cm, sputtering power of 250 W, and $O_2$ flow rate of 0.4 sccm), ITO films with resistivity as low as $0.6\times10^{-3}$ $\Omega \cdot cm$, carrier mobility exceeding 30 $cm^2/V \cdot s$, sheet resistance of approximately 60 $\Omega/\square$, and optical transparency above 80% were achieved. Compared with conventionally sputtered ITO, FTS-grown films exhibited significantly higher carrier mobility while maintaining comparable resistivity.

These findings identify TT distance as a key parameter governing plasma confinement, particle transport, and defect-related scattering in FTS systems. The demonstrated geometric control of film growth provides an effective strategy for improving transparent conductive electrodes intended for advanced photovoltaic and optoelectronic devices.

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# Interface Engineering of $MoO_X$ and $WO_X$ Bilayers for Enhanced Hole-Selective Contacts in Silicon Solar Cells

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Transition metal oxides have emerged as promising hole-selective contact materials for high-efficiency silicon solar cells due to their high work function and compatibility with low-temperature fabrication. Among the most extensively studied transition metal oxides, molybdenum oxide ($MoO_X$) and tungsten oxide ($WO_X$) have both demonstrated desirable properties for dopant-free carrier-selective contacts [1,2]. $MoO_X$ is widely recognized for its excellent hole selectivity and favorable electrical performance, while $WO_X$ has shown improved stability. Despite these advantages, achieving both high electrical performance and long-term stability simultaneously remains a major challenge for oxide-based contacts [1,2]. In this work, we introduce a bilayer hole-selective contact concept based on combining $MoO_X$ and $WO_X$ into $MoO_X/WO_X$ and $WO_X/MoO_X$ multilayer structures. The proposed bilayer approach aims to exploit the complementary advantages of both oxides by integrating the superior electrical characteristics of $MoO_X$ with the enhanced stability of $WO_X$.

To establish the optimal conditions for bilayer fabrication, thermally evaporated $WO_X$ thin films were systematically optimized by varying film thickness, deposition rate, and base pressure. Comprehensive characterization was performed through carrier lifetime measurements and contact resistivity evaluation using the Transfer Length Method (TLM), together with optical transmittance and long-term stability measurements. The optimal $WO_X$ condition was identified as a 10 nm film deposited at 0.3 Å/s under $5\times10^{-4}$ Pa base pressure. While $MoO_X$ demonstrated superior initial passivation quality and lower contact resistivity, $WO_X$ exhibited significantly slower degradation over more than 1000 hours, confirming its outstanding long-term stability.

Based on these results, $MoO_X/WO_X$ and $WO_X/MoO_X$ bilayer hole-selective contacts were fabricated and comparatively investigated. The bilayer structures demonstrated improved balance between electrical performance compared to their single-layer counterparts. In particular, $WO_X$ contributed to reduced degradation and improved optical transmittance, while the presence of $MoO_X$ preserved efficient hole extraction and favorable contact properties. Furthermore, the sequence of oxide deposition was found to influence the optoelectrical behavior of the contacts, indicating the important role of interface formation and interlayer interactions in determining carrier transport and passivation characteristics. The bilayer approach therefore provides an effective strategy for tuning electrical, optical, and stability-related properties through oxide interface engineering.

Finally, proof-of-concept silicon solar cell devices incorporating the optimized oxide contacts were fabricated. The photovoltaic performance of the fabricated devices was evaluated through current density-voltage (J-V) characterization and External Quantum Efficiency (EQE) measurements. The results demonstrated the strong potential of transition metal oxide bilayer engineering for improving carrier-selective contacts [1,2]. This approach provides a promising pathway toward stable, low-temperature, and high-performance photovoltaic technologies.

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# Comparative Life Cycle Assessment of Li-ion Cathode Electrodes with PVDF and PDADMA-DEP Binders

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With the increasing global demand for lithium-ion batteries in electric vehicles, renewable energy storage, and portable electronics, the environmental footprint of battery components needs to be more closely examined. Binders, as polymeric materials that maintain electrode integrity and ensure electrical contact, play a vital role in determining the overall battery sustainability. However they have been less studied. The aim of this study is to compare the life cycle assessment (LCA) of two cathode binder systems, polyvinylidene fluoride (PVDF) processed with the solvent NMP and a water-processed polyionic liquid (PIL) binder PDADMA-DEP.

In this study, the cradle-to-gate boundary system and the CML-IA-based impact assessment method were used, and the environmental performance of both binder-based cathodes was evaluated in several impact categories. According to the results obtained (Figure 1), the PVDF-based cathode shows slightly greater effects on abiotic depletion, global warming potential (GWP100a), human toxicity, photochemical oxidation, eutrophication and specially in marine aquatic ecotoxicity category. However in the ozone layer depletion category PVDF performs better than PDADMA-DEP with a relative effect of approximately 13% compared to 100% for PDADMA-DEP. Meanwhile, PDADMA-DEP shows a greater effect on fresh water aquatic ecotoxicity and acidification. In the terrestrial ecotoxicity category both systems perfom the same.

Overall, the findings of our study suggest that the environmental trade-offs between PVDF and PDADMA-DEP are specific to each impact category, rather than uniformly favoring one binder. As previously mentioned, they may be green in some environmental categories, but the ozone depletion performance of the studied PIL raises concerns about their employment. Therefore, we recommend further research on PILs. These results emphasize the importance of LCA in guiding the development of sustainable binder alternatives for the production of next-generation lithium-ion batteries.

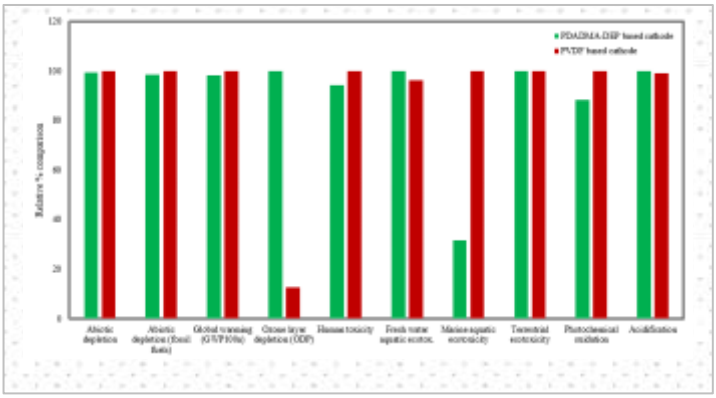


Figure 1. Relative environmental impact comparison (%) of PDADMA-DEP- and PVDF-based Li-ion battery cathodes across CML-IA impact categories.

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# Upcycling Polypropylene Waste into Carbon Anode Materials for Lithium-Ion Batteries

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Polypropylene (PP) waste represents a significant environmental challenge, as it accounts for approximately 20% of global plastic waste with less than 1% currently recycled [1-2]. This work presents a sustainable upcycling strategy for converting PP waste into carbon anode materials for lithium-ion batteries (LIBs) by incorporating montmorillonite (MMT), a naturally occurring clay mineral, as an eco-friendly additive prior to high-temperature carbonization. MMT enhances the thermal stability of PP, preventing complete decomposition at 900 °C and enabling the formation of solid carbon residues. A series of PP/MMT composites with varying MMT loadings (6–20 wt%) were prepared by ball milling and carbonized under argon at 900 °C. The resulting materials were characterized by XRD, Raman spectroscopy, SEM, TEM, CHNS elemental analysis, and XPS. Among all compositions, the M6 sample (6 wt% MMT) demonstrated the most favorable microstructure, featuring well-dispersed MMT-derived inorganic phases and turbostratic carbon domains with high defect density. Electrochemical evaluation revealed that M6 delivers an initial discharge capacity exceeding 400 mAh $g^{-1}$, excellent cycling stability over 100 cycles, and outstanding rate capability of 345.1 mAh $g^{-1}$ at 2 C. The superior performance of M6 is attributed to its optimized balance between carbon content, inorganic phase distribution, and defect density. This approach avoids the hazardous acid-based stabilization treatments commonly employed in PP carbonization while achieving comparable electrochemical performance, demonstrating a viable and environmentally benign route for plastic waste valorization within a circular economy framework.

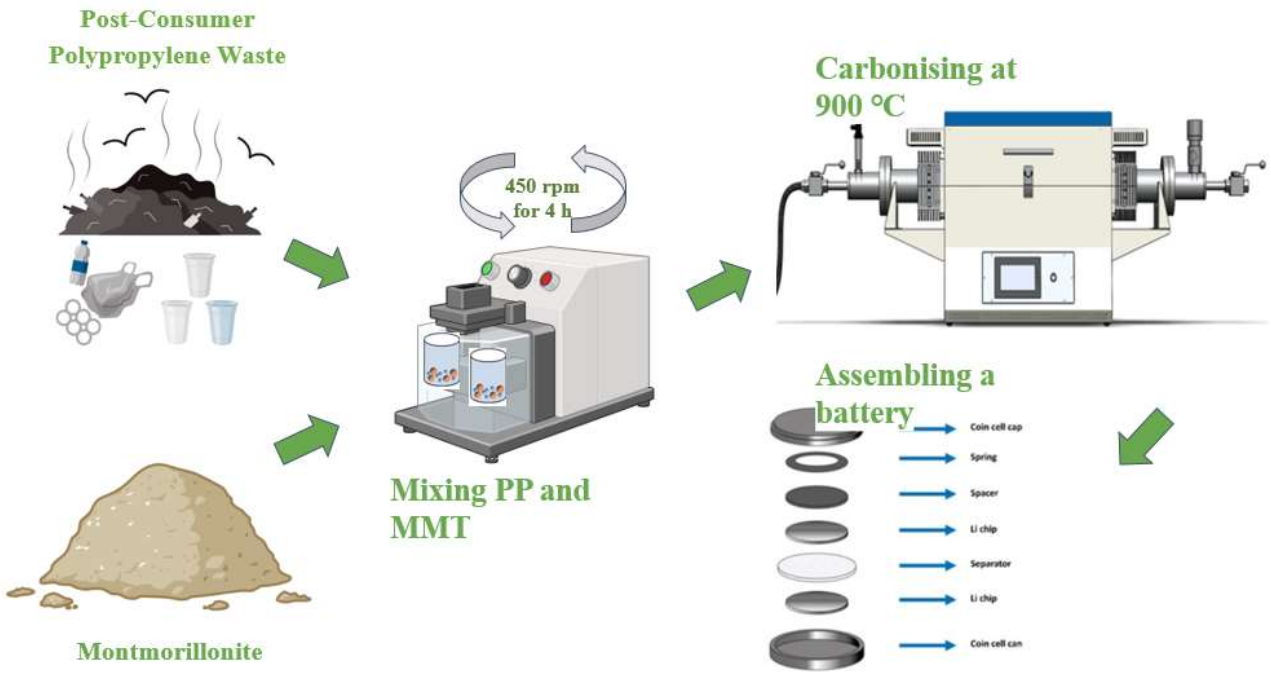



Figure 1. Schematic of PP/MMT composite preparation via ball milling and carbonization

**Acknowledgements**
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# Shape-Resolved Digital Twin Reconstruction of Granular Thermal Storage Particles for Concentrated Solar Power Systems

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Concentrated solar power (CSP) is a solar thermal technology that uses mirrors or lenses to concentrate solar radiation onto a receiver, generating heat that drives a thermodynamic cycle for electricity production. Compared to photovoltaic systems, CSP plants can store energy as heat in thermal storage units, extending operation beyond daylight hours. This storage capability depends heavily on the choice of heat storage medium, which directly affects system efficiency, cost, and durability. Granular powder materials have attracted significant interest for this application due to their excellent thermal stability and heat transfer characteristics at the elevated temperatures encountered in CSP systems. However, their irregular, non-spherical morphology significantly influences particle packing and bulk heat conduction, necessitating precise computational modeling.

The Discrete Element Method (DEM) simulates granular systems by tracking individual particle motion, contact forces, and energy exchange. In contrast to continuum methods, which represent the material as a continuous medium and solve governing field equations on a computational mesh, DEM directly captures particle-scale phenomena. This feature is essential for granular materials, where packing arrangement, contact topology, and particle shape play critical roles in determining heat transfer characteristics. Spherical particle models reduce contact detection to simple center-to-center distance calculations, resulting in high computational efficiency. However, they cannot adequately represent the angularity, aspect ratio, and surface roughness of real granular materials, which can compromise the accuracy of predicted packing structures and effective thermal properties. Non-spherical particle representations provide a more realistic description of fracture-generated particles by capturing their irregular facets and sharp edges. The associated increase in geometric complexity, however, necessitates efficient modeling strategies to maintain computational feasibility for large-scale DEM simulations.

This study extends our previously developed framework for the integrated characterization, classification, and quasi-3D reconstruction of highly irregular calcined bauxite particles for predictive DEM simulations [1]. While the earlier work focused on a bauxite granular material and established the methodology for generating shape-resolved digital particle twins, the present study generalizes the approach to a broader range of granular materials relevant to thermal energy storage applications. By incorporating additional particle systems with distinct morphologies and surface characteristics, the robustness and transferability of the framework are evaluated across different classes of high-temperature granular media. Five particle batches are prepared for analysis, including small (1.0–1.4 mm) and large (1.4–1.8 mm) fractions of calcined bauxite, green silicon carbide, and black silicon carbide. Each batch consists of 200 particles and is sieved to maintain size uniformity. This study develops digital twins of granular particles through multiscale shape analysis and DEM packing simulations. Particle outlines are extracted from microscope images using ImageJ software and analyzed using Elliptic Fourier Analysis (EFA), from which shape descriptors are computed across macro-, meso-, and microscales. EFA-derived indices are supplemented by dimensional size measurements including Feret diameters, projected area, perimeter, and equivalent area diameter.

Three-dimensional geometries are reconstructed from the 2D outlines using a quasi-3D approach (see Figure 1). Three orthogonal projections are drawn from the particle database by statistical criteria: the major projection P1 matches the median elongation ratio of the batch, P2 is varied across the 10th, 25th, 75th, and 90th elongation ratio percentiles to capture the natural range of particle thickness, and P3 is selected at median angularity to represent typical corner sharpness. Volume is generated by a multi-spheres packing procedure based on maximum inscribed circles, each treated as a sphere of equal radius, after which a convex hull produces the final closed polyhedral shape. Face count is reduced through quadric error metric decimation to keep contact detection computationally feasible. Packing simulations using the reconstructed geometries are validated against experimental bulk density measurements, establishing the accuracy of the digital twins under realistic packing conditions.

The framework offers an automated workflow for generating shape-accurate, computationally efficient particle models from 2D images of any granular material, wi ınd heat exchangers in solar energy systems.

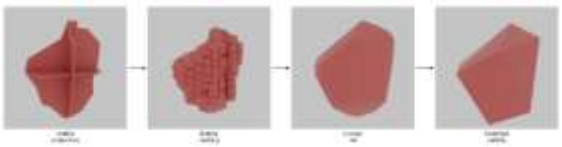


**Figure 1.** 3D Particle Reconstruction Framework.

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# Analysıs and Performance Optımızatıon of a Small Scale Savonıus-Darrıeus, Hybrıd Wınd Turbıne for Low-Wınd Condıtıons in Kazakhstan

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This paper explores ways to reduce the cut-in speed of an H-type Darrieus wind turbine in order to increase its efficiency in low wind conditions. The reason for this research is the low average wind speed in Kazakhstan, average wind speed in many regions ranges between 2–5 m/s, while selected windy regions reach up to 8 m/s. The QBlade platform was used to generate electricity production graphs. As a result of modelling and wind simulation in the programs, it was established that the H-type Darrieus wind turbine is more optimal for low winds than a conventional horizontal axis wind turbine, as it has a cut-in speed allowing it to start rotating at a wind speed of 2 m/s. In comparison, most horizontal turbines require 4 m/s or higher to start the rotor rotation. The second method investigated changing the aerodynamic profile of the H-Darrieus turbine blades NACA 0018, NACA 0012, NACA 0021, NACA 0015, NACA 4412 and using a new airfoil NACA 1920 which increases the lift coefficient and reduces drag at low wind speeds. The results of this work show that the combination of a H-type Darrieus rotor design and a change in the aerodynamic profile of the blades significantly increases electricity generation and reduces the starting speed of the turbine in low winds. The proposed solutions make wind power plants highly effective for use in remote areas with limited access to the power grid.

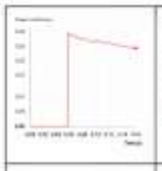
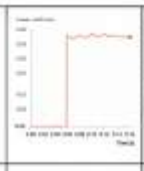
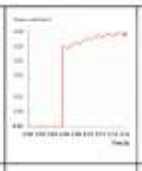
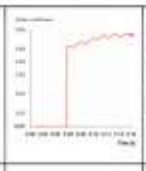
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| NACA 0012 $C_p$ | NACA 0015 $C_p$ | NACA 0018 $C_p$ | NACA 0021 $C_p$ | NACA 1920 $C_p$ | NACA 4412 $C_p$ |

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# Electrospun PCL-$SiO_2$-AgCl/$Ag_3PO_4$ Nanocomposite Membranes for Multifunctional Air Filtration

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Air pollution and the spread of airborne pathogens remain critical global challenges, highlighting the urgent need for efficient air filtration materials with integrated antibacterial and antiviral functionality[1]. Electrospun nanofibrous membranes have attracted significant attention in this context due to their high porosity, large specific surface area, and tunable structural properties[2].

In this work, multifunctional polycaprolactone (PCL)-based nanocomposite membranes incorporating $SiO_2$ and AgCl/$Ag_3PO_4$ nanoparticles were developed for advanced air filtration applications. The electrospinning parameters were systematically optimized to obtain uniform, bead-free nanofibers with a highly porous and interconnected structure, promoting efficient air permeability and particle capture. The morphology of the fabricated membranes was investigated by scanning electron microscopy (SEM), confirming the formation of continuous nanofibrous networks. The chemical structure and successful incorporation of $SiO_2$ and AgCl/$Ag_3PO_4$ components were verified using Fourier-transform infrared spectroscopy (FTIR).

The incorporation of inorganic nanoparticles provides synergistic effects, where $SiO_2$ contributes to structural stability and increased surface area, while AgCl/$Ag_3PO_4$ introduces photocatalytically active sites capable of generating reactive oxygen species (ROS) under light irradiation. As a result, the membranes exhibit antibacterial and antiviral activity, demonstrating effective inhibition of microorganisms.

Filtration efficiency tests showed that the developed nanocomposite membranes are capable of efficient particulate matter removal, highlighting their suitability for air filtration applications.

Overall, the proposed electrospun PCL–$SiO_2$–AgCl/$Ag_3PO_4$ nanofibrous membranes represent a promising multifunctional platform combining particle filtration and antimicrobial functionality. Further studies will focus on optimizing performance and evaluating long-term stability under realistic operating conditions.

**Acknowledgments**

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# Use of Agricultural Waste as a Reducing Agent in Leaching Battery Electrode Mass.

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The rapid growth in consumption of lithium-ion batteries (LIBs) demands the search for environmentally safe disposal methods. Conventional hydrometallurgical processing requires expensive and toxic chemical reducing agents, thereby increasing environmental burden. In the implementation of the “waste-to-waste” concept, the application of coffee grounds, which is a renewable source of polyphenols and melanoidins, capable of effectively reducing the metals (Ni, Co, Mn) from the cathode mass, is promising.

The study presents a detailed analysis of the impact of pre-treatment methods and extraction techniques on the reducing activity of coffee grounds. The research was focused on three methods of drying of raw material: convective, vacuum, and combined. Also, a comparison of three methods of active components extraction was performed: maceration with constant stirring, ultrasonic extraction, and extraction in a Soxhlet apparatus.

The drying kinetics were studied and compared with several models. The most suitable model was the Midilli model with an R2 value of 0.99631 for vacuum drying and 0.99331 for convective drying. The results of the comparative analysis showed that the reducing capacity of coffee grounds depends significantly on the preparation parameters. The best indicators for reducing activity are obtained by using raw materials after combined drying, extracted by maceration with constant agitation. This combination allows for the maximum preservation and mobilization of reactive groups of organic compounds, which guarantees high efficiency of transition of metals in solution.

A detailed study of the chemical profile of the obtained bioreductants was carried out by the analysis of the extracts by high-performance liquid chromatography (HPLC).

The kinetics of leaching using coffee grounds and kinetics of leaching using coffee ground extract were studied. The thermodynamics of the process were investigated and leaching parameters were optimized.

**Acknowledgments**

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# Electorchemıcal Leachıng of Black Mass from Spent Lıthıum-Ion Batterıes Usıng $Fe^{3+}/Fe^{2+}$ Redox Medıator

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The rapidly growing volume of used lithium-ion batteries (LIBs) creates a significant environmental problem: if improperly disposed of, they contaminate the environment with heavy metals (Ni, Mn, Co, etc.) and toxic organic electrolyte. Among the methods for processing lithium-ion batteries (LIBs), hydrometallurgy is the most developed, based on the leaching of black mass using reducing agents (e.g., $H_2O_2$, $Na_2SO_3$, $C_6H_{12}O_6$, etc.) [1]. However, the use of chemical reducing agents inevitably increases the cost of the process and increases the environmental burden. An alternative approach is the use of electrons as a reducing agent – electrochemical reduction leaching [2].

In this work, a simplified design of an electrochemical reactor is proposed (Figure 1a). The principal difference from the designs described in the literature [3,4] is the rejection of expensive electrode materials and highly selective ion-exchange membranes. As the working electrode, glassy carbon was used, and as the auxiliary electrode, a $Pb/PbO_2$ electrode was used. Leaching was carried out in a 1 M $H_2SO_4$ solution with the addition of $Fe^{2+}$. Electrochemical characterizations of the process were carried out by cyclic voltammetry (CV), chronoamperometry and electrochemical impedance spectroscopy (EIS). CV results show that the cathodic peak of $Fe^{3+} \rightarrow Fe^{2+}$ reduction in the leaching reactor appeared at the potential of 0.266 V (vs. Ag/AgCl, 3 M KCl). To conduct the leaching, a working electrode potential of -0.5 V was chosen – more negative than the cathodic peak – ensuring stable reduction of $Fe^{3+}$ in a diffusion-controlled mode and continuous regeneration of the redox mediator $Fe^{2+}$ directly on the electrode surface. The concentration of metals in the solution was determined by the AAS method. The composition of the solid residues was analyzed using XRF and SEM-EDS.

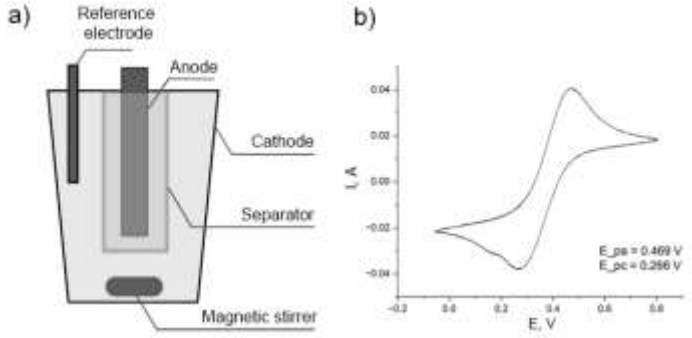



Figure 1 – a) Schematic of the electrochemical leaching reactor; b) cyclic voltammogram of black mass in a 1 M $H_2SO_4$ solution with 20 mmol/L $Fe^{2+}$ and 20 mmol/L $Fe^{3+}$

The proposed method achieved extraction rates for Li, Co, Ni > 90%. Kinetic analysis showed a high degree of conformity between the data and the shrinking core model with the diffusion-limiting stage through the reaction product layer. The developed approach allows for a reduction in the cost of processing and a decrease in environmental impact, which opens up prospects for scaling up the electrochemical recycling of LIBs.

**Acknowledgments**
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**Without their tireless efforts, the conference would not have been possible.**

