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Abstract book

13th INTERNATIONAL CONFERENCE ON NANOMATERIALS & ADVANCED ENERGY STORAGE SYSTEMS

INESS 2025

100th ANNIVERSARY OF YEVNEY BUKETOV

August 6-8, 2025
Nazarbayev University, Astana, Kazakhstan

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POSTER SESSION

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KEYNOTE

Grain Size Engineering of Porous Si-Alloy Anodes for Enhanced Electrochemical Stability

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Silicon (Si) is a highly promising anode material for lithium-ion batteries (LIBs) due to its exceptional theoretical capacity (3589 mAh g^{-1}) and natural abundance [1–3]. However, its large volume change (~300%) during cycling leads to mechanical fracture and unstable SEI formation, limiting practical applications [4]. Nanostructuring is a key strategy to mitigate these issues, as Si particles below ~150 nm avoid pulverization during lithiation [5,6]. Furthermore, grain size below ~60 nm helps suppress the formation of the metastable c-$Li_{3.75}Si$ phase, which is associated with parasitic reactions in carbonate-based electrolytes [7,8]. In this work, we demonstrate a scalable approach to engineer grain-controlled porous Si alloy anodes. Amorphous Si-Al-Fe alloys were synthesized by melt spinning and recrystallized at optimized temperatures to produce uniformly distributed Si nanograins (~60 nm). Subsequent acid etching introduced a porous architecture, which improved lithium-ion kinetics and accommodated volume changes (Figure 1). The resulting anode delivered a reversible capacity of 572.2 mAh g^{-1} with 85.2% retention after 100 cycles and a high Coulombic efficiency (~99.9%). Differential capacity (dQ/dV) analysis confirmed suppression of the detrimental c-$Li_{3.75}Si$ phase. This study highlights the critical role of Si grain size control in stabilizing electrochemical performance and offers a scalable route to high-performance Si-based anodes.

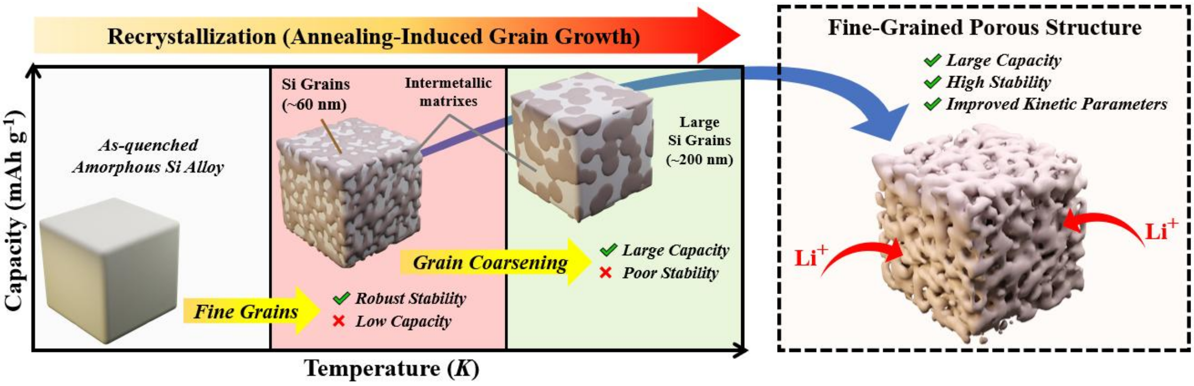

Figure 1. A schematic illustration of the fine-grained and porous Si alloys.

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New Trend of Lithium Ion & Metal Batteries By Using Separator Having Inverse Opal structure

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Lithium ion battery (LIB) has been utilized in various applications, such as portable devices, electric vehicles and energy storage systems, owing to its high energy density and resonable power density. However, there are some problems for a presnt LIB. In this study, we are improving sevelar performances of LIB. In addition, we are developing lithium metal battery (LMB). Our research targets are:

(1) Longer cycle life of LIB, may be more than 10000 cycles. (3) Higher safety of LIB and LMB.
(2) Wide operation temperature of LIB, -10 °C ~ 100 °C. (4) Higher energy density of LMB.

Most important material is an electrolyte to solve these research targets. Non-aqueous organic solvents with lithium salt has been widely utilized in LIB. A standard electrolyte is based on a mixed solvent of liner carbonate and cyclic carbonate with lithium slat, such as a mixed ethylene carbonate and methyl cabonate with $LiPF_6$. These electrolytes can be used in LIB with poly-olefin separator, due to their high wettability of these electrolytes to poly-olefin seprator. In other words, many of other electrolytes without high wettability to poly-olefin separator cannot be utilized in LIB. The poly-olefin separator has limited a kind of electrolytes which can be used in realy LIB. In this study, we have developed new polyimide separator with inverse opal struture (IOP-PI separator), as shown in Figure 1. This seprator has an excellent wettablity to most of electrolytes. For example, a mixed solvent between ethylene carbonayte and propylelne carbonate with lithium salt cannot be used in a present LIB owing to low affinity to poly-olefin separator, but can be used in LIB with IOP-PI separator. The viscosity of this electrolyte is high, so that the electrolyte cannot penatrate into poly-olefin seprator. In the case of IOP-PI seprator, even high viscous electrolytes can penatrate into all of pores in IOP-PI seprator. This property of IOP-PI separator enable to use many kinds of electrolytes. By the way, a mixed solvent between ethylene carbonayte and propylelne carbonate with 1.3 mol dm^{-3} LiFSI $^{+}$ 0.2 mol dm^{-3} $LiPF_6$ electrolyte is very stable at high temperature, such as 60 °C. Even after a storage of this electrolyte at 150 °C, this electrolyte does not change. By using this electrolyte, we have developed LIB with NMC523, graphite, IOP-PI separtor with a mixed solvent between ethylene carbonayte (EC) and propylelne carbonate (PC) with 1.3 mol dm^{-3} LiFSI $^{+}$ 0.2 mol dm^{-3} $LiPF_6$ electrolyte and tested at 60 ºC, Figure 2 shows the discharge capacity retension of the cell operated at 60 ºC. Standard LIB cell usually can be cycled around 500 cycles at this temperature, owing to degradation of electrolyte containg liner carbonate. The LIB with electrolyte containg only cyclic carboonates (PC and EC) showed more stable cycleabiility, as shown in Figure 2. This cell exhibited a high cycleability more than 1000 cycles even at 60 ºC. EC/PC electrolyte is satable at this temperature. After heating this cell at 150 ºC for 2hours, the cell can be discharged and charged. The cell performance is same with that before the heating treatment. This property contibutes a safety of LIB and also long cycle life at ambient temperature. This LIB was also cycled at 30 ºC. The cycle number was estimated to be more than 5000 at least. For LMB, we have to

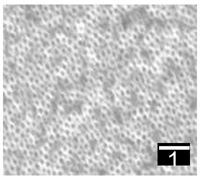

Figure 1. Scanning electron microscope image of IOP seprator. select a proper electrolyte. By using IOP-PI seprator, we can select a suitable one among many of electrolytes including ionic liquids. Thus, IOP-PI seprator provides new world of LIB and enable to realize our four targets described above. These targets are very important for a reduction of carbon dioxide related to rechargeable batteries.

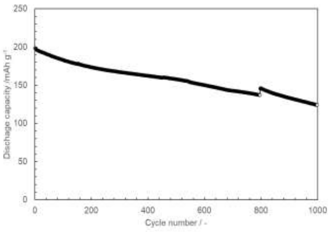

Figure 2. Cycle performance of LIB with NMC523, graphite, IOP-PI seprator and a mixed solvent between ethylene carbonayte and propylelne carbonate with 1.3 mol dm^{-3} LiFSI $^{+}$ 0.2 mol dm^{-3} LiPF6 electrolyte. Charge: CC/CV mode, Cut off 4.3V, 0.01 C, Discharge: CC mode, Cut off 2.5 V, Initial cycles: 0.1 C / 2 cycle, Temperature: 30 °C, Main cycle: 1 C Temperature: 60 °C

Acknowledgements. This study is supported by GteX Project (JPMJGX23S3).

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Poly(ionic liquid)-based Solid-state Electrolyte for High Performance Lithium Metal Batteries

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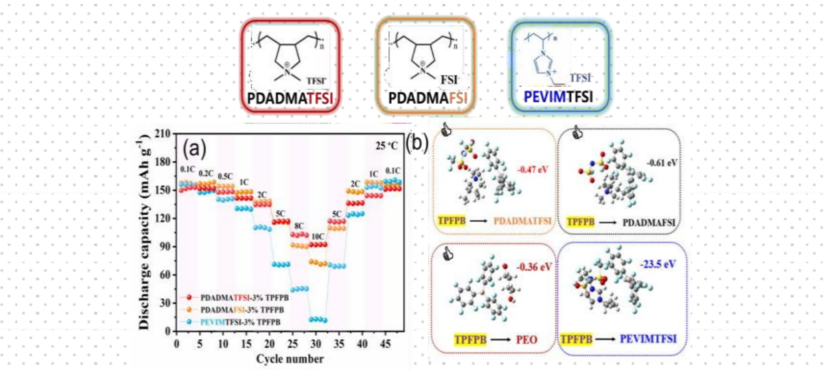
Solid polymer electrolytes (SPE) usually present low ionic conductivity and poor anti-oxidation resistance. which significantly restricts their applications in high-voltage solid-state lithium metal batteries. Recently, we employed molecular engineering method to modify the microstructure of poly(ionic liquid)-based solid-state electrolyte through adjusting the ratio of crystalline to amorphous regions. Firstly, Poly(Ionic Liquid)-based random Copolymers (CPIL) with rigid-flexible segments are successfully synthesized using cross-liked copolymerization reactions by precisely adjusting the ratio of 1-vinyl-3-ethylimidazolium bis(trifluoromethylsulfonyl)imide soft segment to 1-vinyl-3-ethylimidazolium hexafluorophosphate hard segment. As a result, the solid-state $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$/CPIL/Li batteries exhibit an initial discharge capacity of 159.3 mAh g^{-1} and a superior capacity retention of 70.8% after 600 cycles at 1 C.[1]

Secondly, the tris(pentafluorophenyl) boron (TPFPB) is incorporated as an highly effective additive into a poly(ionic liquid)-based solid-state composite polymer electrolyte (CPE) to realize SSLMBs with enhanced high rate performance. The theoretical calculation and experimental analysis demonstrated that the TPFPB serves as an anion immobilizing agent and a modifier of the electrode/electrolyte interphase. In consideration of the role played by TPFPB in PEO-based polymer electrolytes, it is evident that TPFPB is a multifunctional additive suitable for a variety of polymer systems. Its effectiveness is not contingent upon the functional groups of the polymer, but rather, it is determined by the adsorption energy of the polymer (Figure 1). When the adsorption energy between TPFPB and the polymer falls between −0.36 eV and −0.61 eV, TPFPB is capable of functioning in the solid polymer electrolyte. In a notable advancement, the ionic conductivity, lithium transport kinetics, and electrochemical stability of CPE have been significantly enhanced.[2]

Finally, we propose the incorporation of covalent organic framework colloid (COF-C) as an effective modifying agent into SPEs, with the aim of regulating lithium transport and constructing stable electrolyte-electrode interphases. The interaction of COF-C with anions of poly(ionic liquid) has been shown to restrict the growth of PIL spherical crystals and enhance the amorphous area of the electrolyte. As a result, the rational design of SPEs facilitates reaching an ion conductivity of 2.70×10^{-4} S cm^{-1} (25 °C). The solid- state Li/PIL-COF-C/$LiFePO_4$ batteries demonstrate exceptional cycle stability, evidenced by a notable discharge specific capacity of 142.4 mAh g^{-1} at 1 C, along with a commendable capacity retention of 93.1% following 500 cycles.[3]



Figures 1 a) Rate capacities of LFP/Li cells with CPE-3, PDADMAFSI-3%TPFPB and PEVIMTFSI-3%TPFPB at 25°C. b) Adsorption energy of TPFPB with PDADMATFSI, PDADMAFSI, PVEIMTFSI and PEO.

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All-Solid-State Lithium Metal Batteries Integrating Ni-Rich NCM Cathodes and Halide-Based Solid Electrolytes

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All-solid-state Li-ion batteries (ASSLIBs), which replace traditional organic liquid electrolytes (LEs) with solid electrolytes (SEs), are gaining extensive momentum in the development of energy storage technologies. ASSLIBs not only ensure safer operation because of the non-flammable nature and robustness of SEs but also enable the utilization of Li metal anode and bipolar electrode design to enhance battery energy density. However, several challenges persist, such as the kinetic hindrance originating from insufficient interfacial contact between rigid solids, which significantly affects the actual performance of ASSLIBs. Maintaining intimate interfacial contact between SSE and cathode active material (CAM) during ASSLIB operation is particularly challenging due to the different chemo-mechanical responses of these two components to (de)lithiation. Large lattice/volume variations of high-capacity CAMs upon charge-discharge could readily result in extensive interfacial debonding with the surrounding SE matrices, leading to reduced ionic conduction across the interface and higher polarization and severe voltage hysteresis.

Li_3InCl_6 (LIC) is a promising SE because of its high Li-ion conductivities, extraordinary high-voltage stability, and preparation feasibility at low synthesis temperatures. However, its brittle nature is one major concern for its compatibility with equally brittle layered NCM oxide cathodes. Ni-rich NCM cathodes are major CAMs for large-format LIB applications, because of their high specific capacities and lithiation redox potentials, and are known to suffer notable lattice/volume variations during (de)lithiation. This paper reports our recent research in addressing these compatibility challenges. A novel synthesis process of LIC was successfully developed not only to enhances close contact between the two components but also induces interfacial bonding (Figure 1), which substantially reinforces the interface's mechanical robustness to thereby facilitate long-term operation of the composite cathode under low cell assembling and operation stacking pressures.

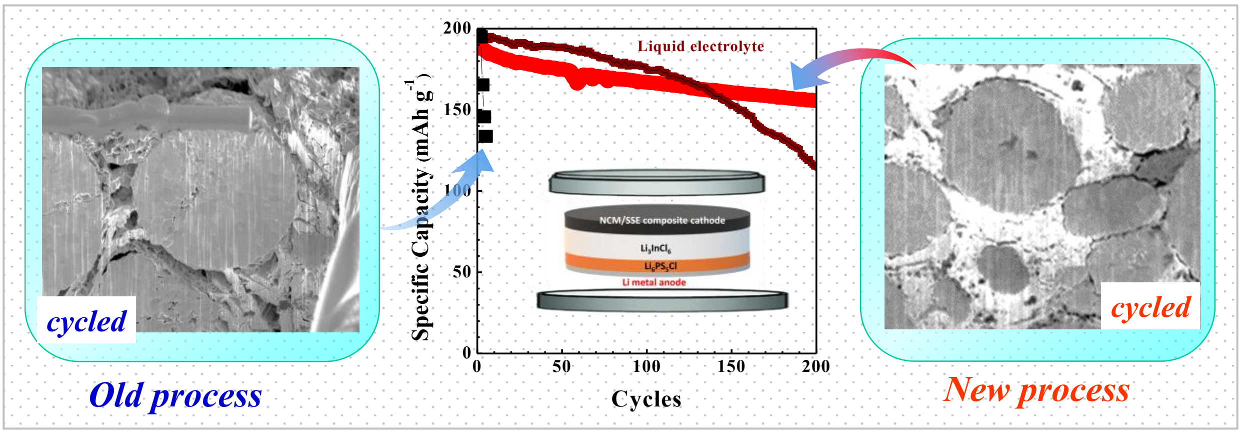

Figure 1. Comparison of NCM-LIC-Li ASSLIBs with different processing methods.

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Nanostructured High-performance Lithium Insertion Materials for Practical Battery Applications

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Ni-enriched layered materials are widely used as electrode materials in Li-ion batteries for electric vehicle applications. Stoichiometric $LiNiO_2$, which utilizes the cationic Ni^{3+}/Ni^{4+} redox couple, is an ideal electrode material. However, its practical applications is hindered by gradual capacity degradation at the high voltage region, primarily due to Ni ion migration.[1] Recently, the critical role of non-stoichiometry and anti-site defects in $LiNiO_2$ has been highlighted. Through defects engineering, highly reversible pure Ni-based layered materials without metal substitution have been successfully developed.[1]

Another important challenge is the development of practical, high-energy Co-/Ni-free Mn-based positive electrode materials, which are essential for the widespread adoption of cost-effective electric vehicles. Nanostructured Mn-based electrode materials have emerged as promising candidates for this purpose.[2, 3] However, these materials are generally synthesized by high-energy milling, a process unsuitable for large-scale production. More recently, nanostructured $LiMnO_2$ with high-energy density (~800 Wh kg^{-1}) has been successfully synthesized through a conventional calcination process, indicating its potential for economical electric vehicle applications.[4]

To realize safe and high-energy Li-ion batteries, the use of solid electrolytes has become a critical strategy. Nevertheless, the inevitable volume changes of electrode materials during cycling pose challenges in maintaining a stable electrode-electrolyte interface. A recently developed nanostructured cation-disordered rocksalt oxide demonstrates a dimensionally invariable character, enabling excellent electrochemical reversibility with solid electrolytes.[5]

These results highlight the importance of nanostructured lithium insertion materials for practical development of high-performance Li-ion batteries.

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Mn-rich layered cathode materials for lithium and sodium intercalation

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In exploring the frontier of high-energy-density cathode materials for lithium-ion batteries, substantial progress has been made by fine-tuning the composition of Ni-rich cathodes tailored for operation to deliver high capacity. Equally promising are Li-rich cathode materials, which leverage the novel mechanism of oxygen-redox chemistry to achieve enhanced capacities. Nonetheless, the practical realization of these capacities remains elusive, falling short of the desired benchmarks. In this work, we pioneer Mn-based Co- free and Ni-less high capacity cathode material, $Li_{0.75}[Li_{0.15}Ni_{0.15}Mn_{0.7}]O_2$ ionic exchanged from $Na_{0.75}[Li_{0.15}Ni_{0.15}Mn_{0.7}]O_2$.1 This material emerges as an O_2-type layered structure, distinguished by honeycomb ordering within the transition-metal layer, as confirmed by comprehensive neutron and X-ray studies and extensive electrostatic screening. This unique structural integrity facilitates the delivery of an exceptional quantity of Li^+ ions via the O^{2-}/O^{n-} redox, circumventing oxygen release and phase transition. The de/lithiation process enables delivery of a substantial reversible capacity of ~284 mAh $(g\text{-oxide})^{-1}$ (956 Wh $(kg\text{-oxide})^{-1}$). Moreover, this structural and chemical stability contributes to an acceptable cycling stability for 500 cycles in full cells to highlight the feasibility of Mn-based Co-free and Ni-less composition, providing improved thermal stability with reduced exothermic heat generation. This investigation marks a pivotal advancement in lithium layered cathode materials.

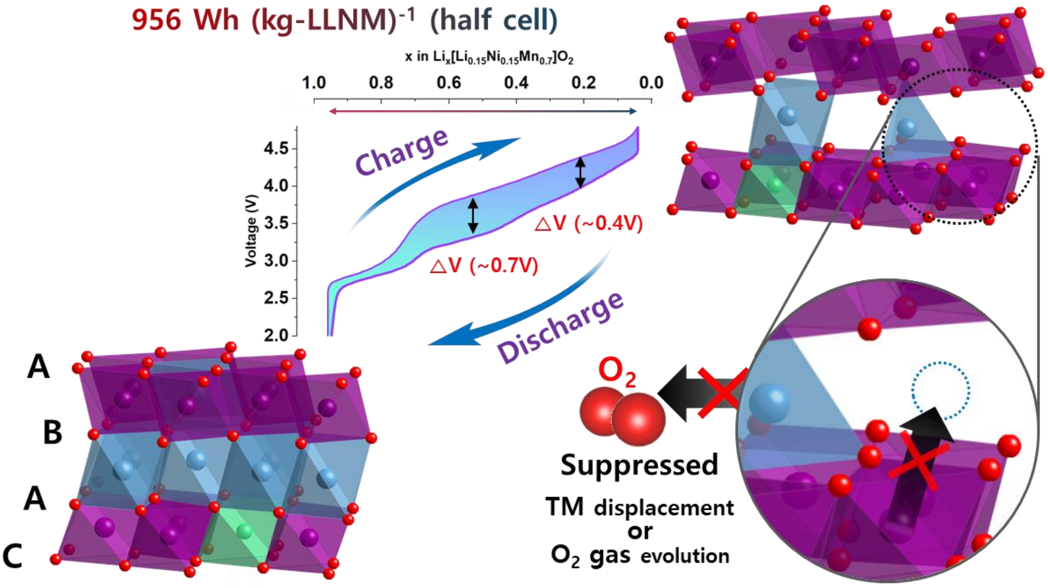

Figure. 1. Illustration of the characteristics of O2 type Li0.75[Li0.15Ni0.15Mn0.7]O2.

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From Materials Science to Market: Recent Progress in Na-Ion Batteries

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Since 2005, we have been challenged to develop new materials for sustainable batteries that are free from costly and toxic metals such as Co, Li, Cu, and Ni. Herein, we study on new materials for sodium-ion and potassium-ion batteries showing a comparable energy density to modern Li-ion batteries.

For attaining high-energy Na-ion batteries, we must develop high-capacity, high-voltage, and highly reversible electrode materials that can be combined with stable, wide electrochemical window electrolytes. Our group has demonstrated high performance hard carbons as promising negative electrode materials which were synthesized via newly developed MgO and ZnO-template methods. These hard carbons show a high reversible capacity exceeding 400 mAh/g, low working potential, fast de/insertion rates and a high initial Coulombic efficiency (ca. 90 %) in Na-half cells. For the positive electrode, layered oxides of the O3-type $Na[Ni,Mn,Ti,Fe]O_2$ have been optimized for high performance. Thus, we could prepare Na-ion full cells based on hard carbon // layered oxide to successfully exhibit a high energy density cell comparable to the Li-ion cells based on graphite // LiFePO4. On the basis of Li- and Na-ion chemistries, we have also succeeded in further expanding the future outlook for K-ion batteries. This includes several critical aspects such as: (1) highly reversible potassium insertion into graphite, (2) new potassium insertion materials of layered oxides and coordination/polyanionic compounds, and (3) development of improved electrolytes and additives for attaining long life K-ion batteries, We will review the Na-ion and K-ion chemistries and discuss their opportunities for sustainable battery technologies and future perspective.

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INVITED SPEAKERS

Phosphate cathode materials for lithium-ion batteries and methods for their improvement

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Phosphate cathode materials are a major alternative to oxide compounds as lithium-ion battery (LIB) cathodes, primarily due to the success story of lithium iron phosphate $LiFePO_4$, often referred to as LFP. The main difference between phosphate materials and oxide ones is the presence of phosphate (PO_4) or pyrophosphate (P_2O_7) groups, which form a reliable structural framework and "bind" oxygen anions. Due to these factors, phosphate-based materials demonstrate stable cycling over thousands of charge-discharge cycles, the ability to quickly charge or discharge, as well as increased thermal stability, i.e. safety of use. Currently, LFP has become the basis of an entire direction both in research activities and in the field of LIB industry - actively developing and extremely promising. However, the issue of increasing the specific energy density of batteries with the transition from oxide materials to LFP arises very acutely, and today there are three main ways to solve it: 1) increasing energy density by replacing part or all of Fe with Mn, with an increase in the average cell voltage from 3.4 V vs. Li/Li^+ for LFP to 4.1 V vs. Li/Li^+ for $LiMnPO_4$ (LMP), 2) improving the density of deposition of active layers and increasing the proportion of active material in the total mass of the battery and 3) transition to solid electrolyte and metal lithium (or so-called "anodeless" systems) at the anode.

The report discusses the results of the main ways to achieve these goals. In particular, the use of the solvothermal method for the synthesis of $Li(Fe,Mn)PO_4$ phosphates in combination with spray drying makes it possible to obtain powders of cathode materials with a fairly high tap density, and the use of water-based binders and single-walled carbon nanotubes improves the electrochemical properties of materials even with a high mass fraction of phosphate in the electrode composite and a load of more than 3 mAh/cm^2. In addition, the report discusses the fundamental difference between LFP and LMP in terms of synthesis and their electrochemical properties. Particularly, to optimize experimental conditions for the synthesis and post-processing of mixed $Li(Fe,Mn)PO_4$ phosphates, we systematically investigated the solvothermal synthesis of $LiFePO_4$ (LFP) and $LiMnPO_4$ (LMP) using water or 1:1 mixtures of water with ethylene glycol, diethylene glycol, or propylene glycol as solvents. LMP consistently formed smaller particles than LFP under identical synthesis conditions. Furthermore, LMP particle size showed significantly less dependence on the solvent composition compared to LFP. Despite this, the co-solvent choice affected the electrochemical properties of LMP, with diethylene glycol yielding the best performance. Using this co-solvent, we synthesized well-crystallized $LiFe_{0.5}Mn_{0.5}PO_4$ (LFMP) nanoparticles exhibiting a fairly high capacity, although with a low initial tap density. Subsequent spray drying increased the LFMP tap density by 70% (from 0.7 to 1.2 g cm^{-3}). Electrodes prepared with water-based binder (carboxymethyl cellulose + styrene-butadiene rubber) and containing 95 wt% active material demonstrated excellent electrochemical performance, delivering a reversible capacity of 150 mAh/g with 89% retention after 300 cycles at a 1C current density.

Acknowledgements. This work was supported by the Russian Science Foundation (Grant No. 24-13-00107).

Electrolytes and interphases in low temperature lithium batteries

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In recent years, lithium deposition on graphite has garnered significant attention. Numerous studies have investigated changes in the internal structure of electrolytes, aiming to optimize the coordination environment around Li^+ by adjusting solvent and lithium salt combinations [1]. The introduction of Helmholtz layer theory has further clarified the impact of solvation structure on the electrode surface. However, the impact of the solvation structure on the electronic behavior at the electrode surface is often overlooked. Li^+ insertion into graphite is essentially an electron transfer process. To this end, we investigated the impact of different solvation structures on the electronic behavior of the graphite electrode surface using anion-poor/rich electrolytes. To bridge the gap between microscopic research and macroscopic interfacial dynamics regulation. We also defined the Electron Migration Potential Energy (EMPE) as a parameter to quantify the interface electronic exchange capability. This parameter assesses the electronic exchange capability of the graphite surface and reveals the effects of solvent structural differences on electron acquire and loss characteristics. Analysis of this parameter reveals a strong correlation between the designed electrolyte systems and both theoretical calculations and experimental results. This study provides new insights into the benefits of anion-rich solvation structures and proposes potential directions for future theoretical research.

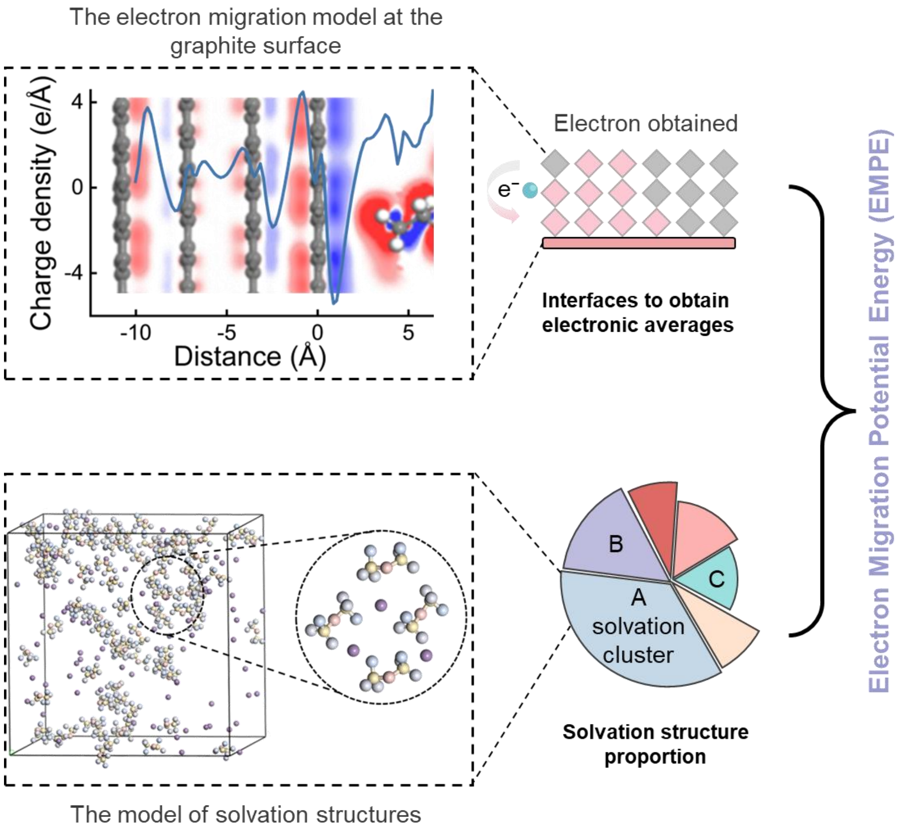

Figure 1. Schematic diagram of EMPE formula.

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Molten Salt Intermediate Energy Storage in a Hybrid Energy System with Multiple Nuclear Power Plants and Multiple Energy Use

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Multiple small modular or micro nuclear reactors maybe economically more feasible than one large size nuclear power plant in some markets. Hybrid and integrated energy systems may at the same site also include multiple energy sources such as solar, wind, nuclear, gas; as well as multiple energy uses such as to produce electricity, steam, hydrogen, or as industrial heat. Load-following capability is hence expected to be a feature in new and advanced small and micro nuclear reactors. However, load following may lead to reduced operational efficiency of nuclear power plants. One approach to decouple the operations of such nuclear power plants from the demand signal is by introducing an intermediate thermal energy storage system. Such an energy storage system can isolate the operations of the nuclear power plant from the rapid fluctuations of the energy demand signal. It can simultaneously also act as means to increase the power available over and above the rated reactor power (to satisfy peak energy demand) for limited periods of time. We will discuss different energy storage options, their control dynamics, and economic feasibility.

Identifying Hidden Trends in Complex Data to Design Best Metal-Organic-Framework Catalysts for Oxygen Evolution Reaction

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Metal-organic frameworks (MOFs) hold great promise in catalyzing the oxygen evolution reaction (OER) due to their high surface area, tunable pore size, structural diversity, stability, and functionalization potential. Moreover, the well-defined catalytic sites make the rational design of MOF catalysts plausible. However, the structure-activity relationship for MOFs remains elusive due to complex interplay between electronic structure and catalytic properties. In this study, we developed a novel artificial-intelligence (AI) approach combining first-principles calculations, machine learning, and data mining to perform high-throughput screening of doped MOFs with TDC ligands to find materials with low OER overpotential. We demonstrate how symbolic regression can be used to find physics-rich features for machine learning to improve model transferrability. Also, a data-mining algorithm was developed to find subgroups of materials that fall out of trend but have non-optimal performance and can therefore be safely removed to improve accuracy of machine-learning model for “interesting” candidates (Figure 1).

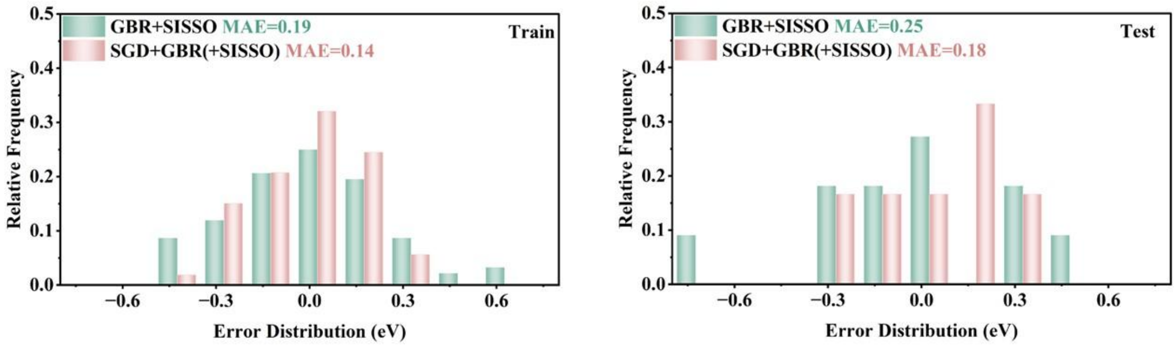

Figure 1: Error distributions for train (right) and test (left) datasets for machine-learning models without and with identified out-of-trend subgroup removed.

Using the developed AI model, we conducted high-throughput screening of more than 800 catalysts, identifying NiFe-TDC, CoIr-TDC, and CoNi-TDC as a highly active OER catalyst. Following the predictions, NiFe-TDC catalyst was synthesized, having overpotential 0.186 V at current 10 mA cm^{-2} and exceptional long-term stability. The outstanding performance of the catalyst is explained by an unusual one-dimensional structure and high oxidation state of active catalyst phase at the reaction conditions. The observed trends in catalytic activity are consistent with feature importance analysis for the AI model, and detailed analysis of electronic structure.

AI/ML for Discovery in the Nuclear Domain

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Deep machine learning is used as a tool for data-driven modeling which in the nuclear domain finds applications to reactor operations, maintenance, diagnostics, prognostics and data brevity. For instance, Physics-Informed Neural Networks (PINNs) can model reactor transients and increase the efficiency of operations through anticipatory control. However, as with all machine learning, development of a PINNs involves laborious and time-consuming training, testing and validation in order to have trustworthy outcomes. Can AI help us accelerate and possibly transfer such learning? The conventional view of AI as a property of machines must be revised to allow for AI that is, actionable, interpretable and, more importantly, transferable. In this way, AI becomes more than a data-driven modeling tool – it can become an instrument of scientific discovery, not unlike the microscope or the telescope. We will examine issues surrounding deep machine learning and AI for scientific discovery along with possibilities to contribute to discovery of new reactor materials. We will discuss theoretical issues and empirical findings from research at Purdue using PUR-1, the first fully digital I&C reactor operational in the US.

Short Bio

Lefteri H. Tsoukalas is the founding director of Purdue’s Center for Intelligent Energy Systems (CiENS) and a professor at Purdue University. He has over three decades of experience in developing AI/ML methods with over 300 publications including the textbooks Fuzzy and Neural Approaches in Engineering (co-authored with Robert E. Uhrig, Wiley, 1997); Fuzzy Logic: Applications in Artificial Intelligence, Big Data, and Machine Learning (McGraw Hill, 2023); and, Energy Transitions: The AI-Energy Nexus (World Scientific, 2025).

Dr. Tsoukalas has served in several advisory and consulting capacities including at the OECD-NEA; the International Atomic Energy Agency (IAEA); the Agency for Science, Technology and Research (ASTAR) of Singapore; and the Secretariat of Research and Technology (GSRT) of Greece. Dr. Tsoukalas is a Fellow of the American Nuclear Society and the 2009 recipient of the Humboldt Prize, Germany’s highest honor for international scientists.

Working Mechanism and Materials Design of Thermoresponsive Electrolytes

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This research focuses on high-energy-density lithium-metal batteries, addressing key issues such as the inadequate safety of liquid electrolytes and the poor interfacial contact and low ionic conductivity of intrinsically safe solid-state electrolytes. A novel thermoresponsive electrolyte system is proposed that maintains favorable liquid-solid interfacial properties during normal operation. Still, it rapidly solidifies under thermal safety hazards, enhancing the battery's intrinsic safety while balancing cycle life and safety. Specifically, this study introduces a host-guest electrolyte system as an internal safety switch for lithium-metal batteries. Upon exposure to thermal risks, the liquid electrolyte swiftly forms a thermally stable gel polymer electrolyte, thereby improving safety without compromising cycle stability. To mitigate safety risks associated with parasitic reactions from residual solvents under extreme conditions, a thermoresponsive mono-solvent electrolyte is further developed. This electrolyte transforms into a solid-polymer electrolyte during high-temperature abuse, significantly enhancing both the battery's lifespan and safety. For lithium-sulfur batteries, a smart thermoresponsive solid electrolyte interphase is designed. During normal operation, lithium iodide additives in the electrolyte accelerate desolvation and construct a highly conductive interface, facilitating lithium-ion transport and deposition. Upon thermal abuse, lithium iodide, lithium polysulfides, and lithium oxides react to form a dense perovskite layer on the lithium surface, suppressing exothermic reactions and increasing the thermal runaway initiation temperature. These intelligent strategies offer innovative and effective solutions for developing safe, long-life, high-energy-density lithium-metal batteries.

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Toward Safer and Cheaper Batteries: Phosphate-Based Cathodes for Li^+ and Na^+ Ion Technologies

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In recent decades, the energy market has undergone a profound transformation driven by three key trends: decarbonization, electrification, and digitalization. The growing demand for clean, renewable energy to combat climate change has led to a rapid expansion of renewable power sources. However, their intermittent nature has made energy storage solutions essential. Among these, rechargeable lithium-ion batteries (LiBs) have become the dominant technology across a range of applications, from consumer electronics to electric vehicles and solar energy storage.

The performance of LiBs is largely determined by their cathode materials, making the development of suitable cathodes critical for enabling future large-scale energy storage. Polyanionic compounds have emerged as promising candidates due to their high operating voltage, excellent structural stability, enhanced safety, low cost, and environmental sustainability. Despite some commercial success, polyanionic cathodes still face challenges such as limited electronic conductivity, suboptimal reversible capacity, and poor rate performance—factors that hinder their broader adoption. To address these issues, various strategies have been explored, including structural engineering, ion doping, surface coating, and electrolyte optimization.

This presentation will explore the significance and key challenges of phosphate-based cathode materials for lithium- and sodium-ion batteries. Recent advancements in several in-house developed cathode materials will also be discussed.

Keywords: Li-ions Batteries; Na-ion Batteries; Fluorophosphates; Cathode materials

Acknowledgements. The R&D activities presented in this work were supported by OCP's Strategic Business Units: Manufacturing and SPS.

Investigation of Anionic and Cationic Redox Chemistry in P3-type $Na_{0.67}[Zn_{0.3}Mn_{0.7}]O_2$ Layered Sodium Cathode

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Oxygen redox-based layered cathode materials, such as P2/P3-types $Na_x[A_yMn_{1-y}]O_2$ (A=Li, Mg, Zn, vacancy), are of great importance for realizing high-energy-density sodium-ion batteries (SIBs). In this work, we introduce an oxygen redox-based layered cathode material, P3-type $Na_{0.67}[Zn_{0.3}Mn_{0.7}]O_2$ (NZMO) with Na-O-Zn local configuration (Figure 1 a,b). We investigate the NZMO material using a variety of methods such as galvanostatic potential cycling (Figure c), *operando*-X-ray diffraction (o-XDR) (Figure d,e), X-ray absorption near-edge structure (XANES), X-ray photoelectron spectroscopy (XPS), nuclear magnetic resonance (^{23}Na NMR), atomic-resolution scanning transmission electron microscopy (STEM) and differential electrochemical mass spectroscopy (DEMS). Moreover, a combined approach of lattice and surface modifications is employed for the P3-type $Na_{0.67}[Zn_{0.3}Mn_{0.7}]O_2$ (NZMO) cathode using a $NaTi_2(PO_4)_3$ (NTP) ionic conductor to improve the long-term stability of NZMO. The Ti integration stabilizes the oxide lattice, and the P-based moieties boost surface stability. This leads to superior long-term capacity retention and charge transfer efficiency. The NTP layer is instrumental in maintaining interfacial stability under high-voltage conditions, counteracting lattice oxygen redox triggered by Zn migration from the transition metal layer to the Na layer in the oxidized $Na_x[Zn_{0.3}Mn_{0.7}]O_2$ O/P phase. The enhanced electrochemical performance can be attributed to improved surface stability, boosted ionic conductivity, and stabilization of the anionic O^{2}-/$(O_2)^{n-}$ redox process at high voltage. Moreover, the NTP layer suppresses electrolyte-induced surface reactions by extracting HF and H_2O, while Ti integration maintains c-axis variations. Ab initio molecular dynamics simulations additionally reveal that the NTP layer serves as a protective shield, preventing electrolyte degradation and HF^- triggered metal ion dissolution, thereby ensuring durability. These findings substantiate the efficacy of NTP coatings in elevating sodium-ion battery cathode material performance.

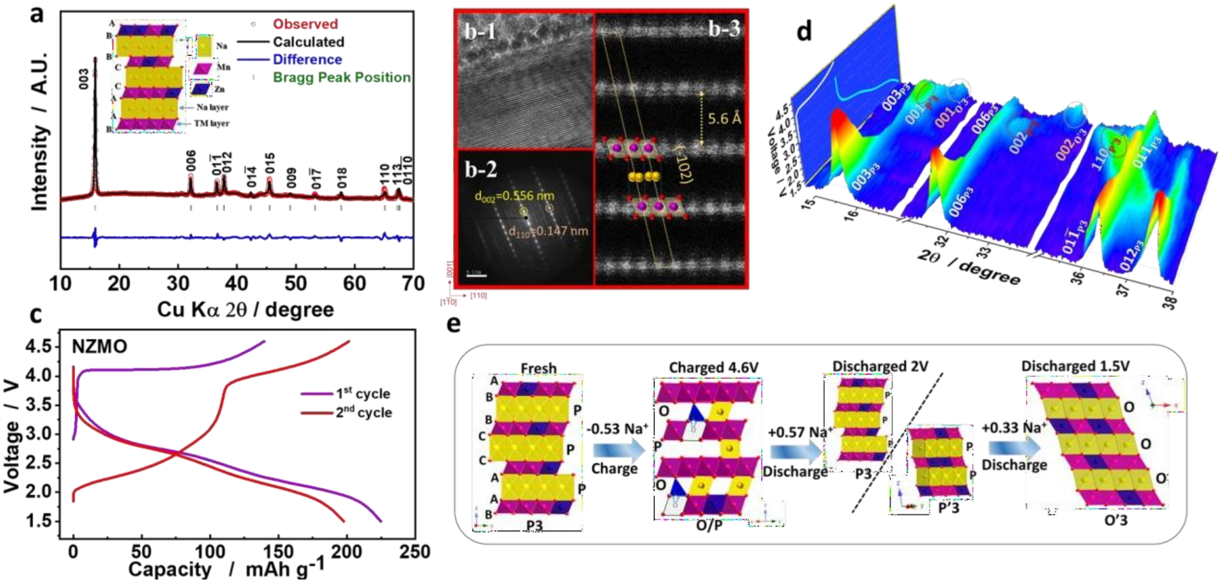

Figure 1. (a) Rietveld refinement of XRD pattern for P3-$Na_{0.67}[Zn_{0.3}Mn_{0.7}]O_2$ (NZMO) (inset: crystal structure of NZMO) (b) STEM- HAADF images of NZMO at fresh state (c) The 1st and 2nd charge-discharge cycles of NZMO tested at 13 mA g^{-1} (0.05 C) (d) Operando-XRD pattern of NZMO electrode during the first charge-discharge cycle (e) Schematic image of structural evolution of NZMO during de/sodiation.

Underground Hydrogen Storage Sites Selection using Fuzzy Logic

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The global push for renewable and clean energy sources is driven by the urgent need to reduce greenhouse gas emissions and combat climate change. Countries around the world are transitioning from traditional fossil fuels to renewable energy sources like solar, wind, and hydropower [1]. This transition is also driven by the desire to strengthen energy security, and create the long-term sustainability of energy systems. However, these energy sources face limitations as they primarily produce electricity, restricting their versatility as energy carriers for various applications [2]. Since many transportation vehicles cannot solely run on electricity, the demand for chemical fuels and feedstocks remains essential.

Hydrogen is emerging as a key energy carrier in the shift towards de-carbonization, offering to store and deliver clean energy across multiple sectors (applications). It can serve as a fuel or be converted to electricity using devices like fuel cells. As a zero-carbon gas, hydrogen emits no greenhouse gases during combustion, provided it is produced from non-fossil fuel feedstocks [3]. When adopted on a large scale as both an energy carrier and a replacement for chemical fuels, hydrogen has the potential to effectively decarbonize the entire fuel supply chain.

At present, compressed hydrogen storage is the most developed and widely used approach, offering simple operation and efficient hydrogen storage and release. There are two main options for storing compressed hydrogen: above-ground storage in hydrogen cylinders and underground storage in porous formations such as depleted gas fields, saline aquifers, or mined salt chambers, commonly known as salt caverns [4, 5]. Storing hydrogen in cylinders on a large scale requires significant ground space, leading to high construction costs [6]. Additionally, due to hydrogen's high flammability, any leaks or potential explosions pose serious safety risks, potentially causing extensive damage to nearby urban areas. Consequently, underground storage is often viewed as a safer and more cost-effective alternative for large-scale hydrogen storage. Various geological formations are used for gas storage, each offering unique advantages for UHS [4, 5].

This study explores the potential for underground hydrogen storage (UHS) in Central Asia, focusing on the evaluation of depleted gas fields, salt caverns, and aquifers as storage options. Utilizing the Fuzzy TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) methodology, a systematic multi-criteria decision-making approach, the research identifies and ranks critical technical, economic, and geological criteria to determine the most suitable UHS sites.

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Large-Scale Production of High-Temperature Superconducting Wires for Fusion, Energy, and Transportation Applications

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The promise of compact fusion energy systems, such as tokamaks and stellarators, increasingly relies on high-temperature superconductors (HTS) to generate and sustain powerful magnetic fields. Faraday Factory Japan (FFJ) has established the world's largest production of second-generation HTS (2G-HTS) wires, with a state-of-the-art facility producing over 3,000 km of superconducting tape annually. These tapes, based on $YBa_2Cu_3O_{6+x}$ (YBCO) materials, are designed to operate in extreme conditions of magnetic fields up to 20 T and temperatures of 4.2 K or 20 K making them ideal for fusion applications.

Beyond fusion, 2G-HTS wires have already found practical use in superconducting cables, fault current limiters, and inductive heaters. There is also strong and growing interest in their use for next-generation transportation systems including electric aircrafts, where they could serve in superconducting generators and motors, as well as in levitation magnets for maglev trains. These diverse applications impose distinct requirements on operating temperature, magnetic field, and critical current density, requireing to tailor superconducting wires for each individual application.

The unprecedented production scale achieved by FFJ has provided extensive datasets that enable systematic refinement of manufacturing processes, quality control, and material properties. Recent developments include precise control of oxygen non- stoichiometry to tune carrier concentration, engineering of artificial pinning landscapes to enhance in-field performance, and optimization of buffer architectures for improved lattice matching and mechanical integrity. Understanding and engineering the real structure of HTS materials, including the landscape of pinning centers, has become of extraordinary importance to meet these varied application demands.

This presentation will highlight how industrial-scale production informs materials science and process engineering, and how these insights drive ongoing improvements in performance, reproducibility, and cost-effectiveness. We aim to demonstrate how HTS technology is transitioning from laboratory-scale developments to enabling real-world solutions across fusion, energy, and transportation sectors.

Nanomaterials and Nanofabrication for Sensing Applications.

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The Recent advancements in nanomaterials and nanofabrication are transforming sensor technology, enabling higher sensitivities, higher integration, and ultra-low power gas sensors and biosensors. In this talk, I will highlight some core microfabrication methods such as lithography, thin-film deposition, and in-situ material growth that used to develop functional nanostructures and microdevices. Drawing on my research, I will share examples on CuO nanowires and graphene-based sensors **[1-4]**, where tailored electronic structures unlock exceptional gas sensitivity and biosensing selectivity. I will also talk about suspended SiO_2 membranes and their versatile utility that supports everything from in-situ material development and Seebeck-effect measurements to emerging quantum-transduction applications.

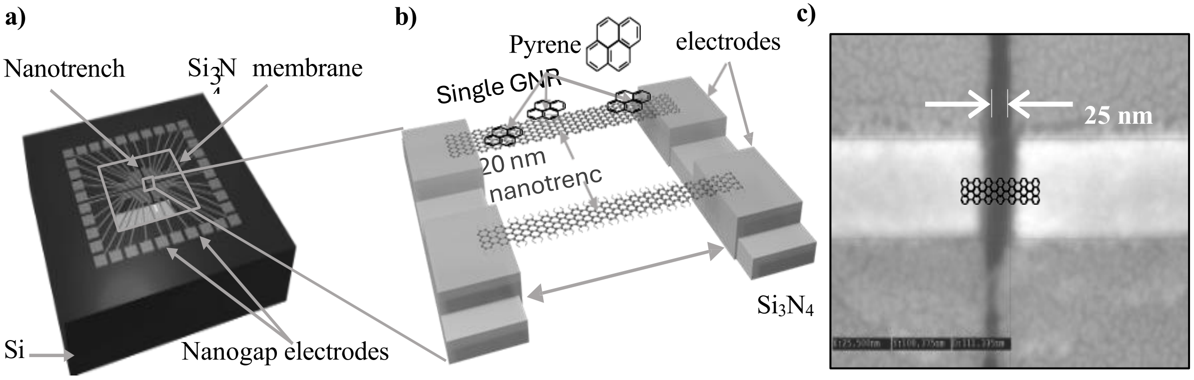

Figure 1. An example of a proposed sensor system to be discussed in this presentation:

a) Schematic of nanoscale integration using atomically precise graphene nanoribbons (GNRs);
b) Two gas sensors based on single GNRs—with and without pyrene functionalization;
c) SEM image of nanogap electrodes fabricated using the proposed method with single GNR

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DEVELOPMENT OF ADVANCED NANOCOMPOSITE MATERIALS FOR ENVIRONMENTAL PROTECTION AND INDUSTRIAL APPLICATIONS

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All of the below work was carried out at the Institute of Combustion Problems, the main directions being in the field of combustion and the production of nanomaterials for various purposes.

Synthesis of nanocarbon sorbents for water purification from heavy metal ions. The synthesis of nanocarbon sorbents for water purification from heavy metal ions involves innovative approaches in material science and environmental engineering. Nanocarbon materials, such as carbon nanotubes, graphene, and activated carbon, exhibit exceptional adsorption properties due to their high surface area (~3000 m^2/g), porosity, and surface chemistry. These sorbents effectively capture heavy metal ions from water sources, mitigating environmental pollution and providing a sustainable solution for water treatment challenges [1].

Synthesis of composites based on semiconductor metal oxides and carbon nanostructures for the detection of toxic gases. These composites leverage the unique properties of metal oxide nanoparticles and carbon nanostructures such as carbon nanotubes or graphene to detect toxic gases through interactions with gas molecules on their surfaces. This opens up promising avenues for gas detection technologies [2].

Gas generator compositions based on activated carbon from a gas mask for destruction of rocks. Gas generator compositions utilizing activated carbon from gas masks offer a novel approach to rock destruction. Activated carbon, known for its high porosity and adsorption properties, serves as a key component in these compositions. Through controlled combustion or chemical reactions, gases generated from the activated carbon interact with rocks, facilitating their disintegration. This innovative method presents a promising alternative for rock demolition in various applications, including mining and construction [3].

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Ultraclean 2D hole system on silicon with mobility beyond the state of the art

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High carrier mobility is the fundamental criterion for frontier fundamental research and for realising advanced classical and quantum electronic devices, as it directly impacts elementary charge transport, device speed performance, energy efficiency and heat dissipation issues. In particular, the development of high-mobility hole two-dimensional (2D) systems epitaxially grown on a silicon (Si) substrate is emerging as a critical enabler for next-generation low-power electronics, quantum computing, and spin-based information processing. Hole transport in the valence band, particularly in low-dimensional systems, offers unique advantages over electron-based platforms — including strong spin–orbit coupling, suppressed hyperfine interaction, and efficient all-electrical spin control.[1-4] These properties make holes particularly attractive for scalable quantum bit architectures and energy-efficient classical logic devices.

However, realising high hole mobilities within a Si-compatible platform has historically faced fundamental and technological barriers. In contrast to electrons, holes experience stronger effective mass anisotropy and enhanced scattering from interfaces and defects, demanding exceptionally high material quality and careful control over strain, composition, and heterointerface abruptness. Traditional III–V hole systems, while capable of high mobility,[5,6] lack compatibility with ultra- large-scale integration (ULSI) and complementary metal oxide semiconductor (CMOS) infrastructure, limiting their practical deployment. Despite their remarkable intrinsic properties, the technological deployment of high-mobility materials has been constrained by challenges in manufacturability and platform compatibility. Si, by contrast, underpins the global semiconductor ecosystem, supported by decades of process optimisation, mature fabrication infrastructure, and robust supply chains. Therefore, the ability to grow high-quality, defect-suppressed epitaxial layers of high-mobility semiconductors directly on a Si substrate is of profound significance. It enables monolithic integration with CMOS technologies, facilitates wafer-scale scalability up to 300 mm diameter, and bridges the gap between emerging materials and industrial adoption.

Compressively strained germanium (cs-Ge) epitaxially grown on Si (cs-GoS) has recently emerged as a leading platform for next-generation quantum devices and electronics, combining unprecedented hole mobility with full compatibility with Si semiconductor technology.[7-9]

In this talk, the results of comprehensive research leading to a record-breaking hole mobility, among all semiconductors epitaxially grown on Si substrate, achieving 7.15×106 $cm^2V^{-1}s^{-1}$ in cs-GoS heterostructure, will be presented.

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Health Risk Implications of Photocatalytic Indoor Air Purification: Challenges and Mitigation Strategies

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Photocatalytic oxidation (PCO) has been widely considered as a promising technology for the removal of volatile organic compounds (VOCs) from indoor air, owing to its ability to degrade organic pollutants under ambient conditions using UV light. However, growing experimental evidence indicates that this process can result in the formation of toxic by-products, including formaldehyde, acetaldehyde, and benzene—compounds with well-established carcinogenic and non-carcinogenic health risks even at low concentrations, casting doubt on the applicability of PCO-based air purification systems for indoor environments.

Despite the expanding literature on PCO systems, the human health implications arising from exposure to by-products remain underexplored. Most investigations focus on VOC removal efficiency and/or catalyst development, while toxicological risk assessment is rarely addressed. At the same time, the increasing commercialization and deployment of PCO-based air purifiers in residential homes underscores the importance and urgency of in-depth safety evaluations of PCO devices under realistic operating conditions.

In this work, recent studies were systematically reviewed, with a focus on compiling data on the concentrations of key by-products measured both at the outlet of PCO reactors and within indoor test chambers under environmentally relevant conditions (e.g., 50% relative humidity, sub-ppm VOC concentrations). Health risks were determined using quantitative risk metrics, including the hazard quotient (HQ), hazard index (HI), and excess lifetime cancer risk (CR). In most cases, calculated values for hazard indicators exceeded acceptable thresholds, highlighting potential health hazards associated with by-product exposure. The study further identifies critical factors influencing the formation of by-products, including catalyst characteristics, airflow rate, relative humidity, UV light wavelength and intensity, and the nature of VOC pollutants. Evidence-based mitigation strategies are proposed, including the optimization of photocatalyst design, improvement of reactor configuration, incorporation of secondary treatment units (e.g., adsorption filters), and the use of predictive modeling tools—both mechanistic and data-driven (i.e., AI-based models). Our findings suggest that although PCO can be a viable approach for indoor air purification, its routine use in residential settings may be premature without comprehensive risk assessment analyses and targeted risk mitigation measures.

Study on the construction of high safety and rapid ion conduction gel polymer lithium battery

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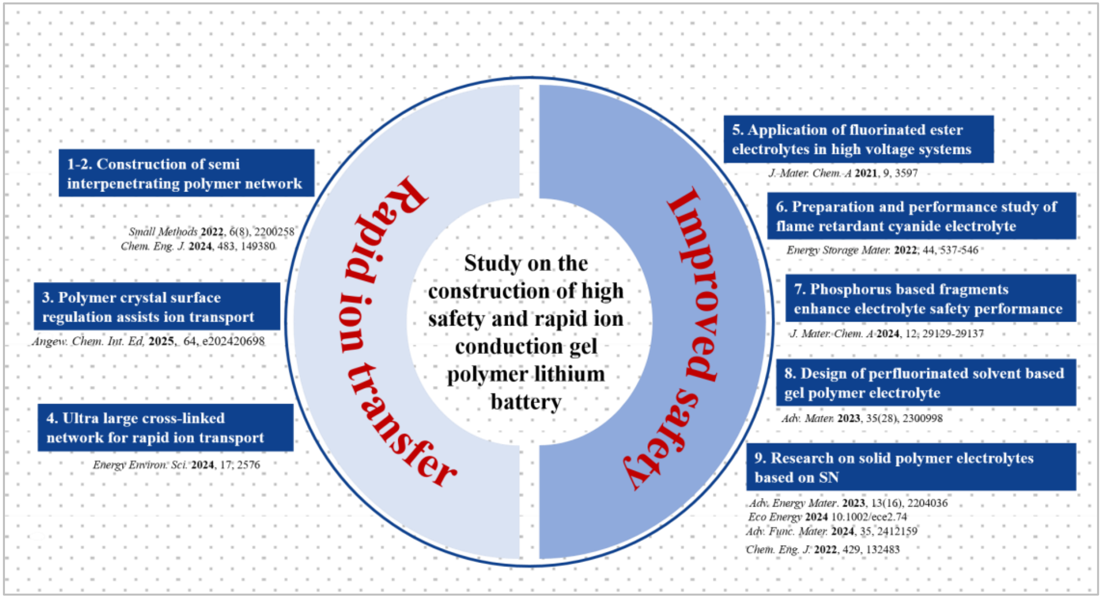
Solid-state electrolytes represent a promising alternative to mitigate the safety concerns associated with liquid electrolytes in lithium batteries. Among solid state electrolytes, polymer based systems demonstrate superior scalability potential owing to exceptional mechanical robustness and favorable electrode/electrolyte interfacial compatibility. Nevertheless, fundamental constraints in lithium- ion transport kinetics coupled with persistent safety vulnerabilities under extreme operating conditions present critical bottlenecks to their practical development.

To address the challenges of weak lithium-ion dissociation and discontinuous matrix structure of polyvinylidene fluoride hexafluoropropylene, two distinct strategies are proposed: constructing a semi-interpenetrating polymer network and regulating crystal facet/phase structures via solvent-processing method. These approaches collectively establish additional lithium-ion transport pathways, thereby achieving improved ion transport characteristics within the electrolyte. Furthermore, the cyclic stability of ether- based sulfidized polyacrylonitrile batteries is remarkably enhanced by designing an oversized cross-linked polymer electrolyte network. In terms of safety, flame-retardant fluoro-, cyano-, and phosphorus-containing moieties are in situ introduced into the polymer electrolyte matrix. Concurrently, the solid content is progressively increased to mitigate combustion risks. The resulting polymer electrolyte exhibit exceptional fire resistance, withstanding continuous exposure to an open flame for 190 s without ignition. Furthermore, gel polymer electrolytes are prepared using fluoroethylene carbonate (FEC) as the sole solvent. The charged pouch cell exhibit a temperature below 50°C during nail penetration tests and showed no thermal runaway in accelerating rate calorimetry (ARC) tests. These works offer valuable insights for constructing high safety, rapid ion conduction polymer lithium batteries.



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Machine Learning (ML) Approach Utilizing FTIR spectroscopy Data for Accurate and Efficient Identification of Organic Components

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Accurate and efficient identification of chemical compounds is essential in various scientific and industrial applications. Vibrational spectroscopy techniques such as Fourier Transform Infrared (FTIR) Spectroscopy have proven invaluable in chemical analysis and materials characterization [1]. In the context of state-of-the-art automated high-throughput experiments, automated data analysis methods become necessary given that manual analysis is time-consuming and prone to human error [2].

This study presents a machine learning approach to identify organic constituents in FTIR spectra. A Random Forest classifier serves as the core modeling technique, and we introduce a novel feature extraction method that effectively captures the signature peaks of each compound, thereby enhancing the model's efficacy. Evaluation on a training set yielded a remarkably low training log loss and an overall accuracy of 98%. The resulting confusion matrix indicates good alignment between predicted and actual classes, with only minor discrepancies observed for certain variants of some few compounds (likely due to labeling inconsistencies). These results demonstrate that our model not only improves identification accuracy but also reduces computational complexity, making it a robust tool for rapid compound detection and facilitating interpretation of FTIR spectra. Our model holds significant potential for applications in environmental monitoring, food analysis, and clinical diagnostics, and chemical manufacturing, where swift and dependable compound analysis is paramount.

Keywords: Machine Learning, FTIR Spectroscopy, Random Forest, Compound Identification, Feature Extraction, Spectral Analysis

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ORAL PRESANTATION

Investigation of Intense Pulsed High-Current Ion Beam interaction with ITO and FTO coatings

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Intense pulsed ion beam (IPIB) irradiation is a highly effective technique for altering material properties through rapid heating and cooling process [1]. This study investigates the impact of IPIB irradiation on different materials, particularly transparent conductive oxides such as FTO (Fluorine-doped Tin Oxide) and ITO (Indium Tin Oxide), and focuses on the modification on their structural, optical, and electrical properties [1].

Our research group at the Innovative Nazarbayev University Research Accelerator (INURA) the radiation resistance of FTO using pulsed high-current ion beams with nanosecond durations. Those materials used in solar cells, touchscreens, and smart windows [2]. The results show that the IPIB irradiation on FTO thin films maintain both transparency and conductivity up to 23 A/cm² (which corresponds to a total fluence of 1013 ions/cm²) and performs strong resistance to radiation, making them suitable for advanced space applications [2].

In the plasmonic active SERS experiments, a simple gold sputter deposition method was used to creates Au thin film (3 nm) on FTO substrate. The IPIB irradiation at 15 A/cm² converted gold thin films into gold nanoparticles (AuNPs) without destroying FTO substrate. The SERS experiments were performed to detect prototype methylene blue (MB) dye.

These samples are characterized using AFM, SEM, UV-Vis absorption spectroscopy, XRD, and Raman spectroscopy to evaluate the amplification of Raman signals. As a result, a low-concentration methylene blue solution (10^{-5} M) will enhance the Raman signal. The highest SERS sensitivity was achieved on Au NPs/FTO substrates fabricated with IPIB irradiation .

This research was supported by the Ministry of Science and Higher Education of the Republic of Kazakhstan grant №AP19674485

Keywords: Flourine doped tin-oxide, surface enhance raman scattering, Intense pulsed ion beam

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Application of Track-Etched membrane decorated by Fe_3O_4-Cr(azide)MIL101 MOF in the sorption of U(VI) ions from aqueous media

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Polyethylene terephthalate-based track-etched membranes (PET TeM) are a unique class of polymers with high porosity and active surface area [1]. Composite track-etched membranes have increased scientific interest due to their potential applications in catalysis, sorption, sensors, and energy sources [2]. With the development of the nuclear industry in Kazakhstan, the need to develop methods for purification from radioactive elements such as uranium has increased. The presence of uranium and its compounds in the aquatic environment and drinking water can increase cancer, kidney illnesses, and genetic mutations [3]. Earlier published literature reported on the effective sorption of uranium compounds using the metal-organic frameworks MIL101 based on chromium (MOF) [4]. We propose an effective method for the sorption of uranyl cations from aqueous media using composite track-etched membranes based on PET TeMs modified with metal-organic frameworks based on chromium MIL101. For successful deposition of MOF onto the surface of the polymer template, we suggest using the click chemistry approach. Firstly, we modified the PET TeM surface by reversible addition-fragmentation chain transfer (RAFT) polymerization of n-vinyl formamide, followed by alkali hydrolysis to obtain the polyvinyl amine (PVAm). The amine group concentration was 26.87 $nmole \cdot cm^{-2}$, after 10 min at 0.1M NaOH. Finally, we found optimal conditions for grafting alkyne groups on PVAm-PET TeMs by coupling amine groups with propionic acid. FTIR analysis allowed to confirm the presence of alkyne functional groups at 2200 cm^{-1} shift. In parallel, we synthesized chromium-based MIL101 MOF and modified it by a post-synthetic strategy to form azide groups instead of amine groups in the MOF as described in [5]. The peak at 2120 cm^{-1} is related to the azide groups in MOF. Integration of Fe^3O^4 nanoparticles (NPs) was performed by two strategies. The first one was based on the reduction of Fe^3O^4 on the prepared MOF. At the same time, the second approach was based on the reduction of Fe_3O_4 NPs on the MOF-modified PET TeMs. In both cases, we used a similar reducing agent – NH_4OH solution. To achieve the deposition of Cr-MOF and Fe_3O_4-Cr-MOF on PET TeM, we varied the concentration of copper catalyst and reaction time. After that, prepared adsorbents were analyzed on SEM-EDX analysis. According to the elemental analysis, the concentration of Cr was around 2.5% and Fe was around 5%, including both sides of the PET TeM. The XRD and XPS analyses demonstrated the presence of magnetite - Fe_3O_4. BET analysis was used to describe the pore size distribution. Sorption is a pH-dependent process; consequently, we defined the pHdzt value for the prepared sorbents, which was 6.4. The time was varied from 6 h to 96 h. The uranyl ion concentration for the experiment was 100 ppm, and all aliquots were measured by ICP – MS. To describe the sorption process, we used the Dubinin-Radushkevich, Freundlich, and Elovich isotherm models.

Acknowledgements. This study (grant IRN AP 19676626) was funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan. Saniya Rakisheva is grateful for a grant from the International Innovation Center of Nanotechnology of the CIS, JINR, Russia.

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Low-Permeability Behavior of Chromium Tailings: A Barrier Material Perspective

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The global mining industry generates substantial volumes of waste, predominantly stored in large-scale tailings storage facilities (TSFs). Ensuring the stability and long-term performance of these structures requires a thorough understanding of the geotechnical behavior of mine tailings. This study investigates the physical and mechanical properties of fine-grained chromium tailings through comprehensive laboratory testing, including particle size distribution, compaction, consolidation, permeability, and shear strength. The tailings were classified as well-graded sand with silt (ML) under the Unified Soil Classification System (USCS), with notably higher dry density compared to typical natural soils. Consolidation tests indicated moderate compressibility, shedding light on deformation behavior under load. The material exhibited very low permeability, posing challenges for seepage and pore pressure control in TSFs. Shear strength parameters confirmed the material's stable mechanical behavior under shear loading. Beyond geotechnical applications, the study also considers the potential of such mine tailings for environmental technologies, particularly as low-permeability media in subsurface containment barriers for carbon capture, utilization, and storage (CCUS) systems. These findings not only contribute to safer and more sustainable TSF design but also open avenues for integrating tailings into broader environmental engineering frameworks.

Tailoring Carrier Suppression in a-IGZO/SiO_x/a-IGZO Ultrathin Laminates

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In this report, we synthesised ultrathin multilayer IGZO/SiO_x/a-IGZO films using radio frequency (RF) magnetron co-sputtering. We systematically varied the SiO_x layer thickness from 1 to 7 nm, while keeping the a-IGZO layer thickness constant. The study focused on how changing the SiO_x thickness influenced the films' electrical characteristics. Notably, electrical performance declined with SiO_x layers up to 3 nm thick but improved as the thickness increased to 7 nm. X-ray photoelectron spectroscopy (XPS) showed that the overall oxygen bonding and chemical structures of the multilayers remained stable. However, it was revealed that the 2 nm SiO_x layer (with $x \approx 1.5$) was nonstoichiometric. We found evidence of Fowler–Nordheim (FN) tunneling across films with different SiO_x thicknesses. Oxygen content was identified as a key factor modifying electron trap states within the SiO_x layer, which facilitated to reduce a reduction in charge carriers. By optimising the oxygen flow during the deposition process, we successfully treated a drop in charge carrier concentration in the a-IGZO20nm/SiO_x(2nm)/a-IGZO10nm and a-IGZO20nm/SiO_x(3nm)/a-IGZO10nm structures. Notably, the ultrathin SiO_x layers in these multilayer structures act as efficient carrier suppression layers, offering a promising alternative to conventional doping methods for tuning electrical properties of materials.

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Multifunctional hybrid conducting polymers and their nanocomposites for highly stable and flexible micro-supercapacitors

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Recent studies underscore the superior performance of three-dimensional (3D) materials over their two-dimensional (2D) counterparts, primarily due to enhanced mass transport, ion diffusion, and storage capabilities. However, the transition from 2D to 3D structures often introduces limitations caused by insulating cross-linkers or templating agents used during synthesis. Additionally, the performance of these materials can be restricted by the nature of their porosity. While continuously porous structures are ideal for fluid and gas diffusion, their synthesis remains a significant challenge.

3D porous nanocomposites based on conducting polymers exhibit exceptional electrocatalytic and diffusion properties, owing to their high specific surface area, increased pore volume, improved charge mobility, and efficient ion and gas transport. This work presents a novel, template-free, one-step, and scalable polymerization strategy based on bicontinuous microemulsion (BME) for synthesizing continuously porous hybrid conducting polymers (HPPs). This method eliminates the need for external templates or matrices while preserving the advantageous properties of the resulting materials.

The unique interpenetrating cross-linked structure of the BME system acts as a self-assembling matrix for monomers, enabling the formation of stable and functionally enhanced porous composites. The use of a nonionic surfactant further stabilizes the process by reducing interfacial tension, ensuring uniform nanoparticle dispersion, and enabling homogeneous current distribution.

This cost-effective and scalable platform supports the synthesis of binary and ternary hybrid conducting polymer composites, where each component retains its intrinsic functionality while being seamlessly integrated into the polymer matrix. This technique provides a versatile route to engineer multifunctional polymer materials with unique morphologies, suitable for applications in flexible energy storage devices, wearable electronics, gas sensors, electrocatalysis, and hydrogen evolution reactions. Our polypyrrole-cobalt oxide (PPy-CoO) composite was studied as an electrode for micro-pseudocapacitor and showed outstanding stability results with 106% capacitance retention under 180 bending and 83% after 10000 bending cycles. The devices demonstrate excellent areal capacitance of 30.58 mF cm^{-2}, energy density of 4.22 µWh cm^{-2}, and power density of 75.97 µW cm^{-2} at 0.2 mA cm^{-2}.

In-situ optical monitoring and morphological evolution of silicon nanowires grown on faceted $Al_2O_3(0001)$ substrates via the ATLAS deposition technique

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Silicon nanowires are attractive building blocks for nano-optoelectronics and energy harvesting, but practical deployment requires catalyst-free routes that guarantee nanometre-scale thickness control and complementary metal–oxide–semiconductor (CMOS) compatibility [1]. Here, we fabricate laterally ordered Si NW arrays on thermally faceted $Al_2O_3(0001)$ by accelerated thermal loading and sublimation (ATLAS) physical vapour deposition, whose source geometry and dedicated vacuum chamber enable real-time tracking of their evolution via in situ reflectance anisotropy spectroscopy (RAS). During deposition, the main $\pi \rightarrow \pi^*$ RAS peak red-shifts linearly at –0.035 eV nm^{-1}, yielding an intrinsic optical thickness calibrator that enables closed-loop growth control with ±0.3 nm precision. Vacuum annealing reveals three regimes reversible quantum-confinement relaxation below ≈485 °C; a crystallisation window centred at

≈640 °C, where the peak blue-shifts by up to 0.15 eV and $\Delta r/r$ triples, signalling solid-phase epitaxy; and collapse of optical anisotropy above 700 °C, attributed to capillarity-driven nanowire reflow. Atomic force microscopy confirms these optical signatures, showing the mean wire height drops from ≈10 nm to <3 nm throughout the crystallisation window, with complete disappearance beyond 800 °C. Correlating RAS peak energy, anisotropy magnitude, and AFM morphology furnishes a process map that flags an optimum growth end-point at 3.90 eV (≈11 nm height) and sets a safe backend-processing ceiling below 640 °C. Because sapphire is insulating, transparent, and CMOS-compatible, the resulting silicon nanowires platform is directly integrable into photonic and sensing architectures. More broadly, the RAS-guided methodology extends earlier surface-optical studies [3] and offers a scalable blueprint for sub-nanometre precision engineering of one-dimensional silicon nanostructures on non-Si substrates [2].

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Development of the New 1D Nickel-Rich NCM Cathode for Lithium-Ion Battery

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The most promising energy system is considered to be lithium-ion batteries (LIBs), which are used in a variety of consumer electronics including laptops, mobile phones, cameras, and electric cars because of its low cost, high energy density, superior performance, and extended lifespan [1]. From the perspective of cathode materials, layered $LiMO_2$ oxides, where M is a combination of Ni, Mn, and Co—known as NCMs, or lithium nickel cobalt manganese oxides—are regarded as a potential next-generation cathode material for LIBs because of their higher specific capacity (more than 150 mAh g^{-1}) and thermal stability. Overall, the chemical properties of LIBs are always evolving [2].

In this work, free-standing one dimensional (1D) NCM811 ($LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$) cathode was fabricated by electrospinning tecnique for LIBs and the conditions of sintering process for obtaining successful structure of the material were optimized. The resultant 1D NCM811 samples' morphology, physico-chemical characteristics, and structure were examined using scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction analysis (XRD), inductively coupled plasma optical emission spectroscopy (ICP-OES), and thermogravimetric analysis (TGA). The XRD patterns of the material under examination showed a set of peaks that exactly matched the NCM811 diffraction patterns, while indicating low cation mixing degree I(003)/I(104) = 1.64. Cyclic voltammetry (CV) and galvanostatic charge-discharge cycling (GDC) were used to examine the electrochemical characterizations of 1D NCM811. Obtained electrochemical properties of the 1D NCM811 demonstrated that compared to conventional slurry casted electrodes (electrode-specific capacity-49 mAh g^{-1}), the free-standing electrodes with low cation mixing degree have stable electrode-specific capacity about 150-160 mAh g^{-1} within the initial 20 cycles. Hence, it is highly expected that the results will offer some new ideas for the creation of free-standing 1D NCM811 cathodes and morphological modification, which will aid in the logical design and manufacturing of LIBs with high energy densities.

Acknowledgments. This research was funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. AP19679855).

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Optimizing hybrid carbon matrices: synthesis and electrochemical characterization of buckwheat-derived HC and SWCNT composites for Li-S batteries

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Lithium-sulfur (Li-S) batteries are promising candidates for next-generation energy storage due to their high theoretical capacity and environmental sustainability. However, challenges such as poor electrical conductivity, polysulfide dissolution, and volume expansion hinder their commercial viability [1-3]. In this work, we developed hybrid cathode composites using hard carbon (HC) derived from buckwheat waste and single-walled carbon nanotubes (SWCNTs) to address these limitations.

Electrochemical testing revealed that an optimal SWCNT content of 6 wt% significantly enhanced conductivity, sulfur utilization, and capacity retention, delivering an initial capacity of 1144 mAh g^{-1} with excellent cycling stability. Furthermore, HC synthesized at 1000 °C showed the highest initial capacity (1259.89 mAh g^{-1}), whereas HC prepared at 1200 °C exhibited superior long-term stability (retaining 55.31% capacity after 100 cycles). However, HC synthesized at 600 °C provided a favorable balance between performance, energy efficiency, and safety, making it a more practical candidate for large-scale applications. These results highlight the potential of biomass-derived carbon and SWCNT-based hybrid matrices to overcome critical barriers in Li–S battery technology.

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Biomass-derived porous carbon for high-performance hydrogen storage at ambient and cryogenic temperatures

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Hydrogen is considered a promising energy carrier due to its exceptional properties: as the lightest element, it possesses the highest specific energy density - releasing approximately three times more energy than gasoline upon combustion (140 MJ/kg vs. 44 MJ/kg), while producing only water vapor as a byproduct [1]. These characteristics make it an attractive option for decarbonizing energy- intensive sectors. However, the widespread adoption of hydrogen is hindered by challenges related to its efficient and safe storage, necessitating the development of new technologies and solutions to ensure its cost-effective utilization [2]. Biomass-derived porous carbon materials have gained attention as promising adsorbents for hydrogen storage due to their high specific surface area, tunable porosity, and environmental friendliness. Owing to these features, they are actively studied as effective hydrogen carriers, playing a crucial role in the advancement of hydrogen energy technologies [3].

The aim of this study is to synthesize a highly porous carbon material from rice husk biomass for further investigation of its hydrogen sorption capacity. The carbon material was produced via thermochemical activation of pre-carbonized rice husk using KOH as the activating agent. Characterization revealed a high specific surface area of 3386 m2/g, a total pore volume of 1.94 cm^3/g, and an average pore diameter of 2.29 nm. The nitrogen adsorption-desorption isotherm indicated a predominantly microporous structure. Pore size distribution analysis further confirmed the dominance of micropores - a critical feature for efficient hydrogen storage in carbon-based materials. According to pressure-composition-temperature (PCT) measurements carried out at both room and cryogenic temperatures, the highest hydrogen uptake was observed at a pressure of 80 bar: 0.73 wt.% at room temperature and 8.97 wt.% at cryogenic temperature. The highest hydrogen sorption values were observed at the maximum applied pressure of 80 bar, suggesting that the material had not reached full saturation and that the isotherm lacked a distinct plateau. The strong correlation with the Langmuir model indicates that the adsorption predominantly follows a monolayer mechanism, which is typical for microporous materials employed in hydrogen storage applications.

Acknowledgments. This research was funded by the research project OPCRP2024013 “Advanced Porous Carbon Materials for High-Performance Hydrogen Storage: Biomass-Derived, Theoretically-Informed, and Experimental Approach” from the Nazarbayev University.

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Development of a Zn/$LiFePO_4$ Aqueous Battery System with $ZnCl_2$/LiCl Binary Electrolyte for Commercial Applications

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The accelerating global shift toward sustainable energy infrastructures has underscored the urgent need for advanced energy storage technologies that are not only safe and cost-effective but also environmentally benign. Conventional lithium-ion batteries, despite their widespread deployment, depend on flammable organic electrolytes and resource-intensive materials, thereby raising significant safety and ecological concerns. Similarly, while lead-acid batteries offer economic advantages, their inherently low energy density and the environmental hazards associated with toxic lead content limit their broader applicability.

In response, aqueous rechargeable batteries have attracted considerable attention as a compelling alternative, leveraging water-based electrolytes to enhance safety, reduce production costs, and support environmentally sustainable design—all while delivering competitive electrochemical performance [1,2]. Among these, Zn/$LiFePO_4$ rechargeable aqueous hybrid-ion batteries (ReHABs) have emerged as a promising system, synergistically combining the favorable characteristics of zinc and lithium iron phosphate within an aqueous electrolyte environment.

The hybrid-ion configuration, which enables the co-utilization of Zn^{2+} and Li^+ ions in a shared aqueous medium, offers notable improvements in energy density, cycling stability, and intrinsic safety compared to conventional aqueous battery chemistries. The implementation of nonflammable, low-toxicity binary electrolytes—such as $ZnCl_2$/LiCl—further enhances system safety, simplifies manufacturing processes, and aligns with green chemistry principles. As such, Zn/$LiFePO_4$ ReHABs present a viable and sustainable platform for scalable energy storage applications.

Nonetheless, several critical challenges hinder the widespread commercialization of this technology. These include cathode delamination from the current collector, restricted energy density due to limited active material loading, and zinc dendrite formation during repeated cycling, all of which compromise battery performance and long-term stability. Addressing these issues will require concerted efforts in advanced electrode architecture, electrolyte engineering. This research work introduces the Zn/$LiFePO_4$ ReHAB system, emphasizing its strategic advantages while outlining the key scientific and technological innovations needed to establish it as a next-generation solution for safe, sustainable, and high-performance energy storage.

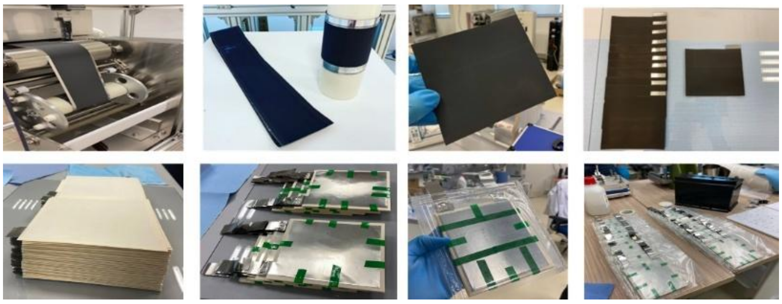

Figure 1. Zn/$LiFePO_4$ battery prototyping

Acknowledgements. This research was funded by the research targeted program #BR21882402 “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.

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Development and Fabrication of Lithium-Ion Battery Pouch Cells Using a Pilot Production Line

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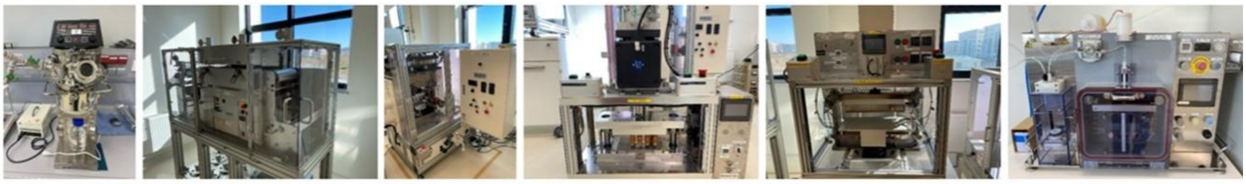
The advancement of lithium-ion battery (LIB) technologies requires not only the discovery of novel materials but also effective upscaling strategies to bridge laboratory research with industrial cell formats. In this work, we report the successful prototyping of LIB pouch cells using a pilot-scale manufacturing line, focusing on the engineering aspects necessary for high-performance and reproducible cell fabrication.

$LiFePO_4$-based cathodes and graphite anodes were systematically optimized with respect to composition, porosity, mass loading, and electrode density to ensure a balance between energy density and mechanical integrity. Key process steps—such as calendaring, electrode punching, stacking, and tab welding—were carefully controlled to minimize variation and improve electrode alignment. Electrolyte formulations were tailored to ensure interfacial compatibility, promoting stable SEI formation while suppressing gas evolution and capacity fade during extended cycling. Additionally, electrolyte filling methods were evaluated to ensure uniform wetting and pressure control within the sealed cells.

Pouch cell design was guided by targeted energy and power requirements, with detailed considerations of electrode dimensions, separator properties, tab positioning, and packaging geometry. All unit operations, including slurry preparation, coating, drying, calendaring, stacking, pouch forming, electrolyte filling, and heat sealing, were performed on an integrated pilot line to simulate scalable production conditions.

The resulting prototype cells exhibited stable electrochemical performance, low variability, and manufacturing consistency. This study highlights the importance of coupling materials development with process engineering to accelerate the transition of LIB technologies from laboratory innovation to industrial readiness.



Slurry mixer
Coating machine
Calendaring machine
Pouch forming machine
3-side sealer
Final sealer

Figure 1. Pilot line for Pouch Cell Production and Assemble Process

Acknowledgements. This research was funded by the research targeted program #BR21882402 “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.

Li-coated poly(ethylene oxide)-poly(vinylidene fluoride-co-hexafluoropropylene)-based membrane as gel polymer electrolyte for lithium-ion batteries

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The growing demand for high-energy-density lithium-ion batteries (LIBs) has accelerated the development of advanced electrolytes that enhance both performance and safety [1][2]. This study introduces an metallic lithium-coated gel-polymer electrolyte (GPE) system based on a poly(ethylene oxide)-poly(vinylidene fluoride-co-hexafluoropropylene) (PEO-PVDF-co-HFP) matrix incorporating 0.5-2.0 wt% graphene oxide (GO) particles (Fig.1 (a)). The GO dopant serves a dual function: its high surface area and oxygen-containing functional groups facilitate improved Li-ion transport while enhancing electrolyte-electrode interfacial interactions [3]. Complementing this design, metallic lithium deposited via magnetron sputtering further boosts electrochemical stability and interfacial compatibility, collectively enabling superior cycling performance. To evaluate the GPE, $ZnO-Zn_3N_2$ thin-film anodes were fabricated by RF reactive magnetron sputtering. The integrated system of Li-coated 1.5wt% GO-PEO-PVDF-co-HFP GPE and $ZnO-Zn_3N_2$ anodes demonstrated exceptional stability. The cell exhibits rapid capacity fade from ~800 mAh g^{-1} (1st cycle) to 350 mAh g^{-1} (5th cycle) during the formation stage, followed by cycling stability with only ~90 mAh g^{-1} total degradation (350 → 260 mAh g^{-1}) over the subsequent 195 cycles (Fig.1 (a)). These results underscore the synergistic effects of the engineered electrolyte-anode interface in facilitating efficient charge transport and prolonged cycle life.

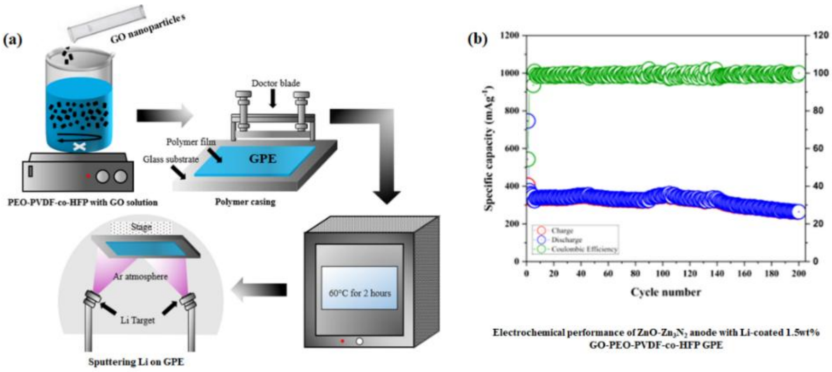

Fig 1: (a) Schematic synthesis of Li-sputtered PVDF-co-HFP-PEO gel polymer electrolyte (GPE) modified with 1.5 wt% graphene oxide (GO), showing polymer matrix preparation with GO incorporation, and metallic Li deposition via magnetron sputtering. (b) Electrochemical performance of $ZnO-Zn_3N_2$/GPE/Li half-cell.

Acknowledgments. This research was funded by the research project AP19680567 “Advanced nanocomposite 3D thin film electrodes for lithium-ion batteries” from the Ministry of Science and Higher Education of the Republic of Kazakhstan.

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Tailoring Mn–Fe–Ni Layered Oxides for High-Performance Sodium-Ion Battery Cathodes

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Sodium-ion batteries (SIBs) are attracting increasing attention for large-scale energy storage due to sodium's abundance and low cost. Layered Na_xMeO_2 (Me = Mn, Fe, Ni) oxides are among the most promising cathode candidates owing to their high theoretical capacity, simple synthesis, and tunable structure. Their structural versatility enables phase engineering between O3- and P2-type frameworks, allowing optimization of sodium diffusion pathways and electrochemical behavior. Moreover, the strategic selection and ratio adjustment of transition metals can enhance redox activity, suppress irreversible phase transitions, and improve cycling stability [1-2].

In this study, a series of P3- and O3-type Na-layered oxides with varying Mn, Fe, and Ni contents were systematically investigated to optimize their phase stability, electrochemical performance, and redox activity. X-ray diffraction and high-resolution transmission electron microscopy confirmed well-developed layered structures with varying degrees of stacking and transition metal ordering. Operando XANES and Mössbauer spectroscopy revealed that Ni^{2+}/Ni^{4+} and Fe^{3+}/Fe^{4+} redox couples dominate charge compensation during cycling, while Mn remains largely inactive but structurally stabilizing. Among the tested compositions, $Na_{0.95}Mn_{0.4}Ni_{0.35}Fe_{0.25}O_2$ exhibited excellent reversible capacity (≈170 mAh g^{-1} at 20 mAg^{-1}) and cycle stability over 100 cycles. These findings align with previous studies demonstrating the importance of redox synergy and transition metal ordering in Na-layered oxides. The work provides valuable insights into the design of cost-effective, high-performance cathode materials for sustainable sodium-ion energy storage.

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Analysis of morphological features of binder-free metal electrodes for a sodium-ion battery

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Currently, lithium-ion batteries are the dominant technology in the field of energy storage devices. However, the finite nature of lithium resources encourages scientists to search for alternative energy storage systems. Sodium-ion batteries are one of the most promising candidates. Although carbon-based anodes are the most prevalent [1], their low specific power can not fully sustain high-power cathode materials [2]. One of the promising alternaitves are p-block elements with their alloyng mechanism of sodium storaging [3,4]. These alloying-type materials have a high energy density with acceptable cycling stability. One of the major issues is the large volume expansion of these materials during cycling, which has the tendency to lead to high mechanical degradation and loss of electrical contact. One of the possible ways to reduce these issues is to obtain such anodes by physical vapor deposition (PVD) techniques [5]. This method enables the production of 100% active electrodes without binders or electrochemically inactive carbon additives.

In this work, we investigated vacuum metal deposition as a tool for producing mechanically stable and high-performance anode materials for sodium-ion batteries. Particular focus was placed on the morphological evolution of deposited metal films and cycling-induced structures. X-ray diffraction analysis confirmed the formation of bismuth films with preferred (003) orientation. Scanning electron microscopy (SEM) found that the as-deposited films consisted of well-ordered crystallites with sizes ranging from 50 to 300 nm. Following electrochemical cycling, these films experienced a drastic transformation: the original dense morphology gave way to very porous, sponge-type structures composed of a random network of interconnected pores and residual crystallites. The sponge type is an expression of extensive volume change in the course of alloying/dealloying and is vital in sustaining mechanical stability and pathways of ion conduction on sustained service. In situ XRD measurements also revealed that the original crystallographic texture of the films was lost following the first charge/discharge cycle, consistent with observation of widespread structural rearrangement. Electrochemical testing in CR2032-type cells with an ether-based electrolyte demonstrated stable performance: following 600 cycles at 1C, bismuth retained a capacity of 370 mAh/g (from an initial 384 mAh/g), and lead retained 425 mAh/g (initially 484 mAh/g). At high levels (10C), bismuth films maintained 90% of its capacity , but there was a 52% loss in capacity with lead. Saturated-cell Bi||NaSICON and Pb||NaSICON stacks supported the functional viability of these sponge-like anode architectures. The formation of a porous framework and stability by cycling appear to buffer volumetric change and offer electrochemical contact, resulting in stable long-term cycling.

The report will place particular emphasis on the morphological evolution of the anode films, emphasizing the formation, structure, and functional significance of the sponge-like architectures that form upon cycling. The morphological features of the resulting anode materials will be studied in detail both before and after cycling. For this purpose, atomic force microscopy data, micrographs of the films produced, as well as EDX data on various phase transitions will be discussed. Electrochemical cycling data for various loads of anode material, as well as system operation at low temperatures, will be presented to represent all the operating possibilities of the system. Finally, alloying caused by cycling will be graphically illustrated in an attempt to show visually the evolution of the material volume.

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Effect of Ni and Fe redox transformations on electrochemical properties of O3-$NaFe_{1-x-y}Ni_xMn_yO_2$ materials as cathodes for Na-ion batteries

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Na-ion batteries are considered as future alternative to Li-ion due to low cost and wide abundance of sodium. In turn, O3-type $NaNi_{1-x-y}Fe_xMn_yO_2$ cathode materials are an excellent alternative to Li-containing layered oxides such as $LiCoO_2$ and its derivatives [1]. These compounds are isostructural to α-$NaFeO_2$ (s.g. $R\bar{3}m$) with Ni, Fe, and Mn in $NaNi_{1/3}Fe_{1/3}Mn_{1/3}O_2$ being in the 2+, 3+, and 4+ oxidation states, respectively. The possibility of using Fe^{3+}/Fe^{4+} redox pair in cathode materials for SIBs is one of the main features of the Na-ion system in contrast to Li-ion. However, the peculiar crystal chemistry of iron cations introduces certain problems in the (de)sodiation process of layered sodium oxides.

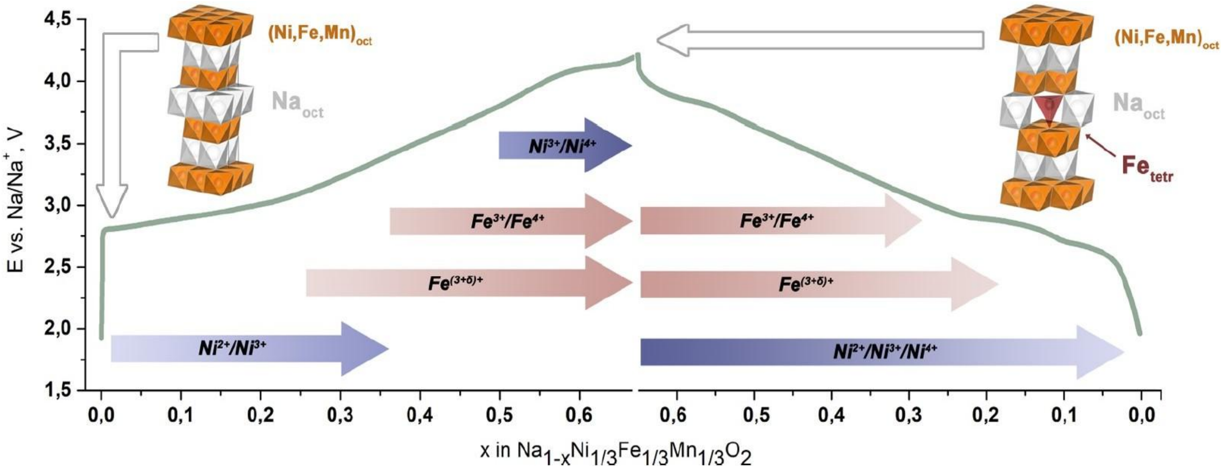

Figure 1. Redox transformations of Fe and Ni cations in O3-$Na_{1-x}Ni_{1/3}Fe_{1/3}Mn_{1/3}O_2$ during charge/discharge.

Here, we present operando and ex situ studies of O3-$NaNi_{1/3}Fe_{1/3}Mn_{1/3}O_2$ using powder X-ray diffraction (PXRD) and X-Ray absorption spectroscopy (XAS) combined with ^{57}Fe Mössbauer spectroscopy (MS). Our approach revealed the sequence of the redox transitions and allowed us to observe ≈12% of the Fe^{4+} cations that occupied tetrahedral positions. To the best of our knowledge, this is the first instance of Mossbauer spectroscopy detecting the presence of iron cations in the sodium layer in $NaMO_2$ oxides, as well as the first indication of its oxidation state [2]. Furthermore, we accurately analyzed the effect of the Mn/Fe/Ni ratio on the iron migration and kinetics of Na^+ (de)intercalation in O3-$NaMO_2$ oxides [1]. Our study demonstrates that Mn has a clear positive effect on such important electrochemical properties as cyclic stability and thermal safety. Increase in Ni amount reduces average working potential and the kinetics of sodium (de)intercalation, and lowers the onset temperature of thermal decomposition, which makes nickel-rich oxides potentially dangerous for large size power sources. Excess of iron also reduces the cyclic stability and leads to large heat release from the charged electrode. We are planning to use our approach to investigate the effect of some other possible dopants on iron migration in O3-$NaMO_2$ oxides.

Acknowledgements. This work was supported by the Russian Science Foundation (grant no. 25-43-00007).

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Sodium and iron mixed phosphate cathode materials: phase composition and electrochemical performance relations

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An increasing demand for electricity in the modern world leads to the necessity of production of efficient energy storage systems. One of the promising energy storage systems are sodium-ion batteries (SIBs). A key task for the successful commercialization of SIBs is the development of new efficient electrode materials, which will allow the production of batteries with specified electrochemical characteristics.

Sodium-iron mixed phosphate - $Na_4Fe_3(PO_4)_2P_2O_7$ (often referred to as NFPP) is a promising cathode material for SIBs. NFPP attracts attention due to its potential low cost (caused by a wide abundance of the elements in its structure), relatively high Fe^{3+}/Fe^{2+} redox potential, high cycling and thermal stability [1]. One of the key problems related to the implementation of NFPP is that its synthesis is accompanied by the formation of impurities in the resulting samples (namely, $NaFePO_4$ and $Na_2FeP_2O_7$ phases), which impact the electrochemical characteristics of the resulting cathode material [2]. Besides the obvious need for correct identification of impurities, the important step towards further investigation and optimization of NFPP as cathode material is finding a correlation between the type and content of impurity phases and the electrochemical performance of the materials.

In this work we suggest a novel approach to identification and quantitative estimation of peculiar phase activity in multiphase NFPP- based cathode materials using electrochemical data. The approach is based on comparing experimentally obtained galvanostatic curves with model galvanostatic curves derived from quantitative phase analysis based on powder X-ray diffraction (PXRD) data.

NFPP samples were synthesized by sol-gel method using different sodium-to-iron ratios (4:3.0, 4:2.9 and 4:2.8) and different annealing temperatures (400 °C, 500 °C, 600 °C, 700 °C). The phase composition of the obtained samples was analyzed using PXRD. The relative weight content of $NaFePO_4$ and $Na_2FeP_2O_7$ phases in the samples was determined by a structural analysis using Rietveld refinement. The electrochemical characteristics of obtained materials were investigated by galvanostatic charge-discharge in two-electrode cells with sodium metal as counter electrode.

According to PXRD data, the optimal conditions for synthesis of NFPP phase are the following: Na to Fe ratio = 4.0:2.9 and 500 °C or 600 °C as annealing temperature. The quantitative analysis of phase composition showed that the content of the particular impurity phase could be influenced by both the initial compound's stoichiometry and annealing temperature. The obtained values of phase weight fractions were used for further analysis of correlation between materials phase composition and galvanostatic charge-discharge curves profile.

The analysis of the model and experimental curves allowed us to distinguish the three voltage areas which correspond to the activity of different phases: 2.00 – 2.64 V vs Na^+/Na (activity of $NaFePO_4$ and $Na_2FeP_2O_7$), 2.80 – 3.15 V vs Na^+/Na (activity of $Na_2FeP_2O_7$ and NFPP) and 3.15 – 3.40 V vs Na^+/Na (activity of NFPP). The correlation between the weight fraction of the phases in the samples and the discharge curves profile was shown. The analysis of differential capacity curves for both model and experimental data allowed us to separate the impact of $NaFePO_4$ and $Na_2FeP_2O_7$ impurities in 2.0 – 2.6 V voltage area. It was shown that the electrochemical activity of each of the impurities is different for samples obtained by annealing at different temperatures.

Thus, in this work the correlation between the amount of $NaFePO_4$ and $Na_2FeP_2O_7$ impurities in NFPP samples and galvanostatic discharge curves profiles was firstly shown. The implementation of galvanostatic discharge model curves in comparison with experimental data allowed us to distinguish the contribution of NFPP, $NaFePO_4$ and $Na_2FeP_2O_7$ phases into galvanostatic discharge curves profile.

This work was supported by the Russian Science Foundation, project 24-13-00107.

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The new polyanionic $NaMNb(PO_4)_3$ (M=Cr, V) multielectron anode materials for Na-ion batteries based on the $Nb^{5+}/Nb^{4+}/Nb^{3+}$ redox transfer

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Rapid implementation of Na-ion batteries in the new areas of application, such as electric vehicles and large-scale energy storage systems, provokes the evolution of electrode materials towards enhanced safety, sustainability, lifespan, and energy density. In this work we introduce the NASICON-type niobium phosphates $NaCrNb(PO_4)_3$ (**CNP**) and $NaVNb(PO_4)_3$ (**VNP**) as the three-electron anode materials based on the $Nb^{5+}/Nb^{4+}/Nb^{3+}$ and M^{3+}/M^{2+} reversible redox processes [1–2]. Both of the compounds were prepared in the form of submicron particles by the Pechini sol-gel technique followed by a two-step annealing at 400-600°C and 700-850°C in air for **CNP** and in argon flow for **VNP**. $NaMNb(PO_4)_3$ (M=Cr, V) maintain the NASICON framework (S.G. R-3c) without any Nb/M ordering, and sodium ions occupy only Na1 6b position, while the Na2 18e site remains vacant and could be thoroughly filled on sodiation. To improve the electric conductivity of **CNP** powder, the carbon-coated samples were prepared via pyrolysis of polyacrylonitrile with further introduction of single-walled carbon nanotubes (SWCNT), resulted in the materials' conductivity gain of about 7 order of magnitude. The carbon-containing $NaMNb(PO_4)_3/C$ samples were used for electrodes fabrication (80-85 mass.% of the active material).

CNP and **VNP** show a reversible electrochemical activity in the Na-half cell within the 0.8–2.2 V (vs. Na^+/Na) interval. The robust polyanionic NASICON framework maintains a facile sodium diffusion and provides the attractive electrochemical performance. The first-cycle discharge capacities of 168 and 175 $mAh \cdot g^{-1}$ were achieved at 0.1C current rate for **CNP** and **VNP**, respectively, being close to the theoretical value for a $3e^-$ process (178 $mAh \cdot g^{-1}$). The initial Coulombic efficiency (ICE) of 95–98% was reached for both materials. **CNP** renders a discharge capacity of 160 $mAh \cdot g^{-1}$ at 1C rate and retains 82.6% capacity after 300 cycles. **VNP** exhibits an outstanding rate capability delivering the initial discharge capacity of 162 $mAh \cdot g^{-1}$ at 10C rate with a capacity retention of 92.3% after 150 cycles.

Niobium K-egde XANES spectroscopy revealed the Nb^{5+}/Nb^{4+} couple activation at 2.2–1.6 V and the Nb^{4+}/Nb^{3+} one at 1.3–0.8 V, thus supporting the $Nb^{5+}/Nb^{4+}/Nb^{3+}$ multielectron redox transition. The M^{3+}/M^{2+} transfer in both cases occurs at 1.6–1.3 V. Moreover, for **CNP** by chromium K-egde XANES data we elicited a direct proof of the $Cr^{3+} \leftrightarrow Cr^{2+}$ reversible transformation, being the first example of the Cr^{3+}/Cr^{2+} couple activation in the NASICON structure. Operando X-ray powder diffraction study unveiled the single-phase mechanism of sodium (de)intercalation within the intervals of Nb^{5+}/Nb^{4+} and Nb^{4+}/Nb^{3+} activity, while in case of Cr^{3+}/Cr^{2+} a biphasic area was disclosed. The appearance of the biphasic region obviously arises from a Jahn-Teller distortion of $Cr^{2+}O^6$ octahedra and may be responsible for the reduced rate capability of **CNP** comparing to **VNP**. The total cell volume increase on the full sodiation process ($NaMNb(PO_4)_3 + 3Na^+ + 3e- \leftrightarrow Na_4MNb(PO_4)_3$) was found to be about 9%.

Besides improved ICE and rate capability, the high thermal stability in a sodiated form may be considered as an attractive advantage of $NaMNb(PO_4)_3/C$ anode materials comparing to hard carbon ones. Indeed, our DSC experiments unveiled both sodiated **CNP** and **VNP** are stable until the electrolyte decomposition point (292°C for 1M $NaPF_6$ in 1:1 EC:DEC), while for sodiated hard carbon exothermic process starts at already 150°C. Thus, the new $NaMNb(PO_4)_3/C$ anode materials exhibit the clear benefits to be proposed as the high-stable and safe alternative to hard carbon ones, somewhat resembling LTO ($Li_4Ti_5O_{12}$) vs graphite in Li-ion systems.

Acknowledgements. The work was supported by Russian Science Foundation (grant No. 23−13−00071).

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Carbon Nanofibers Embedded with Nickel Phosphide for Enhanced Sulfur Immobilization in Li–S Batteries

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Lithium–sulfur batteries (LSBs) are widely regarded as a highly promising next-generation energy storage system due to their high specific energy density, cost-effectiveness, environmental friendliness, and the natural abundance of sulfur. Despite these advantages, the intrinsic insulating nature of sulfur and the shuttle effect of lithium polysulfides (LiPSs) lead to low active material utilization, poor Coulombic efficiency, and rapid capacity fading, which hinder their practical deployment [1,2]. To address these issues and improve the electrochemical performance of LSBs, numerous strategies have been proposed. In our work, we investigate nickel phosphide/carbon (Ni_xP/C) composite nanofibers as a sulfur host material. The conductive and porous carbon nanofiber framework facilitates efficient sulfur utilization and accommodates volume changes, while the polar Ni_xP nanoparticles enhance electron transport and chemically anchor LiPSs during cycling [3]. These composite nanofibers were synthesized via a one-step electrospinning technique followed by carbothermal reduction, employing polyvinylpyrrolidone (PVP) as the carbon source [4]. Recognizing the significant impact of humidity during electrospinning on nanofiber morphology and properties, we prepared samples at relative humidity levels of 25%, 30%, and 35%, and systematically compared their performance as sulfur hosts. Furthermore, X- ray photoelectron spectroscopy (XPS) was used to study the LiPS adsorption mechanism, as shown in Figure 1a. Among the tested conditions, the nanofibers fabricated at 30% relative humidity delivered the best electrochemical performance, achieving the highest initial discharge capacity of 1344.9 mAh g^{-1} at a current density of 0.1C (Figure 1b).

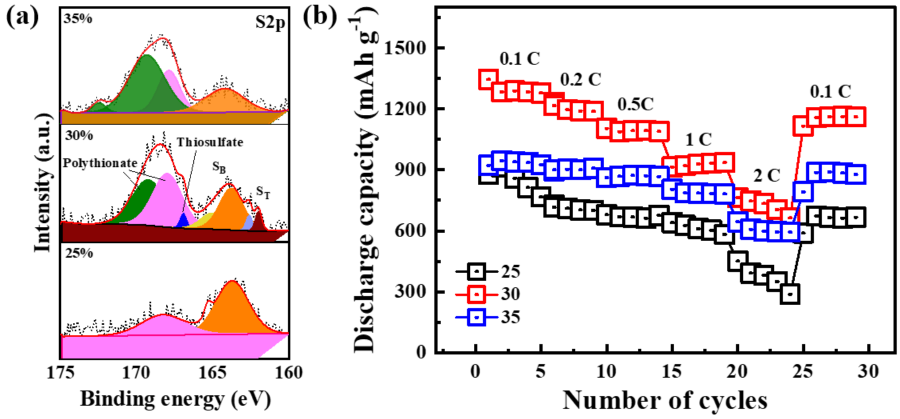

Figure 1. (a) S 2p XPS spectra for Li_2S_6 adsorbed by NixP/C composite nanofibers; (b) rate performance of NixP/C composite nanofibers of different humidity levels.

Acknowledgements. This research was funded by the research targeted program BR21882402 “Development of new material technologies and energy storage systems for a green economy” and project AP19675260 “Development of nanofibrous electrode materials for next-generation lithium-ion batteries” from the Ministry of Science and Higher Education of the Republic of Kazakhstan.

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Influence of electrolyte composition on the photoelectrochemical performance of electrodeposited Bi_2S_3 thin films

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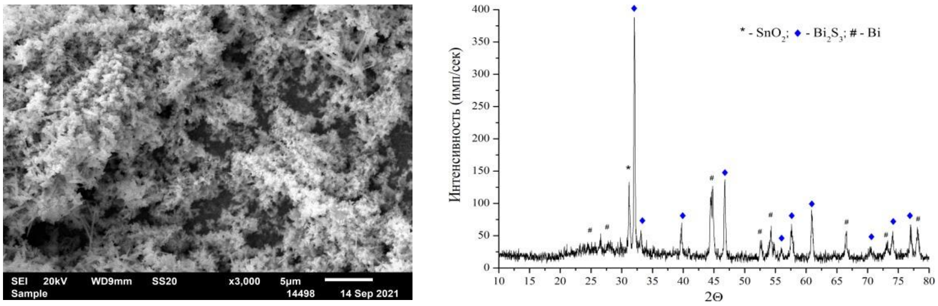
Bismuth sulfide (Bi_2S_3) is a promising n-type semiconductor for photoelectrochemical (PEC) and solar cell applications due to its high absorption coefficient ($\alpha > 105\ cm^{-1}$), narrow band gap (1.5–1.9 eV) and photocatalytic stability. These properties determine its high potential efficiency in photovoltaic and photoelectrochemical devices [1]. Thermal stability and environmental safety of bismuth compounds expand the prospects for their use in sustainable energy technologies.

Bi_2S_3 is used as an active layer in thin-film solar cells, including as part of heterostructures with other semiconductors, as well as in liquid photoelectrochemical cells (PEC) and photocatalytic processes, such as the reduction of CO_2 and Cr(VI) ions [2, 3].

Numerous techniques have been developed to synthesize Bi_2S_3 thin films, including spray pyrolysis, chemical bath deposition, solvothermal and hydrothermal methods, vacuum thermal evaporation, and spin coating. However, autoclave- and vacuum-based techniques typically require high temperatures, long synthesis durations, and complex equipment, which hinder scalability.

Electrochemical deposition offers a simple, energy-efficient, and scalable route for Bi_2S_3 thin-film synthesis. This work investigates the impact of electrolyte composition on the photoelectrochemical properties of Bi2S3 thin films obtained by electrodeposition, with the goal of optimizing their application in PEC devices.

As a result of electrodeposition at a potential of -750 mV from an electrolyte with the addition of EDTA (pH = 4), uniform thin films of Bi2S3 of dark gray color were obtained. SEM analysis (Figure 1a) revealed that the films exhibited a feather-like morphology with a uniform particle distribution on the FTO substrate. XRD patterns (Figure 1b) confirmed the formation of the orthorhombic Bi2S3 phase (JCPDS 17-0320).



a b

Figure 1. SEM image (a) and XRD pattern (b) of electrodeposited Bi_2S_3 thin films

The photoelectrochemical behavior of the films was investigated in 0.01 M Na_2S and 0.5 M Na_2SO_4 at 0 mV (vs. RHE) under AM 1.5G illumination (100 mW/cm^2). In both electrolytes, a stable anodic photocurrent typical of n-type semiconductors was observed. The maximum photocurrent density reached 3.3 μA/cm^2 in Na_2S and 22 μA/cm^2 in Na_2SO_4, highlighting the significant influence of pH and electrolyte composition on charge carrier dynamics.

Thus, the electrolyte composition critically affects the photoresponse and stability of Bi_2S_3 films. The obtained data demonstrate the high potential for using such films as an active material for photoanodes in photoelectrochemical cells, as well as in photodetectors and other photovoltaic devices, due to their high photosensitivity, resistance to degradation and the possibility of low-temperature synthesis using available reagents.

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New electrochemical methods for obtainig ultradispersed metal powders

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One of the promising directions in the creation of new pharmaceuticals, including those with wound-healing properties, is the incorporation of nanomaterials. It has been established that metal powders possess physicochemical properties that differ from those of bulk metallic objects and individual atoms. When nanometer-sized metal particles enter living organisms, they trigger a biological response that differs from the action of traditional ionic forms of elements. It has been shown that nanoparticles of d-elements, when administered parenterally, are 7-50 times less toxic than metals in ionic form. Nanoparticles easily penetrate all organs and tissues and have a prolonged effect. In biotic doses, they stimulate metabolic processes and exhibit multifunctional actions [1]. In this context, the development of new methods for obtaining ultrafine metal powders is a pressing issue of modern times.

We have developed a number of fundamentally new methods for producing ultrafine and nanoscale metal powders, with current efficiency increasing by more than 10-15%. Dispersed metal powders can be produced through various mechanisms. For example, in the case of copper, depending on the conditions of electrolysis, dispersed powders can be produced by three mechanisms.

In a sulfuric acid solution of copper (II) containing tetravalent titanium ions, these ions are reduced at the cathode to produce titanium (III) ions (reaction 1):

$$Ti^{4+} + e \rightarrow Ti^{3+} \qquad (1)$$

The resulting titanium (III) ions interact in the cathode space with copper (II) ions (reaction 2).

$$2Ti^{3+} + Cu^{2+} \rightarrow CuO + 2Ti^{4+} \qquad (2)$$

in this process, the reduced copper produces as a dispersed powder.

In this case, the part of the current that is consumed for hydrogen evolution in the classical methods of powder production is used for the reduction of titanium (IV) ions and, effectively, for the production of copper powder. As a result, current efficiency increases, as the discharge rate of hydrogen ions decreases.

During reaction (2), titanium (IV) ions are simultaneously regenerated, which are then reduced again at the cathode and participate in the next cycle of the process. In this manner, titanium (IV) ions act as a catalyst.

In the case of electrolysis conducted in a titanium (IV) sulfate solution with a copper anode and a titanium cathode, the copper electrode dissolves to produce copper (II) ions (reaction 3).

$$Cu - 2e \rightarrow Cu^{2+} \qquad (3)$$

and the titanium (IV) ions are reduced to titanium (III) at the cathode. The resulting copper (II) and titanium (III) ions interact with each other in the solution volume, leading to the reduction of copper (II) to its elemental state in the form of a dispersed powder.

The titanium (IV) ions produced in reactions (2) are again reduced at the cathode to the trivalent state and interact with copper (II) ions in the solution volume, with these reactions continuously repeating cyclically.

We have also proposed an electrolysis method whereby, upon immersing a copper anode and a titanium cathode in a titanium (III) sulfate solution, the resulting copper (II) ions instantly interact with the titanium (III) ions, producing a dispersed copper powder in the anode space.

It has been established that depending on the mechanism of powder production, dispersity of their particles varies in the range of 10 to 500 nm.

Our patented methods open new approaches to obtaining dispersed metal powders with varying dispersity. The work was completed in accordance with project No. AP 23486503.

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Thermoelectric and Electronic Properties of Bi_2S_3 Synthesized via Green Mechanochemical and Conventional Routes

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Bismuth sulfide (Bi^2S^3) is a promising material for thermoelectric and photocatalytic applications due to its narrow band gap and favorable electronic properties. While several solvothermal[1], thermal[2], sonochemical[3], and other synthesis methods have been reported, solvent-free approaches remain underexplored. In this work, we propose a facile and environmentally friendly mechanochemical synthesis of Bi_2S_3 via solid-state reactions using a planetary ball mill. The process achieves full conversion in just 20 minutes, comparable in speed to sonochemical synthesis using an ultrasonic bath, but with the added advantage of being solvent-free and more sustainable. To compare the effectiveness of different synthesis routes, Bi_2S_3 was also synthesized via thermal and solvothermal methods. SEM analysis revealed significant morphological differences: the mechanochemically synthesized Bi_2S_3 consisted of small, non-tubular particles; the thermally synthesized sample showed rod-like or tubular-like structures; while the solvothermal method yielded larger, layered crystallites. XRD confirmed crystalline structures for thermal and solvothermal products, whereas the mechanochemical product showed broader peaks, indicating nanocrystallinity or partial amorphousness (Figure 1).

To evaluate structure–property relationships, Bi_2S_3 was also synthesized via thermal and solvothermal methods. SEM revealed significant morphological differences: Bi_2S_3-M showed agglomerated nanostructures; Bi_2S_3-T exhibited rod-like/tubular forms; Bi_2S_3-S formed layered crystallites. XRD confirmed crystalline structures for Bi_2S_3-T and Bi_2S_3-S, while Bi_2S_3-M displayed broader peaks, suggesting nanocrystallinity or partial amorphousness.

The electronic transport properties were further investigated using Hall-effect measurements. Bi_2S_3-T exhibited the highest carrier concentration (~10^{17} cm^{-3}), attributed to abundant sulfur vacancies from high-temperature synthesis. Bi_2S_3-S showed the lowest n due to reduced defect formation in mild solvothermal conditions, while Bi_2S_3-M displayed intermediate carrier density. In contrast, carrier mobility peaked in Bi_2S_3-S (μ ~16 $cm^2/V \cdot s$), suggesting fewer scattering centers. Bi_2S_3-T and Bi_2S_3-M had lower mobilities, leading to respective resistivities of ~0.1, ~0.5, and ~0.3 $\Omega \cdot cm$.

Thermoelectric properties were assessed for Bi_2S_3-M over 300–350 K. The material exhibited a moderate Seebeck coefficient (~25 μV/K at 300 K), electrical conductivity of ~420 S/m, and low thermal conductivity (~1.5 W/m·K), resulting in a modest dimensionless figure of merit $zT \approx 0.00006$. These values reflect the balance between defect-induced carrier density and limited phonon scattering suppression, indicating the need for further optimization.

This work demonstrates a scalable and eco-friendly approach to Bi_2S_3 synthesis, with direct correlations between synthesis method, microstructure, and transport behavior—paving the way for performance-tuned materials in energy conversion and photocatalysis.

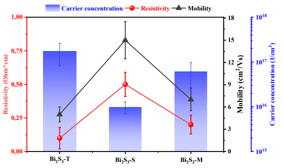

Figure 1. Hall effect results of Bi_2S_3 Samples Prepared by Thermal (Bi_2S_3-T), Solvothermal (Bi_2S_3-S), and Mechanochemical (Bi_2S_3-M) Methods

Keywords: Solid-state reactions, thermoelectrical, photocatalysis

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Investigation of a Dual Photo-Thermally Crosslinked PVA-based Gel Polymer Electrolyte for Robust Lithium-Sulfur Battery Applications

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Lithium-sulfur (Li-S) batteries are highly attractive for next-generation energy storage, offering substantial theoretical capacity and cost-effectiveness. However, a significant obstacle to their widespread adoption is the detrimental polysulfide shuttling effect, which causes rapid capacity fade and compromise cycling stability. A promising approach to overcome this challenge involves replacing conventional liquid electrolytes with the gel polymer electrolytes (GPEs). This research investigates the application of a dual photo-thermally crosslinked PVA-based (PVA-MPHT) GPE in Li-S cells, leveraging its proven efficacy in lithium-ion battery systems. The GPE was meticulously prepared through a dual crosslinking process involving photo-UV and thermal treatment, utilizing maleated poly(vinyl alcohol) (PVA-M), poly(vinyl alcohol) (PVA), polyethylene glycol diacrylate (PEGDA) and tetraethyl orthosilicate (TEOS), with the aim of improving both electrolyte stability and the retention of polysulfides.

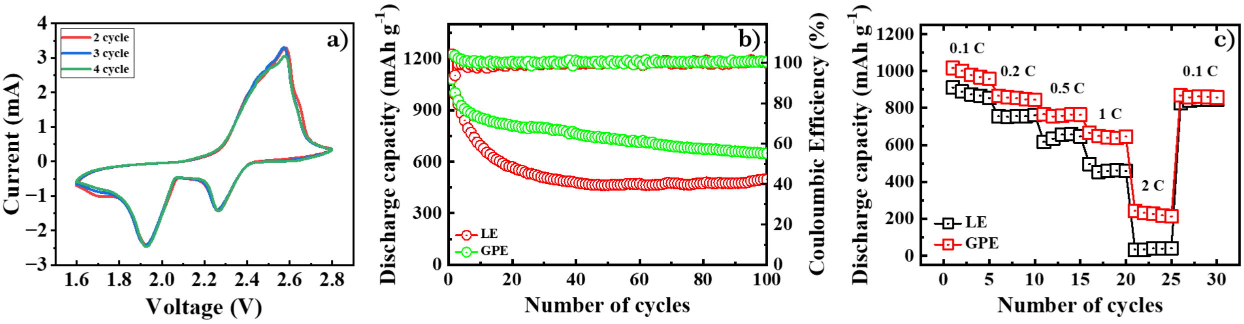

Figure 1. (a) CV curves of the RHG@S GPE half-cell; (b) charge-discharge cycling stability GPE comparison with LE; (c) Rate performances of the assembled half cells with GPE and LE.

The Li-S cell utilized a biomass carbon from rice husk (RHG) and sulfur cathode with a 4:6 carbon-to-sulfur ratio. The overlapping CV curves from the 2nd to 4th cycles (Figure 1 a) indicate good electrochemical reversibility and stability. The cycling performance of the GPE cell demonstrated an initial discharge capacity of 1082.4 mAh g^{-1}, which decreased to 648.7 mAh g^{-1} after 100 cycles at 0.1C, as depicted in Figure 1 b. for comparison, the cell with a conventional LE exhibited an initial discharge capacity of 1226 mAh g^{-1}, decreasing to 496.7 mAh g^{-1} after 100 cycles at 0.1C. the average Coulombic efficiency for the GPE cell was observed to be around 98%. The rate capability test (Figure 1 c) showed that the GPE delivered discharge capacities of approximately 900, 800, 700, 600 and 400 mAh g^{-1} at 0.1C, 0.2C, 0.5C, 1C and 2C respectively, which were superior to the LE.

The superior polysulfide blocking capability of this GPE is attributed to a synergistic effect. Firstly, the crosslinked polymer matrix, forming a nanofibrous structure upon swelling, acts as an effective physical barrier by restricting pore size and increasing tortuosity, thus hindering polysulfide migration. Secondly, chemical interactions between the GPE's polymer chains (e.g., through oxygen-containing functional groups like hydroxyl (-OH) and carboxylic (-COOH) groups, as indicated by XPS analysis) and lithium polysulfides species induce electrostatic and steric hindrance, promoting their adsorption onto the membrane surface. These results suggest the potential of this dual crosslinked PVA-based GPE as a viable electrolyte for Li-S batteries, offering an alternative to traditional liquid electrolytes and effectively addressing the polysulfide shuttling issue. This study contributes to the development of safer and more efficient Li-S batteries through the application of a successful GPE formulation.

A Review of Challenges associated with On-Board Hydrogen Energy Storage for use with Fuel-Cells in Electric Aircraft

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Aircraft are responsible for significant green-house gas emissions (GHGs) resulting from the combustion of aviation fuels. The emissions consists of such gases as CO_2, NO_x, SO_x, particulates and water vapour, all of which lead to contrails that contribute to radiative forcing and global warming [1]. Also, the aviation sector worldwide is expected to grow by about 5% per year for the foreseeable future and attempts to reduce CO_2 emissions originating from the combustion of fossil fuels are insufficient to off-set this growth [2]. All-electric, hybrid-electric and turbo-electric aircraft have the potential to slow this trend in the near future, with all- electric having the ability to eliminate CO_2 emissions and air pollution [3].

Currently electric aircraft are being developed so as to reduce gas emissions harmful to the atmosphere. Likely scenarios to alleviate such emissions are the use of on-board battery power or, on-board hydrogen chemical energy which is converted to electrical energy using fuel cell technology and hence the provision of power for electric motors. Current battery energy density combined with current aircraft performance does not approach a viable solution, and progress within this field would seem to take decades. Hybrid technological arrangements would cope with some current limitations of civil aviation but would still rely on aviation outside the up- to-date combustion engines metrics. Also, battery performance, availability, and costs of electric energy may essentially grow into the limiting factor for large-scale operations after many technological breakthroughs [4]. The long-term solution for civil aviation may be therefore to use hydrogen propulsion.

Hydrogen is emerging as a key energy carrier in the shift towards de-carbonization, offering to store and deliver clean energy across multiple sectors (applications). It can serve as a fuel or be converted to electricity using devices like fuel cells. As a zero-carbon gas, hydrogen emits no greenhouse gases during combustion, provided it is produced from non-fossil fuel feedstocks [3]. When adopted on a large scale as both an energy carrier and a replacement for chemical fuels, hydrogen has the potential to effectively decarbonize the entire fuel supply chain.

However the use of hydrogen as the primary fuel also offers challenges and a review of these is the main aim of this presentation. As well known, hydrogen has a low density at room temperature requiring large storage volumes and reinforced heavy tanks. As weight is important for an aircraft operation, this could be a limitation for available space on-board and payload capability. This would increase the need for enhanced thrust during take-off.

The ability to store hydrogen on-board an aircraft would also depend on such factors as economic viability, safety aspects, the ability for quick release of hydrogen, development of current technology and environmental sustainability.

This presentation will review all of the foregoing challenges together with some suggestions as to possible solutions.

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Advancing Energy Devices through Molecular Engineering of Conducting Polymers and Polyelectrolytes

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This work presents the design and synthesis of novel self-doped conducting polymers and conjugated polyelectrolytes as advanced hole transport layers (HTLs) for third-generation polymer solar cells (PSCs). By introducing mobile and molecular counterions directly into the polymer backbone, we aim to overcome limitations of traditional HTL materials such as PEDOT:PSS, including poor stability, limited conductivity, and sensitivity to humidity and pH (Figure 1). The new materials are engineered with varied ionic group spacing and tailored dipole alignment to improve charge extraction and interfacial energy alignment. Structural and optoelectronic properties are studied using UV-Vis, cyclic voltammetry, and Hall effect measurements. Preliminary results demonstrate enhanced hole mobility and device performance, offering a promising strategy for improving the efficiency and durability of low-cost, scalable PSC technologies.

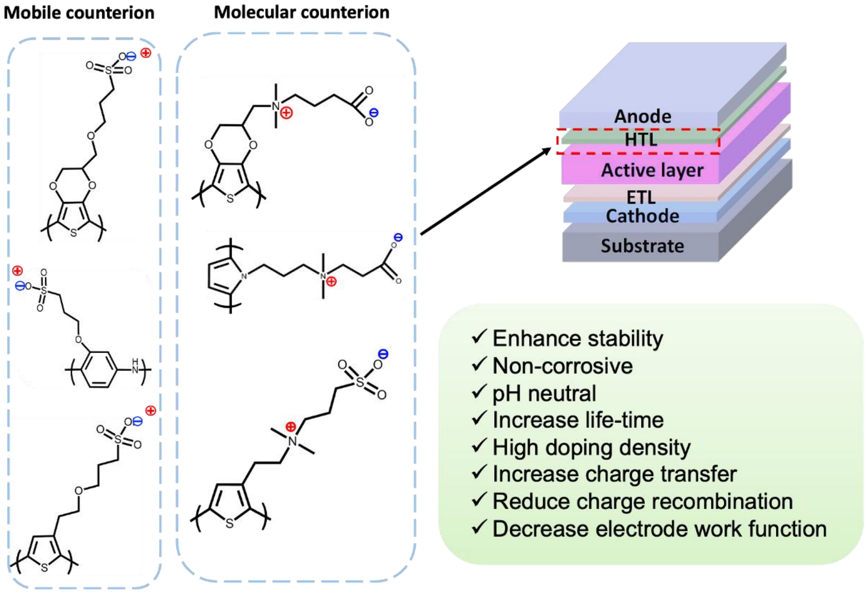

Figure 1. Schematic illustration of polyelectrolytes for PSC

Determining the structure of functionalized graphene for tailored thermomechanical properties using ML techniques

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Chemical functionalization of graphene unlocks an infinite space of graphene-based nanosheet structures with varying properties. Each functional group and its corresponding distribution on the graphene sheet may distinctly impact the thermal and mechanical properties of the resulting nanosheet, hence paving the way for the design of structures tailored to specific applications. Although we can accurately estimate the nanosheets' thermomechanical properties using Molecular Dynamics (MD) simulations, their high computational cost does not permit an extensive search of the design space. To address this issue, we developed a family of regression models which were successfully trained on a selected dataset of functionalized graphene nanosheets and their corresponding thermomechanical properties, estimated via MD simulations. Hence, by combining MD simulations with Machine Learning (ML) models we enabled the cost-effective deployment of global optimization approaches to rapidly and accurately identify the atomic layout of functionalized graphene sheets that meet given sets of user-prescribed thermomechanical properties.

600 unique single-layer graphene nanosheets were generated, each containing hydrogen and/or methyl functional groups at controlled surface coverages of up to 15 %. These nanosheets were of identical dimensions (220Å by 100Å) with ≈ 8500 carbon atoms which permitted the accurate estimation of their thermomechanical properties of interest via MD simulations. Specifically, we evaluated the following property values: thermal conductivity, Young's modulus, as well as maximum stress and strain. The estimated values were compared and validated using results from pertinent literature. Subsequently, a range of ML-based regression models were trained using 5 fold cross-validation on the aforementioned dataset, with 90% of it comprising the training dataset and the remaining 10% being reserved for testing. Support Vector Regressions (SVRs), Neural Networks (NNs) and Gaussian Process Regression (GPR) demonstrated the highest predictive performance among the tested models, with very high coefficients of determination (R2>0.98) and mean absolute errors below 1% for Young's Modulus, thermal conductivity and maximum stress. However, estimation of maximum strain was less successful in our study regardless of the trained model type. Hence, at the end of this stage, we were equipped with a set of ML-based regression models that could predict, with sufficient accuracy, the thermomechanical properties of each nanosheet in a negligible fraction of the time required by MD simulations, i.e., a couple of milliseconds using a standard PC instead of a couple of hours on a high-performance computing cluster (up to 7 orders of magnitude speed increase).

Finally, the best-performing ML models were coupled with a global optimization framework that permitted the performance of inverse design, i.e., the automatic identification of the functionalized graphene layout that exhibits a user-defined set of thermomechanical properties. The resulting layouts were subsequently evaluated using MD simulations to validate the model's predictions. These results demonstrate that a data-driven ML-based design optimization framework can be effectively used for designing customized graphene-based nanosheets with prescribed properties that may satisfy specific requirements stemming from the applications at hand. Future steps will study the applicability of this approach to a wide variety of graphene-modification techniques, including functionalization, doping, defects' introduction, as well as their combinations.

Acknowledgements. This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP23488419) "Design Optimization of Graphene-based materials and devices with computational and Machine Learning approaches (DOG-ML)" and from Nazarbayev University FDCRGP: "Machine Learning-Assisted Design of Membranes for Wastewater Treatment, Desalination and Gas-Separation - ML-BRANES", Grant Award No.: 040225FD4734.

Integrating Computational Materials Science into Engineering Education and Energy Innovation

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With its abundant natural resources, expanding research capabilities, and strategic commitment to sustainability, Kazakhstan is uniquely positioned to become a regional leader in clean energy and advanced materials innovation. As the nation accelerates its transition toward low-carbon and sustainable technologies, the ability to rapidly and efficiently develop advanced materials and optimize complex engineering processes is increasingly critical. Kazakhstan's abundant mineral reserves, rich wind and solar energy resources, and growing research infrastructure present opportunities to lead in targeted innovation. Meeting these demands requires moving beyond traditional trial-and-error approaches to materials development.

At the CMS Lab, we are advancing a "computation-first" approach that integrates physics-based multiscale modeling and AI-assisted design. This framework enables precise prediction of material properties, identification of fundamental mechanisms, and targeted support for experimental validation.

Our studies span critical areas of national interest. For hydrogen energy systems, we employ Density Functional Theory (DFT) and molecular simulations to investigate hydrogen adsorption on pristine, doped, and defect-engineered graphene [1]. We examine how nitrogen and boron doping, lithium modifications, and defects influence binding strength, storage capacity, and desorption reversibility, helping identify optimal design strategies for high-performance hydrogen storage materials.

In nuclear energy materials research, we conduct large-scale molecular dynamics simulations to examine radiation effects in silicon carbide (SiC), a leading candidate material for structural applications in fusion and fission reactors. Our results show that stacking faults can serve as recombination sinks for Frenkel pairs, significantly mitigating radiation-induced damage and restoring phonon transport, which is essential for thermal management under demanding reactor conditions [2].

In fossil energy recovery, we use atomistic simulations to explore gas-enhanced methane extraction in nanostructured carbon materials. Focusing on CO_2 and N_2 injections into graphene nanoslits pre-saturated with methane, we characterize competitive adsorption, displacement efficiency, and molecular transport. Our findings demonstrate the potential for CO_2-assisted methane recovery while simultaneously enabling in situ CO_2 storage, offering a dual-purpose strategy for enhancing unconventional gas extraction and geological carbon sequestration [3].

In the built environment, we develop analytical models for predicting pressure losses during concrete pumping. These models provide practical tools for optimizing energy use and operational safety in infrastructure projects involving large-scale concrete placement [4].

Crucially, many of these research initiatives actively involve students and early-career researchers, underscoring our commitment to integrating research and education. By embedding computational methods into the engineering curriculum, we equip students with the tools needed to address complex, interdisciplinary challenges across scales, drawing on decades of rapid advances in computational power and algorithmic development. This integration not only accelerates innovation in energy and sustainability but also builds national capacity in computational-assisted research and development. Computational materials science is emerging as a scalable, high-impact driver of clean technology development in Kazakhstan and beyond.

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Advanced Polymer-Based Emulsion Modeling for Efficient Hydrocarbon Recovery in Kazakhstan's Oil Fields

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Kazakhstan's petroleum industry plays a central role in the national economy, contributing approximately 17% of GDP, 60% of total exports, and a significant portion of government revenues [1,2]. However, the country's oil production has experienced a notable decline over recent years, falling from approximately 1.903 million barrels per day (mb/d) in 2019 to 1.771 mb/d in 2023, a drop of over 7%. This includes a 6.4% year-over-year decrease between 2022 and 2023 alone, with further reductions of around 2% reported in 2024 due to maintenance at major fields such as Tengiz and Kashagan [3,4]. Many oil fields across Kazakhstan continue to rely on conventional waterflooding methods, which often result in water cuts exceeding 90%, particularly in sandstone and heavy oil reservoirs [5]. These factors have led to reduced oil recovery and increased water handling costs, highlighting the urgent need for cost-effective, enhanced oil recovery (EOR) technologies that can improve production efficiency in oil fields.

The use of polymer-based emulsions, characterized by non-Newtonian and shear-thinning behavior, represents one of the most promising approaches among EOR methods. These fluids offer multiple advantages for subsurface injection, including mobility control, improved sweep efficiency, and stabilized displacement fronts. In contrast to conventional polymer flooding or surfactant injection methods, polymer-surfactant-based emulsion formulations are capable of reducing viscous fingering and bypassing effects that are common in high-water-cut environments. However, effective field application of these emulsions depends on a thorough understanding of their transport behavior in porous media, supported by experimental validation and numerical modeling.

This study combines one-dimensional laboratory-scale experiments with numerical simulations to evaluate the performance of optimized polymer-based emulsions for hydrocarbon recovery. The work builds upon experimental investigations conducted by Sabyrbay et al. (2025) [6], which demonstrated that a stable emulsion composed of xanthan gum, sodium decyl sulfate surfactant, and alcohol achieved complete diesel recovery in sand-packed columns. The emulsion exhibited controlled viscosity and stable displacement behavior during injection.

A numerical model was developed using CMG STARS and was calibrated using experimental data, including core dimensions, permeability, porosity, fluid viscosities, and injection flow rates. The model incorporated the shear-thinning behavior of the emulsion, adjusted endpoint relative permeabilities, and neglected capillary pressure to align with experimental conditions. The simulation results accurately reproduced the formation of a stable displacement front and complete oil recovery, validating the experimental results. These results demonstrate the effectiveness of the emulsion formulation and its stable flow characteristics in homogeneous porous media.

The modeling results highlight the potential of polymer-surfactant-based emulsion EOR and provide a validated framework for further development. The next phase of the study will focus on upscaling to three-dimensional reservoir models and applying the approach to real-life field scenarios. This will involve adapting the model to heterogeneous conditions and implementing realistic injection and production well configurations. Particular emphasis will be placed on optimizing injection rates, emulsion slug design, and breakthrough timing to maximize oil recovery while minimizing water production.

In conclusion, this work demonstrates the feasibility and effectiveness of polymer-based emulsion injection as an innovative EOR technique for Kazakhstan's oil fields. The combination of laboratory validation with predictive modeling provides a strong foundation for future field trials and informed decision-making within Kazakhstan's evolving energy landscape. This approach enables improvements in oil recovery rates, extends the productive life of mature reservoirs, and enhances overall energy efficiency, aligning with the strategic goals of the country's long-term energy development plans.

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Acid rainwater-assisted mineral dissolution using Kazakhstan's industrial waste for CO_2 mineral carbonation

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The growing need to address climate change has driven the advancement of sustainable technologies for carbon dioxide (CO_2) capture and storage [1]. To date, no attempt has been made to study CO_2 mineral trapping using industrial wastes in post-Soviet countries. In this sense, Kazakhstan has generated approximately 4 billion tons of industrial waste [2]. This research explores the feasibility of using naturally occurring acidic rainwater as a reactive agent for mineral dissolution from steel slag originating from the North Kazakhstan Ferroalloy Plant. The refining steel slag sourced from North Kazakhstan was initially analyzed through X-ray fluorescence (XRF) and X-ray diffraction (XRD) techniques. Comprising mainly diluted sulfuric and nitric acids resulting from human-induced emissions, acid rain offers a low-cost and environmentally compatible medium for extracting divalent cations (Ca^{2+}, Mg^{2+}) from silicate-rich minerals such as wollastonite and serpentine present in the industrial wastes. Both the experimental analysis and the equilibrium model simulation results under synthetic acid rain conditions revealed the mineral dissolution and leaching of Ca^{2+}, which can increase the CO_2 uptake by carbonate precipitation along with dissolution trapping of CO_2 (Figure 1).

This is the first attempt at CO_2 mineral trapping by industrial wastes in the Commonwealth of Independent States (CIS). The proposed methodology presents a synergistic and environmentally sustainable approach to atmospheric CO_2 mitigation, concurrently addressing the ecological concerns associated with acid rain and wastewater reuse. The outcomes of this study affirm the technical feasibility and economic viability of employing acid rainwater to facilitate mineral carbonation, positioning it as a scalable and low- impact strategy within the broader framework of carbon capture and storage (CCS) technologies.

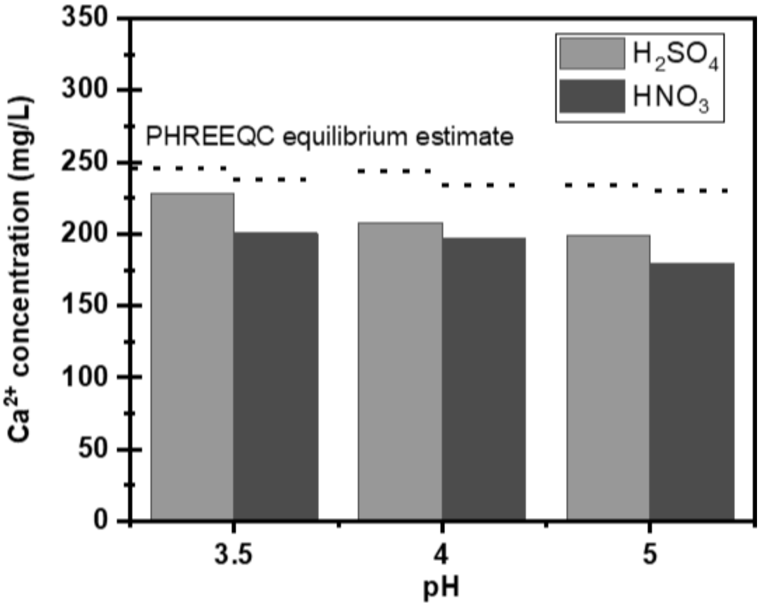

Figure 1. Comparison of experimental results and the simulation estimate of calcium leaching under different conditions.

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1 ppm-detectable hydrogen gas sensor based on nanostructured polyaniline

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In this work, a new type of relatively fast and responsive conducting polymer sensor has been demonstrated for tracing H2 gas in a nitrogen environment. Three different PANI morphologies consisting of hollow tube, a film and short nanofibers were evaluated for hydrogen sensing. Among them, the PANI hollow nanotubes exhibited excellent detection performance compared to the thin film sensors and obtained a response of 29% sensitivity with a response time of 15 s, which has better performance than PANI thin film (20% and 65s). The sensing performance of the hollow tubes were directly proportional to their carrier mobility and carrier concentration. In addition, the hollow nanotube structure polyaniline provided the best conductivity (9.15 S/cm), followed by PANI thin film (0.60 S/cm) and PANI nanofiber (0.05 S/cm). Compared with the polyaniline thin film and short nanofibers, the obtained hollow nanotubes polyaniline has a tubular structure similar to carbon nanotubes, which provides a better connection network to conduct electrons better. This finding gives some insight into structure-property studies of polyaniline nanostructures and H2 gas sensing mechanism.

Enhancement of NO Gas Sensing Properties of Titanium-Doped ZnO Nanostructures via Intense Pulsed Ion Beam Irradiation

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In this work, we report on the significant enhancement of gas sensing performance in titanium-doped zinc oxide (TZO) nanostructures through the application of intense pulsed ion beam (IPIB) irradiation. TZO thin films were synthesized via the sequential ion-layer adsorption and reaction (SILAR) method [1] and subsequently subjected to either thermal annealing at 500 °C in nitrogen or IPIB treatment. A comprehensive investigation of their morphological, structural, optical, and electrical properties was carried out with a focus on nitrogen monoxide (NO) detection.

The IPIB-treated films (iTZO) exhibited pronounced lattice distortion and an increase in surface roughness, contributing to enhanced gas adsorption and charge transport. Compared to thermally annealed samples (aTZO), the iTZO films demonstrated a remarkable 1300% improvement in sensor response to 100 ppm NO at 200 °C. Complementary density functional theory (DFT) calculations confirmed stronger interaction of NO molecules with defective TZO surfaces, providing insights into the observed sensing behavior.

These findings highlight the potential of IPIB irradiation as an effective post- synthesis modification technique for tuning the gas sensing characteristics of metal oxide semiconductors. The approach offers promising prospects for the development of high-performance sensors in environmental and industrial monitoring applications.

Acknowledgements. This research has been funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No AP22785922).

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ZIF-derived Co/NC as an Efficient Catalyst for Biomimetic CO_2 mineral carbonation under Ambient Conditions

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With the rapid progression of climate change, it is essential to advance innovative catalytic platforms for carbon capture and mineralization. [1]Among emerging strategies, biomimetic catalysis, drawing inspiration from the function of carbonic anhydrase (CA), a natural enzyme that facilitates the swift hydration of CO_2 to bicarbonate, has attracted considerable interest.[2] Although CA demonstrates remarkable activity, its application on a large scale is constrained by thermal instability, a narrow pH tolerance, and elevated production costs. To address these challenges, metal-organic frameworks (MOFs) and their derivatives present a promising solution, characterized by their exceptional tunability, porosity, and thermal stability.[3] This study assesses carbonised ZIF-67 (Co/NC), produced by pyrolyzing cobalt-based ZIF-67 at 800 °C in an inert atmosphere, as a biomimetic catalyst for the mineralization of aqueous CO_2 into calcium carbonate. The resulting Co/NC maintains the morphology of the parent MOF while evolving into a porous, graphitized carbon matrix that incorporates catalytically active cobalt nanoparticles. The process of carbonisation brings about numerous advantageous physicochemical characteristics, including heightened electrical conductivity, a wealth of surface defects, and uniformly distributed cobalt–carbon interfaces. These features collectively contribute to improved CO_2 hydration and the formation of carbonates. The features were meticulously characterized through the application of SEM, EDS, FTIR, and porosimetry. SEM validate the presence of rough, microporous surfaces containing embedded cobalt particles (Figure 1); and BET analysis indicates a significant surface area, facilitating extensive interaction with CO_2-laden water. Aqueous CO_2 mineralization reactions were carried out at ambient temperature and pressure to mimic the catalytic behavior of carbonic anhydrase. In every trial, ice-cold CO_2-saturated water was combined with a Ca^{2+}-rich solution in the presence of Co/NC. The extent of CO_2 conversion was assessed by quantifying inorganic carbon (IC) levels prior to and following the reaction with a TOC-TN analyzer. Notably, Co/NC catalysis resulted in >60% reduction in IC, demonstrating the effective mineralization of CO_2 into $CaCO_3$ and affirming the material's enzyme-mimetic capabilities. This investigation highlights the promise of carbonised MOFs such as Co/NC as stable, efficient, and scalable substitutes for natural carbonic anhydrase.

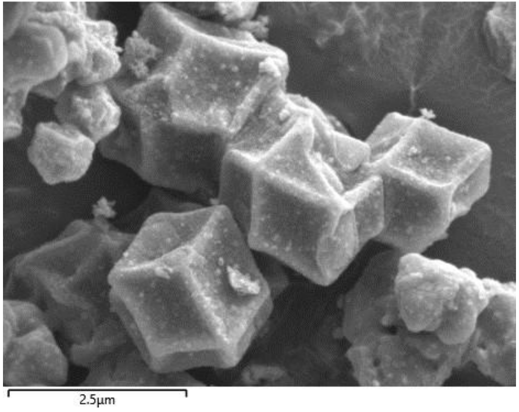

Figure 1. SEM image of synthesized Co/NC

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Syngas production by carbon dioxide conversion of methane over the Co-based nanocomposite catalysts with high stable activity

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Climate change and the depletion of oil resources are the main problems facing the entire world community. In the interests of sustainable development, a search is being made for new alternative cheap and renewable sources of energy, petrochemistry, and environmental protection. In the long term, carbon dioxide can serve as a source of renewable raw materials. In recent years, carbon dioxide reforming of methane, also called as dry reforming of methane (DRM), has generated a lot of interest because it can convert two major greenhouse gases (CO_2 and CH_4) to syngas ($CO+H_2$).

This work deals with the production of synthesis gas by dry reforming of methane over the nanocomposite catalysts containing of Co as base metal modified with Pt and supported on a matrix composed of alumina modified with zirconia and rare-earth metal oxides. Also, the catalytic activity was tested in combined dry-steam reforming of methane (bireforming, BRM). The catalysts were characterised by BET, XRD, SEM, TEM, and TPR methods.

The multicomponent 5% Co-M/Al_2O_3-ZrO_2-R catalysts, where M is a noble metal (Pt) and R is Ce or/and La oxides were synthesized by impregnation method. The processes, DRM and BRM, were carried out in a quartz flow reactor supplied with programmed heating, controlled feed velocity, a programmable syringe pump, and GCs. Stainless steel reactor with catalyst volume – 100 mL was used in order to carry out the long-term tests. The DRM and BRM have been studied under atmospheric pressure, varying gas hourly space velocity (GHSV) within 1000-3000 h^{-1} with using a feed with a ratio of CH_4/CO_2=1:1 and varying temperature within a range of 300- 800ºC. The 0.5-2.0 vol. parts of steam has been added to a feed to provide bireforming of methane. To elucidate the stability the 5% Co-Pt/Al_2O_3-ZrO_2-CeO_2-La_2O_3 catalyst was continuously tested for a long-term period: 400 hours in DRM and 100 hours in bireforming of methane. The catalysts were characterised by BET, XRD, SEM, TEM, and TPR methods.

The catalysts perform a high activity in both dry and steam reforming of methane. Methane is almost completely converted at 750- 800ºC depending on the catalyst composition and process type. Adding steam in amount 0.1^{-1} volume parts to a feed of carbon dioxide + methane always leads to decrease in temperature of methane complete conversion and enriching syngas with hydrogen over the synthesized catalysts. The 5% Co-Pt/Al_2O_3-ZrO_2-CeO_2-La_2O_3 catalyst showed a high stable activity for all period of testing in both processes: for 400 hours in DRM and for 100 hours in bireforming of methane. Under conditions t=700ºC, P=1 atm, GHSV=1000 h^{-1}, CH_4:CO_2=1:1, methane conversion was varied within 96.0-96.6%, while the extent of carbon dioxide conversion was insignificantly less and varied within 90.4-92.3% (Figure 1). The ratio of H2/CO in the syngas formed in DRM was 0.9. In combined steam-dry reforming of methane (CH_4:CO_2:H2O=1:1:1), H_2/CO ratio was increased to 1.3 under the same conditions.

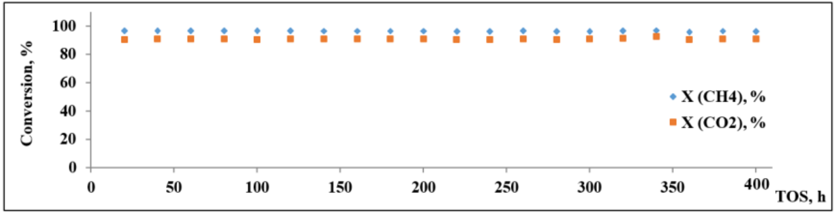

Figure 1. Dependence of conversion of CO_2 and CH_4 on DRM duration over the 5%Co-Pt/Al_2O_3-ZrO_2-CeO_2-La_2O_3 (t=700ºC, P=1 atm, GHSV=1000 h^{-1}, CH_4/CO_2=1:1)

The multicomponent 5%Co-Pt/Al_2O_3-ZrO_2-CeO_2-La_2O_3 developed performs the extremely high activity and stability in syngas production carbon dioxide reforming of methane. The synthesis gas composition can be controlled by adjusting the composition of the feed. A high dispersed state of metals was observed by TEM. The effect of the second metal on reducibility of Co was revealed by TPR method.

Acknowledgements. This research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan, Grant No AP19679439.

Real-time observation of molecular dynamics and chemical reactions in STEM

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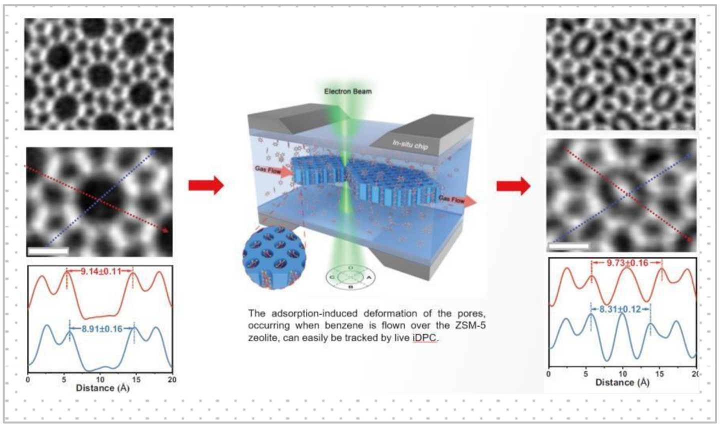
In situ transmission electron microscopy (TEM) has opened novel ways to study chemical reactions and molecular dynamics real- time at atomic scale. Nowadays, thanks to MEMS-based technology, we can easily observe samples in a state that is very close to real-application conditions. However, regardless of the technological advances of MEMS-based holders, some reactions are still extremely difficult to observe, either because of the intrinsic beam-sensitive nature of the sample or because we are limited by the non-ideal collection efficiencies of the common analytical techniques, such as energy dispersive X-ray spectroscopy (EDS) or experimental complications of electron energy loss spectroscopy (EELS).

An example of such beam-sensitive samples is zeolite. Zeolites are very versatile compounds with many present and future applications. Their porous structure makes them ideal molecular sieves. Unfortunately, due to beam-sensitivity issue, imaging zeolites requires special care to preserve their native structure. Using integrated differential phase contrast scanning TEM (iDPC- STEM), a method developed by Thermo Fisher Scientific [1], we routinely image beam sensitive materials with up to orders of magnitude lower electron doses compared to conventional STEM techniques such as high-angle annular dark-field (HAADF). This method, coupled with newly developed single-electron-sensitive detectors such as Panther STEM, can provide precise information on small molecules; and by using advanced in situ gas/liquid/heating holders, the whole reactions can be recorded with high frame speeds. Among many advantages of iDPC-STEM, we point out that it has the potential of providing ultimate spatial resolution under low-dose conditions. We show the capabilities of this technique through an in situ gas experiment on zeolite ZSM-5. As shown in the figure, we clearly observe the molecular dynamics of interactions between small molecules and zeolite ZSM-5 [2,3].

When applying stimuli to samples, TEM/STEM imaging can be performed relatively easily. However, spectroscopy faces more technical difficulties, e.g. complication of EELS experiment setup, or the sensitivity of EDS detectors, hindering the tracking of compositional changes during reactions. The second part of the talk will highlight the advantages of recent technological developments with EELS and EDS. As an example, we show in situ STEM-EDS chemical mapping of Au-Ag core-shell nanorods throughout a heating experiment and observe the chemical reactions in real time. Using such technologies make a dramatic impact on the way such materials behave in real-world applications such as catalysis and renewable energies.



The adsorption-induced deformation of the pores, occurring when benzene is flown over the ZSM-5 zeolite, can easily be tracked by live iDPC.

Figure 1. in situ iDPC STEM observation of beam-sensitive zeolite ZSM-5 used for gas capturing [2].

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Key factors influencing photocatalytic degradation of microplastics

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The persistence of microplastics (MPs) in natural environments raises serious ecological and health-related concerns, prompting the search for efficient removal methods [1]. Photocatalysis is considered a promising and sustainable approach to MP degradation. However, the process involves a complex interplay of numerous factors such as environmental conditions, photocatalyst properties, and polymer characteristics that significantly influence the final outcome [2,3]. These interdependent variables are often difficult to isolate and control, making a comprehensive understanding essential for the effective design and application of photocatalytic systems. This study explores the impact of key operational parameters on degradation efficiency and provides fundamental insights into the photocatalytic transformation of MPs. The findings contribute to developing reliable treatment strategies and addressing global environmental challenges.

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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POSTER SESSION

End-of-life lithium ion battery graphite anode upcycling: exfoliated graphene like material for Hydrogen storage

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Graphite is a naturally occurring crystalline form of carbon that exhibits excellent thermal and electrical conductivity, high chemical stability, and lubricating properties. These attributes make it valuable in numerous industrial applications, including refractories in steelmaking, lubricants, and electrodes in electric arc furnaces. Additionally, graphite is used in nuclear reactors as a neutron moderator due to its high purity and thermal resistance [1]. Among all its applications, the most significant and rapidly expanding use of graphite lies in advanced energy storage systems, particularly as the anode material in lithium-ion batteries (LIBs). Its layered structure allows lithium ions to intercalate and deintercalate reversibly with minimal volume change, offering high efficiency, long cycle life, and stability [2].

The intercalation and deintercalation of lithium ions in graphite are essential processes in lithium-ion batteries (Figure 1a-c), but they can also lead to significant structural degradation over time. During repeated cycling, the insertion of lithium ions causes the interlayer distance of graphite to increase from its natural spacing of approximately 0.335 nm to as much as 0.3703 nm in recovered graphite [3]. This expansion - about 10% - is primarily attributed to the formation and growth of lithium dendrites, which wedge between the graphite layers and weaken the van der Waals forces holding them together [4]. As a result, the graphite structure experiences mechanical fatigue, leading to dislocations, crack formation, and eventual particle fragmentation. Additionally, prolonged cycling causes a measurable increase in graphite particle diameter and overall volume-by 10–20% and 30–70%, respectively, depending on the number of cycles - further compromising the mechanical and electrochemical stability of the anode [5]. These findings highlight the need for improved structural engineering of graphite anodes to enhance battery longevity and performance.

A novel exfoliation method using sodium intercalation in liquid ammonia followed by thermal decomposition (Figure 1d) has also been shown to significantly expand the graphite structure, producing nanometer-thick flakes with increased surface area [6]. This expanded, porous architecture is expected to enhance hydrogen adsorption capacity, making such materials promising for hydrogen storage and other gas sorption applications.

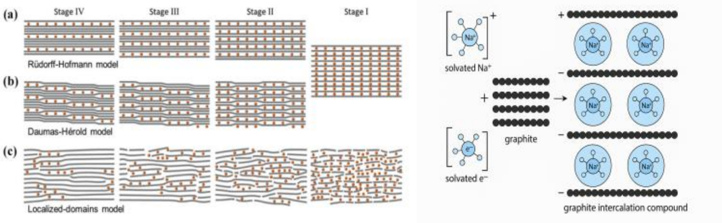

Figure 1. (a–c) Schematic illustration of lithium intercalation and deintercalation in graphite anodes and the resulting structural degradation due to dendrite formation and volume expansion [6]; (d) Exfoliated graphite obtained via sodium intercalation in liquid ammonia followed by thermal decomposition, showing expanded morphology suitable for enhanced hydrogen adsorption [7].

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Hydrophobic nanofibrous membrane for efficient ultrafine PM removal

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Air pollution, driven by fine particulate matters at different sizes, remains a critical global health concern, demanding innovative filtration technologies 1,2. This study introduces the fabrication of a novel PCL-SiO_2-FAS (Polycaprolactone – SiO_2 - Fluoroalkylsilane) nanofibrous membrane for efficient air filtration. This study presents the fabrication of a novel dual-layer nanofibrous membrane PCL-SiO_2-FAS as the first filtration layer and Polyvinyl Chloride (PVC) as a Triboelectric Nanogenerator (TENG) material in the second layer. The biodegradable PCL ensures environmental sustainability, while SiO_2 and FAS enhance mechanical stability and hydrophobicity 3,4. The PVC-TENG layer further improves particle capture efficiency through electrostatic adsorption.

The membranes were fabricated via electrospinning under optimized conditions and solvents and subsequently combined to form dual-layer filtrating system. To systematically evaluate filtration performance, three combinations of layers were tested: (i) PCL-PCL (dual PCL-SiO_2-FAS), (ii) PCL-PVC (PCL-SiO_2-FAS paired with PVC), and (iii) PVC-PVC (dual PVC).

Comprehensive characterization including FTIR, SEM, WCA, and filtration efficiency measurements were conducted. SEM images of PCL-SiO_2-FAS structure showed incorporation of SiO_2 nanoparticles and increased roughness and porosity due to FAS addition. WCA measurements confirmed the PCL-SiO_2-FAS membrane's high hydrophobicity (121.27°) compared to pristine PCL (109.74°) and PCL-SiO_2 (110.06°), indicating enhanced moisture resistance for durable filtration. The dual-layer PCL/PVC membrane demonstrated filtration efficiency exceeding 90% for PM particles.

This study highlights the potential of hybrid PCL/PVC membranes for high-efficiency, sustainable air filtration. Future work will focus on scaling up production, optimizing triboelectric performance, and real-world durability testing under varying environmental conditions.

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Some aspects of MOF-74 (Zn_2DOBDC) metal-organic framework formation using THF as the solvent

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This study presents the synthesis of zinc-based metal-organic frameworks (MOFs) using tetrahydrofuran (THF) as a solvent, with a focus on the formation of distinct phases potentially applicable in energy storage systems. Contrary to expectations, the synthesis did not yield the classical Zn-MOF-74 structure but instead resulted in the formation of three new phases: α, β, and a modified Zn-MOF-74a. The results highlight the critical influence of solvent choice, temperature, and pH on the phase behavior of the system.

Comprehensive structural characterization using X-ray diffraction, infrared spectroscopy, and thermogravimetric analysis provided insight into the coordination environments, thermal stability, and solvent interactions of each phase. The Zn-MOF-74a phase exhibits a unique porous architecture and crystallographic features distinct from those of conventional MOF-74. Its key advantage lies in the use of THF, which can be more readily removed from the pores during or after synthesis. This promotes the formation of smaller pores, which may enhance performance in applications such as gas adsorption and molecular separation.

In addition, the crystal structure of the dry H2DOBDC precursor was determined for the first time, serving as a valuable reference point for future research. Further investigation of the β-phase structure and the properties of Zn-MOF-74a may broaden the application potential of these materials in energy-related and other functional technologies.

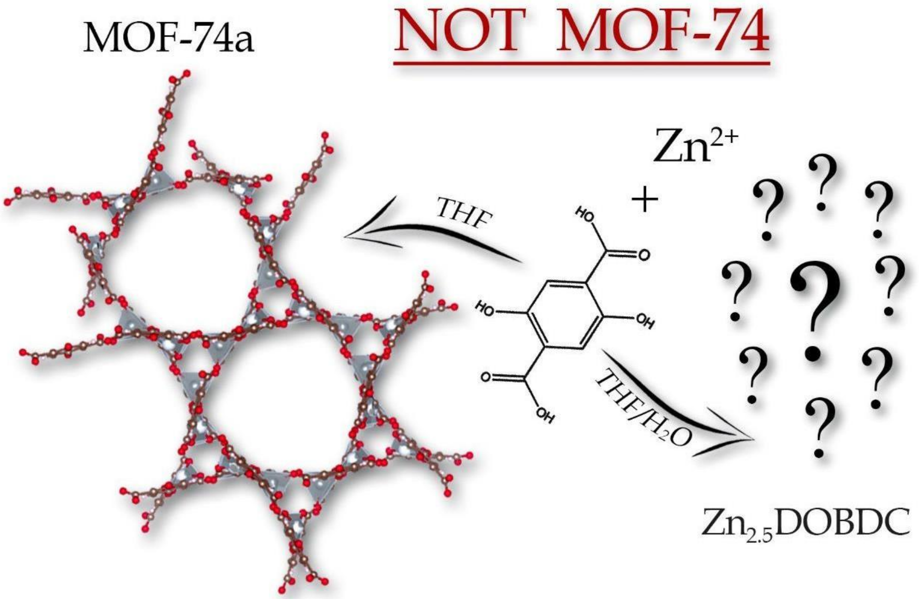

Figure 1. Synthesis of Zinc-Based Metal-Organic Frameworks using THF as a Solvent

Evaluation of perspectives for the synthesis of Ti_3AlC_2 in Kazakhstan for supercapacitor application

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Two-dimensional (2D) materials known as MXenes demonstrate significant potential as electrode materials for modern energy storage systems, including supercapacitors, due to their layered structure, high surface area-to-volume ratio, and the presence of active surface functional groups. Titanium carbide (Ti_3C_2Tx), obtained by selective etching of the corresponding MAX phase Ti_3AlC_2, is of particular interest. However, the high cost of synthesizing the Ti_3AlC_2 MAX phase, accounting for up to 34% of the total cost of MXene production, significantly limits its industrial application.

This study investigates the feasibility of synthesizing the Ti_3AlC_2 MAX phase using locally available raw materials from Kazakhstan, specifically Ti, Al, and TiC. Experimental results show that optimizing synthesis parameters, including increasing the temperature to 1350 °C, pressing the precursors into pellets with an Al_2O_3 coating, and increasing the aluminum excess to 60%, allows for a Ti_3AlC_2 phase yield of up to 91.2%.

The electrochemical performance of the resulting Ti_3C_2Tx is comparable to that of commercial samples, demonstrating its suitability for use in supercapacitor electrodes. An economic analysis revealed that the production cost of one gram of Ti_3AlC_2 synthesized from local precursors is $0.22, which is more than 19 times lower than the cost of commercially available materials. This approach offers a cost-effective route for MXene production and highlights the potential of using local resources to develop competitive functional materials.

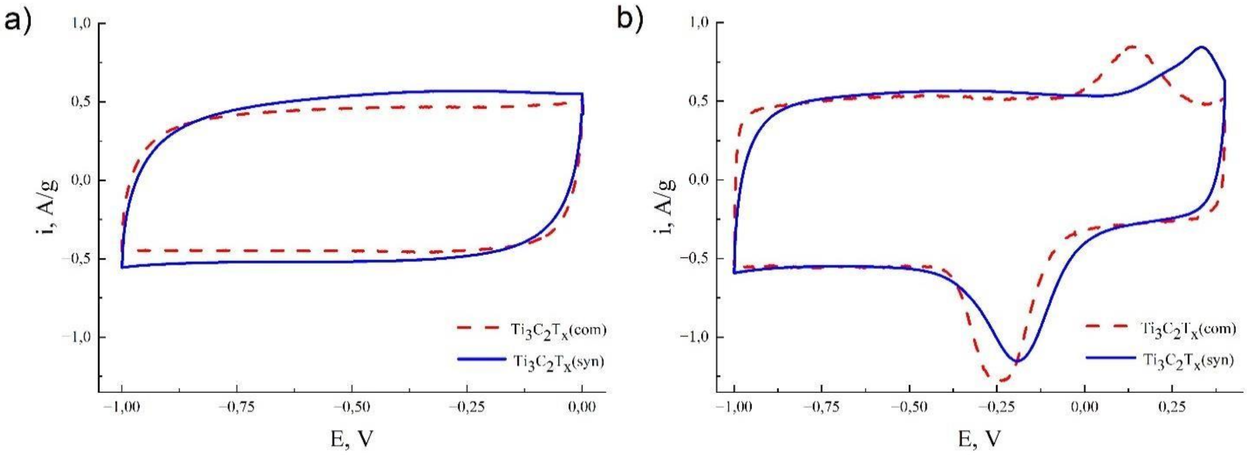

Figure 1. CV curves of 2 cycles of synthesized and commercial MXene Ti_3C_2Tx at a scan rate of 5 mV/s: a) -1 to 0 V range; b) -1 to 0.4 V range.

Optimization of the Ti_2AlC synthesis process by using Kazakhstani precursors

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Two-dimensional (2D) materials from the MXene family have emerged as a highly promising class of functional materials, widely studied due to their excellent electronic, thermal, and catalytic properties. These materials are derived from layered MAX phases, which are synthesized through high-temperature processes typically ranging from 1100 to 1450 °C. Among them, Ti_2AlC stands out as the main precursor for producing the MXene Ti_2C, a material that exhibits significant potential in applications such as supercapacitor electrodes and catalytic platforms for hydrogen evolution reactions (HER).

This work presents a comprehensive study on the multilevel optimization of Ti_2AlC synthesis, targeting the improvement of product yield, material quality, and process scalability. The novelty of this study lies in the use of locally sourced precursors from Kazakhstan, which not only reduces dependency on imported materials but also enables the development of a localized supply chain for advanced materials production. Specifically, the starting materials include titanium (Ti) and titanium carbide (TiC) powders, aluminum (Al) and aluminum carbide (Al_4C_3) powders from the Kazakhstan.

In this work we investigated two synthesis routes: a conventional Ti–TiC–Al system and an alternative Ti–C– Al_4C_3 system. The latter demonstrated superior performance in terms of product purity and process control, as Al_4C_3 offers higher thermal stability and better aluminium distribution, minimising its losses due to sublimation. Experiments revealed that optimal synthesis conditions are a temperature of 1350 °C and a dwell time of 2 hours, which yielded the highest Ti_2AlC content of 71.3%. These conditions were found to be reproducible and scalable, with a minimal drop in yield when the batch size was increased from 1 g to 100 g, thus validating the feasibility of industrial-scale production.

The synthesized Ti_2AlC was then successfully converted into MXene Ti_2CTx via selective etching using HCl and LiF, followed by delamination to form colloidal suspensions. A comparative analysis with commercial Ti_2AlC (Carbon-Ukraine) demonstrated that the synthesised material exhibited comparable morphology and electrochemical behaviour, confirming its viability for practical use. Electrochemical tests, including cyclic voltammetry, showed that Ti_2CTx derived from the Kazakhstan-sourced MAX phase exhibited a specific capacitance of 41–46 mAh/g, closely matching or somewhere even exceeding the commercial reference (37–44.2 mAh/g). Minor differences were attributed to variations in particle size, which influence the effective surface area and reactivity.

In summary, this study not only identifies optimal parameters for Ti_2AlC synthesis using local Kazakhstani resources but also confirms that the resulting MXene performs identically with international commercial standards. These findings open the path for the establishment of domestic production of MAX and MXene materials in Kazakhstan, fostering advancements in energy storage, hydrogen technologies, and high-performance nanomaterials. The approach demonstrates economic and technological relevance, offering a sustainable and scalable route toward next-generation functional materials based on 2D carbides.

Acknowledgments. This work is funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. BR27198753).

Application of Statistical Experimental Design for the Optimization of Synthesis Conditions: A Case Study of 3,4-Dihydropyrimidinethiones

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Microwave-assisted organic synthesis allows chemical reactions to proceed tens, hundreds, or even thousands of times faster. Reactions that previously required many hours to complete can now be finished within minutes. This shift in the temporal scale of chemical transformations significantly increases the importance of each second during the process. Both insufficient exposure time and excessive reaction duration can lead to reduced yields of the desired product. Various strategies have been proposed to identify optimal reaction conditions, including Full Factorial Design, Response Surface Methodology (RSM), Central Composite Design (CCD), Hartley’s method, Orthogonal Design, as well as gradient search techniques and evolutionary algorithms [1-4]. However, in most cases, these approaches involve a systematic exploration of factor combinations within predefined ranges, which considerably extends the overall duration of the investigation. Thus, determining optimal process conditions remains a highly relevant challenge.

To address this issue, we employed an orthogonal-composite experimental design method, which enables the simultaneous assessment of multiple factors, the construction of a regression model, and the reliable identification of optimal synthesis parameters. The solvent-free synthesis of 3,4-dihydropyrimidinethiones was carried out according to the following scheme:

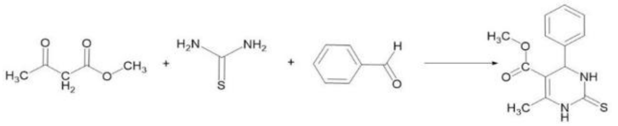

Figure 1. Scheme of the synthesis of 5-(ethoxycarbonyl)-6-methyl-4-phenyl-3,4-dihydropyrimidine-2(1H)-thione

The yield of the target product is influenced by a complex interplay of factors. In our initial model, we investigated the effects of microwave irradiation time and power using a two-factor, two-level experimental design. To perform a more comprehensive assessment that also included the molar ratios of ethyl acetoacetate, thiourea, benzaldehyde, and catalyst, we applied a six-factor second-order orthogonal-composite design. This approach enabled the construction of an adequate regression model and the determination of optimal synthesis conditions with high reliability.

As part of the experimental studies, over 27 trials were conducted to build the two-factor model and assess the influence of microwave power and reaction time. For the extended six-factor second-order orthogonal-composite model, more than 68 experimental runs were performed, covering a wide range of parameter variations. Quantitative determination of the product yield was carried out by thin-layer chromatography using spot area measurement, following the procedure described in reference [5].

The reliability of the experimental results was confirmed by spectral analysis methods (IR, NMR). Optimization of the synthesis conditions was performed using the desirability function approach in specialized software. The validity of the model was supported by statistical analysis. Data processing revealed that microwave power, reaction time, and catalyst amount had the most significant effect on the product yield. Under optimal conditions, the model predicted a yield of 76.93%. The application of the orthogonal- composite design allowed a 70% reduction in the number of required experiments.

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Bioactive Filament for 3D Printing of Medical Devices: A New Paradigm in Personalized Medicine

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Life expectancy, as well as the global population, continues to increase steadily. According to forecasts, by 2025 the number of musculoskeletal diseases leading to disability will rise by 30% compared to 2005 - from 2.1 to 3 million cases [1]. This trend highlights the urgent need for new technologies and materials aimed at the treatment and regeneration of bone tissue. Today, personalized medicine is becoming the standard in healthcare. One of its most effective tools is 3D printing - a precise, flexible, and rapid method for creating medical devices tailored to the unique anatomy of each patient. Software solutions for constructing 3D models based on CT and X-ray data are already well-developed and widely used. However, the range of bioactive filaments for the fabrication of personalized implants and scaffolds remains extremely limited - primarily consisting of polylactic acid (PLA) composites with calcium salts. This makes the development of novel filaments particularly relevant - materials that not only possess the necessary mechanical strength but also perform biologically significant functions, such as antibacterial protection and the stimulation of tissue regeneration. This is especially important for the treatment of bone defects, chronic inflammation, and prevention of implant-associated infections. In this study, we present the development of a bioactive filament fabrication technology [2-4]. The scheme is shown in the figure below:

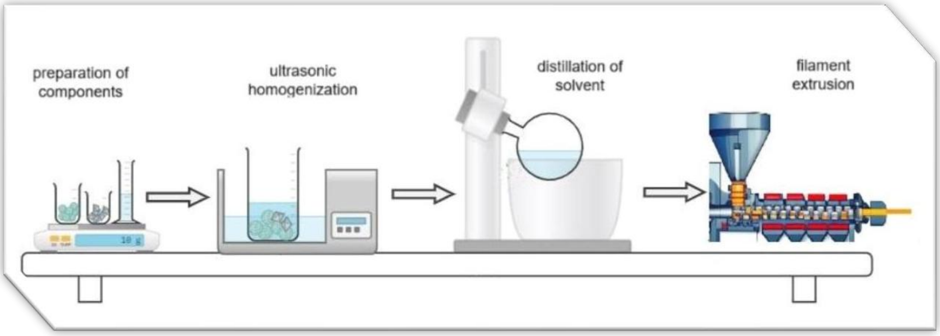

Figure 1. Flowchart of bioactive filament fabrication for 3D printing

The material's foundation is a biodegradable polymer matrix incorporating a complex of biofunctional additives: calcium salts, trace elements, and anti-inflammatory and antimicrobial agents with proven osteogenic and antimicrobial properties.

The material's comprehensive characterization included mechanical testing and microbiological testing per pharmacopoeial standards. The resulting composite demonstrated a combination of key properties: sufficient mechanical strength and pronounced antimicrobial activity against test strains—Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa and Bacillus subtilis.

These results confirm the developed material's potential for biomedical applications, including as part of functional, personalized implants created via additive manufacturing. This opens opportunities for further in vitro and in vivo studies and the translation of the technology into clinical practice.

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Sustainable Biomass-Derived Carbons for High-Performance Hydrogen Storage and Composite Integration with TiFe Alloys

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Hydrogen is a promising clean energy carrier, but the development of safe, efficient, and scalable hydrogen storage materials remains a major challenge. This study explores the use of abundant and renewable biomass resources—garlic peel, spent coffee grounds, and onion peel—as precursors for synthesizing high-surface-area activated carbons for hydrogen storage applications. Through chemical activation and carbonization, each biomass source was converted into porous carbon, with garlic peel-derived carbon (Cg) showing the highest performance. At 298.15 K and 100 bar, Cg exhibited an impressive excess hydrogen uptake of 1.51 wt%, among the highest reported for physisorption-based hydrogen storage under ambient temperature. In comparison, carbon derived from onion peel (Co) and spent coffee grounds (Cc) achieved 1.06 wt% and 0.68 wt%, respectively. The superior performance of Cg is attributed to its optimized pore structure and high surface area, which facilitate efficient hydrogen adsorption.To further enhance the practical utility of this material, a nanocomposite was synthesized by incorporating 1 wt% Cg into a TiFe intermetallic alloy via high-energy ball milling under an inert atmosphere to prevent oxidation. The resulting TiFe–Cg composite exhibited a significant increase in total hydrogen storage capacity, from 1.3 wt% to 1.6 wt%, along with improved oxidation resistance and accelerated sorption kinetics.

Study of YBCO superconductor thin film deposition using RF magnetron sputtering at NLA

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The second generation superconductor tapes have become a key element of modern energy and technology solutions. $YBa_2Cu_3O_{7-x}$ superconductor can transmit current densities more than 106A/cm^2.The production of 2G superconductor tapes is based on advanced thin-film technologies. The basis of such superconductor tapes are metal substrate Hastelloy C276, buffer layers (Al_2O_3,Y_2O_3, IBAD MgO, MgO-epi, $LaMnO_3$) and $YBa_2Cu_3O_{7-x}$ superconductor layer. Our main goal of the study is $YBa_2Cu_3O_{7-x}$ thin film fabrication by magnetron sputtering.

YBCO films have been deposited on $LaMnO_3$ substrates using ex-situ off-axis RF magnetron sputtering. Stoichiometric YBCO ($YBa_2Cu_3O_{7-x}$) ceramic targets were synthesized by the solid-state reaction method. High-purity Y_2O_3, $BaCO_3$, and CuO powders were mixed in a stoichiometric ratio of 1:2:3, ground thoroughly, and calcined at 950°C for 20 hours in air, followed by regrinding, pellet pressing at 300 bar.

The deposition system and thin film growth process are described in detail. Preliminary results demonstrate a significant improvement in film stoichiometry and surface morphology when using the off-axis geometry compared to the conventional on-axis configuration. Off-axis sputtering effectively minimizes the resputtering effect [1,2], leading to more uniform elemental distribution and better crystallinity.

The YBCO precursor were characterized using scanning electron microscopy to evaluate surface morphology. Additionally, energy-dispersive X-ray spectroscopy coupled with SEM was used to compare the elemental stoichiometry of films deposited using both off-axis and on-axis sputtering configurations. The analysis revealed that off-axis sputtering results in a composition significantly closer to the ideal Y:Ba:Cu = 1:2:3 ratio, while on-axis films showed noticeable deviations due to enhanced resputtering effects and non-uniform element distribution.

Additionally, optimal conditions for growing high-quality YBCO precuresor were established. These include:

1. Substrate positioned 8.0 cm horizontally and 5.0 cm vertically from the center of the target;
2. Substrate temperature is root temperature for $LaMnO_3$;
3. Sputtering atmosphere composed of $Ar:O_2$ in a 5:1 ratio at a total pressure of 10 mTorr.

These findings contribute to the development of a reliable method for fabricating high-quality YBCO films and provide a deeper understanding of growth mechanisms under off-axis ex-situ sputtering conditions.

The influence of deposition parameters—particularly temperature and oxygen pressure—on the ex-situ growth and superconducting properties of YBCO films is currently being optimized based on the approaches proposed by R. H. Hammond and R. Bormann [3]. This study outlines key components of the sputtering system, step-by-step optimization of sputtering parameters, and insights into the growth mechanism of YBCO superconducting films.

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Microbial water treatment combined with H_2 generation using GO-modified polymer membranes

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Water purification is a critical global issue, especially with the rising levels of organic contaminants in water sources, 25 billion people projected to be affected by 2050 [1]. The increasing demand for sustainable energy solutions has driven advancements in technologies that address both environmental concerns and energy needs. Here in we present a promising approach: the integration of microbial electrolysis cells (MECs) with wastewater treatment processes, offering a potential pathway for sustainable hydrogen production. This method leverages the unique capabilities of MECs, utilizing microbial activity to facilitate electrolysis and generate hydrogen gas efficiently. For this purpose, polymer polysulfone (PSF), polyamide (PA) and proton exchange (PE) membrane substrates were modified using graphene oxide (GO), owing its high surface area, reduce biofouling on the surface, hence enhancing selectivity due to GO's functional group. Batch of 23 bacteria (primarily Lactobacillus group) was used to further facilitate hydrogen generation. Graphite electrode was pretreated and modified using GO to reduce biofouling on the surface of the electrodes. Finally, two simultaneous MFCs illustrated in Figure 1 were assembled, where Cell (A) contains waste water with cultivated bacteria (left to react for 48 hrs) which was purified via polymer membrane and collected in Cell (B). Generation of H_2 was further analyzed in Gas Chromatograph (GC). Preliminary qualitative experiments revealed that electrogenic bacteria degrade organic pollutants from waste- water, leaading to efficient electron transfer and subsequent hydrogen production 5 times more when PE membranes and electrodes were coated with GO. Modification of the surface reduced membrane fouling and improved microbial access to pollutants. Higher H_2 yields linked to improved electron transfer facilitated by GO.

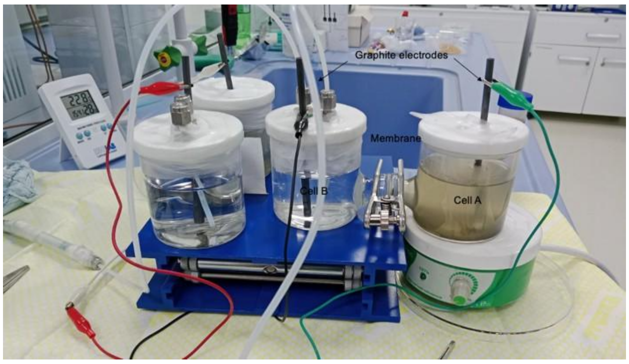

Figure 1. Assembled two simultaneous MECs with polymer membranes interconnecting cells.

Figures and tables should be referred to in the text with the proper numbering. The figures are reproduced in gray scale.

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Molten-Salt Synthesis of $LaNiO_3$ in Eutectic Media

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The synthesis of rare-earth nickelates, such as $LaNiO_3$, is of significant interest in contemporary materials science due to their distinctive electronic, magnetic, and catalytic properties [1]. These compounds, containing Ni^{3+}, are utilized in supercapacitors, heterogeneous catalysis, and are considered as key precursors for the preparation of infinite-layer nickelates with superconducting behavior [2][3][4]. Conventional solid-state methods typically require high temperatures and elevated oxygen pressures to stabilize Ni^{3+}, which limits the reproducibility and scalability of the process [5][6].

In this work, a soft-chemistry route for $LaNiO_3$ synthesis is proposed, based on a low-temperature reaction in a KI-KCl eutectic melt with KNO_3 serving as an oxidizing agent. A mixture of oxide precursors and salts was homogenized and annealed in quartz crucibles at 700 °C for 11 hours. Systematic optimization of synthesis conditions revealed that the oxide-to-salt ratio and KNO_3 content are critical for phase selectivity. According to X-ray diffraction analysis, the highest yield of the $LaNiO_3$ phase, with NiO impurities, was obtained at 20 wt% KNO_3.(See Figure 1). In contrast, the absence of either the molten medium, the oxidizer, or the use of excessive amounts of KNO_3 led to the formation of undesirable phases, including unreacted starting materials, La_2O_3, and mixed-valence nickelates containing both Ni^{2+} and Ni^{3+}. Remarkably, $LaNiO_3$ formation was observed at both low (1:1) and high (1:10) oxide-to-salt ratios. The results confirm the applicability of molten-salt synthesis with controlled oxidation for stabilizing high-valent nickelates such as $LaNiO_3$, and indicate its potential for broader use across the $RNiO_3$ family.

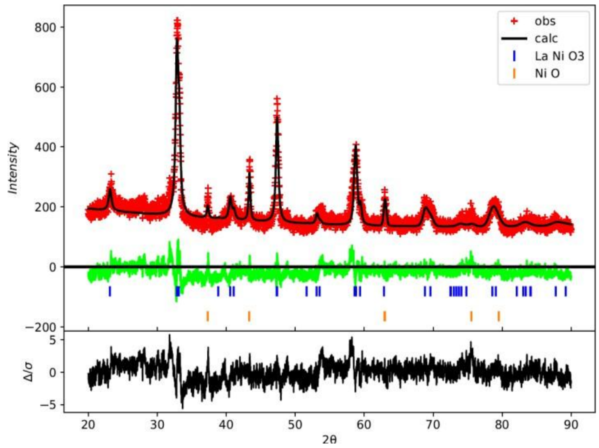

Figure 1. Experimental (red) and calculated (black) X-ray diffraction patterns and their difference profile (blue) for the X-ray diffraction pattern of $LaNiO_3$ using the Le Bail method by GSAS-II program

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PEDOT:PSS-Integrated Hydrogel Electrolyte for Biocompatible Energy Storage Device

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The increasing global demand for efficient and reliable energy storage systems has led to intensive research in developing advanced materials for batteries, supercapacitors, and hybrid devices [1-2]. However, most commercial materials currently used in these systems are derived from fossil fuels, are non-biodegradable, and often involve toxic synthesis routes [3]. This brings major concerns about long-term environmental sustainability and safety, especially in emerging fields like wearable and implantable electronics. PEDOT:PSS-based soft conductive hydrogels are considered promising materials for flexible and biocompatible energy storage systems due to their electronic conductivity and ability to retain electrolyte. However, their low structural integrity and lack of integration with ionic-conductive matrices limit their practical use [4].

In this study, we report the development of a biocompatible hydrogel matrix integrated with a conductive polymer, PEDOT:PSS, for application as a solid-state electrolyte in zinc-based energy storage systems. The hydrogel was synthesized via thermal polymerization of a precursor solution containing N-vinylpyrrolidone (NVP), tetraethylene glycol dimethacrylate (TEGDMA), and polyethylene glycol (PEG-400), using Luperox as an initiator at 80 °C. PEDOT:PSS was introduced directly into the monomer mixture prior to crosslinking, resulting in a uniform dispersion within the polymer network. Post-polymerization, the hydrogel was immersed in $ZnSO_4$ solution to impart ionic conductivity.

The designed hydrogel exhibits high swelling capacity in aqueous electrolytes, mechanical robustness, and sufficient flexibility for self-supporting use in different devices. The formulation is currently being optimized with respect to PEG content and crosslinking density to enhance porosity and ion transport. Characterization of the material's structural and physicochemical properties is performed using Fourier-transform infrared spectroscopy (FTIR), swelling ratio analysis, and scanning electron microscopy (SEM). Electrochemical performance will be assessed via impedance spectroscopy (EIS), cyclic voltammetry (CV), and charge–discharge cycling (GCD).

This study provides insight into the development of multifunctional hydrogel-based electrolytes that combine ionic and electronic transport, with potential use in flexible, biocompatible energy storage systems.

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Sustainable Upcycling of Acrylonitrile Butadiene Styrene (ABS) Plastic into Carbon Material for Lithium-Ion Battery Anodes

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The extensive usage of 3D printing technology has resulted in a large buildup of plastic waste, especially Acrylonitrile Butadiene Styrene (ABS), a thermoplastic that is frequently utilized but presents major environmental problems because it is not biodegradable. This study offers a sustainable upcycling method for turning waste ABS plastic from 3D printing into carbon material, which may then be used as an anode material in lithium-ion batteries (LIBs). ABS plastic waste was crushed and crosslinked using sulfuric acid at 120 °C. Prior to carbonization, the ABS waste was pre-oxidized in air at 300 °C to improve thermal stability and avoid melting. To create carbon material with a disordered structure, carbonization was then performed at temperatures between 600 and 1100 °C in a argon environment. The carbon material with enlarged interlayer spacing and appropriate surface characteristics for lithium storage was confirmed by material characterization using X-ray diffraction (XRD), Raman spectroscopy, and scanning electron microscopy (SEM) analysis. The active material obtained was used to fabricate an anode material, which demonstrated a reversible specific capacity of around 200 mAh/g. Ongoing efforts are focused on improving its properties to develop a stable anode with high coulombic efficiency and good cycling stability. This work illustrates an economical and sustainable method of turning plastic waste into high-performance energy storage materials, supporting the development of lithium-ion battery technology as well as the objectives of the circular economy. A brief summary of this work is presented in Figure 1.

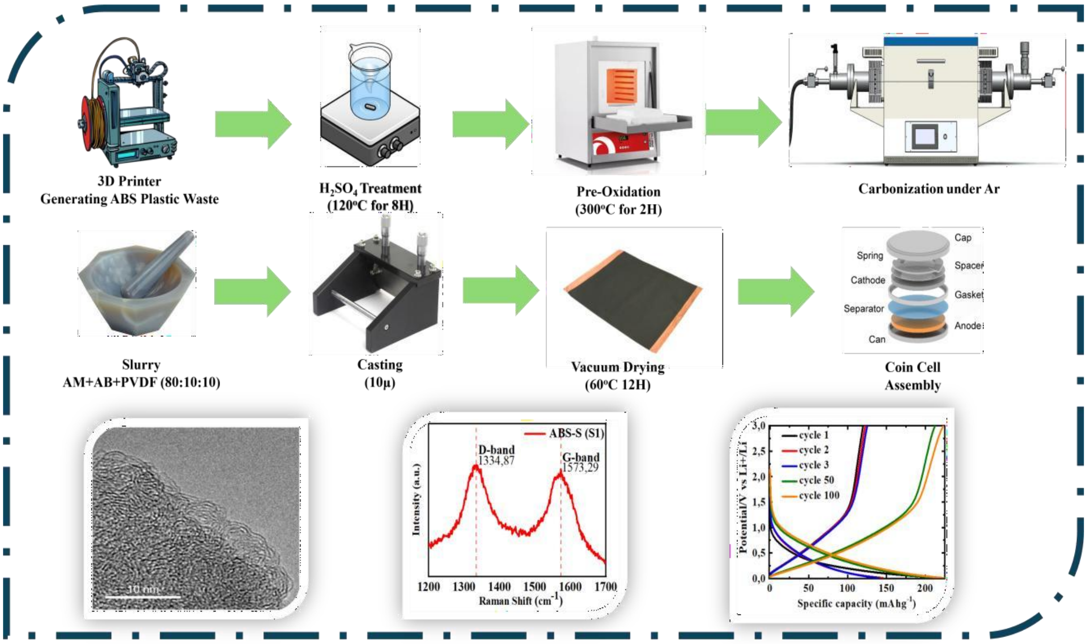

Figure 1. Schematic illustration of the upcycling process of ABS plastic waste into carbon anode material for lithium-ion batteries

Keywords: Acrylonitrile Butadiene Styrene (ABS), hard carbon, lithium-ion batteries, anode material, plastic upcycling, sustainable energy storage, carbonization, pre-oxidation.

Acknowledgements. This study was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (grant No. BR24992766, grant No. AP23483880).

Fabrication of Versatile Nanocomposite Materials For Advanced Electrochemical Applications

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Lithium-sulfur batteries gain interest based on the potential of high theoretical capacity, abundance of sulfur, and eco-friendliness. The practical realization of lithium-sulfur batteries is, nonetheless, subject to innumerable challenges like poor electrical conductance of sulfur and its reduction products, lithium polysulfide solubility and diffusion, shuttle effect, and enormous charge-discharge- induced volume changes. These lead to rapid capacity fading, low efficiency, and short durability. This study focuses on the synthesis and characterization of titanium dioxide (TiO_2) nanotubes modified with nickel to enhance electrochemical performance in lithium-sulfur (Li–S) batteries. The hydrothermally synthesized TiO_2 nanotubes were decorated with nickel and nickel oxide to enhance conductance and overcome Li–S battery's limitations like the polysulfide-based shuttle effect and poor cycling life. The development of these nanocomposites was confirmed by SEM, EDS, and XRD. Electrochemical characterization through electrochemical impedance spectroscopy, cyclic voltammetry, and cycling charge-discharge tests are underway to analyze their properties. Preliminary results reveal initial specific capacities as high as 1192 mAh g^{-1} at 0.2 C and demonstrate excellent cycling stability with a low-capacity decay rate of approximately 0.078% per cycle over 100 cycles. The results demonstrate that the nickel- decorated, TiO_2 nanotubes-based nanocomposites significantly enhance the lithium polysulfide's reaction throughput and overall efficiency and durability of Li–S batteries and hold a bright future to be the one powering the next generation of energy storage devices.

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Sustainable Hydrogen Storage via Upcycled Graphite from End-of-Life Lithium- Ion Batteries

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The accelerating growth of electric vehicles and portable electronics has driven a sharp increase in lithium-ion battery (LIB) production, with global demand expected to exceed 1100 GWh by 2025. As these batteries reach end-of-life, they produce substantial waste-particularly graphite anodes, which account for 12-21 wt% of LIBs and up to 15% of their economic value, yet remain underutilized in current recycling processes [1]. This study proposes an upcycling approach to convert spent graphite anodes into functional materials for hydrogen storage.

Graphite undergoes structural degradation during cycling, including increased interlayer spacing (from 0.335 nm to >0.370 nm) and the formation of defects such as cracks and unstable SEI layers [2]. While unfavorable for battery reuse, these features increase porosity and surface area-key properties for hydrogen adsorption via physisorption. Hydrogen storage in carbon materials is highly surface-dependent, with reported capacities up to 6.5 wt% for carbon nanofibers and 4.48 wt% for graphite [3]. Performance can be further enhanced through doping and composite strategies [4].

We present a selective binder-removal technique that preserves intercalated lithium ions, enabling chemisorption-driven hydrogen uptake. Spent LIBs were disassembled, and the anodes treated either by deionized water washing or heat treatment at 550 °C. Thermogravimetric analysis (TGA) revealed that both methods yielded similar organic content removal, but heat treatment more effectively preserved lithium, thus improving hydrogen storage potential.

The resulting upcycled graphite exhibits expanded interlayer spacing and defect structures conducive to both physisorption and chemisorption. Further modification via exfoliation, heteroatom doping, and metal nanoparticle decoration enhances porosity, active sites, and hydrogen binding energy. These engineered characteristics highlight the promise of spent LIB graphite anodes as multifunctional materials for solid-state hydrogen storage.

Acknowledgments. This work was supported by the Collaborative Research Project (CRP) titled "End-of-Life" Lithium-Ion Batteries Graphite Anode Upcycling: Fundamentals and Application in Hydrogen Storage under project number 111024CRP2005.

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Temperature-driven phase transition and defect engineering in $Na_2Mn_3O_7$ layered cathodes for sodium-ion batteries

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Interest in lithium-ion battery (LIB) substitutes has increased globally due to the rising need for sustainable and reasonably priced energy storage technologies. Among these, sodium-ion batteries (SIBs) have emerged as a promising next-generation solution, particularly for large-scale stationary applications. Owing to the natural abundance, wide geographic distribution, and lower cost of sodium resources compared to lithium, SIBs offer an economically viable and environmentally friendly alternative [1]. One of the most extensively researched and realistically feasible cathode families for SIBs is represented by layered transition metal oxides Na_xTMO_2 (TM = transition metal). Because of their extensive redox chemistry, these materials can accommodate various transition metal oxidation states, have a wide range of structural versatility, and have high theoretical capacities. Because manganese is abundant, inexpensive, and non-toxic, manganese-based layered oxides in particular have garnered a lot of interest. $Na_2Mn_3O_7$, a layered oxide with a high manganese content, stands out due to its high Na content and unique structure, making it a potential candidate for high-energy-density cathodes. Yet to reach its full potential, issues such as capacity fading, slow kinetics, and structural phase transitions need to be resolved [2].

In this work, we report a systematic study on the synthesis of $Na_2Mn_3O_7$ at temperatures ranging from 500 ºC to 900 ºC for 10 hours in an oxygen atmosphere. Structural characterization using X-ray diffraction (XRD) reveals a clear temperature-driven phase transformation: samples synthesized at 500-600 ºC adopt a triclinic P-1 space group, whereas those synthesized at 650 ºC and above crystallize in a hexagonal P2-type structure. This phase transition is accompanied by a significant increase in crystallite size and a reduction in structural disorder. Electrochemical testing demonstrates that the sample synthesized at 500 ºC delivers a slightly higher specific capacity compared to those prepared at 550 ºC and 600 ºC, despite its lower crystallinity. The intensity increase in the diffraction peaks with temperature suggests improved crystallinity, but this correlates with a reduction in capacity, likely due to decreased sodium diffusivity and reduced redox-active defect sites. Our findings highlight the importance of defect engineering and phase control in tuning the electrochemical performance of $Na_2Mn_3O_7$.This study provides new insights into the structure–property relationships of layered Mn-based oxides and offers a foundation for optimizing synthesis parameters to enhance SIB cathode performance. These results contribute to the growing understanding of metastable low-temperature phases and their potential advantages for high-energy sodium-ion battery applications.

Acknowledgements. This research was funded by Nazarbayev University under Collaborative Research Program Grant No. 20122022P1611, AK.

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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) are widely regarded as the leading energy storage technology, owing to their low cost, high energy density, reliable performance, and extended lifespan. These attributes make LIBs indispensable for a wide range of applications, especially in the transportation sector where they power electric vehicles (EVs), and in the energy sector where they enable the integration and storage of renewable energy sources such as solar and wind. As the demand for more efficient and higher-capacity batteries grows, researchers have turned their attention to the development of advanced cathode materials capable of delivering better performance.

Among various lithium-ion battery (LIB) cathodes, nickel-rich layered oxides have attracted widespread attention due to their ability to achieve higher specific capacities and energy densities, attributed to their high nickel content [1]. Notably, NCM811 ($LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$) and NCA811 ($LiNi_{0.8}Co_{0.1}Al_{0.1}O_2$) are two prominent examples, sharing similar compositions and layered crystal structures [2]. Both materials can deliver capacities of approximately 200 mAh g^{-1} at an average voltage of 3.6 V. These materials feature similar layered crystal structures and have demonstrated promising electrochemical behavior in various studies [3].

In this research, we focus specifically on NCA811 and explore its synthesis using the electrospinning technique, which provides a novel approach to producing free-standing, binder-free cathodes [4]. The process involves electrospinning a polymer solution mixed with metal salts to form one-dimensional nanofibers, followed by a multi-step thermal treatment to obtain the final crystalline product. Characterization using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) confirmed the formation of uniform, well-crystallized nanofibers. Furthermore, energy-dispersive X-ray spectroscopy (EDS) showed a homogeneous distribution of nickel, cobalt, and aluminum, while X-ray diffraction (XRD) patterns verified the successful formation of a pure layered NCA811 phase.

Despite ongoing challenges such as phase transitions and microcrack formation during cycling at high voltages, Ni-rich cathodes like NCA811 continue to show great promise. The free-standing NCA811 electrode demonstrated good initial electrochemical performance. Continued testing will help evaluate long-term stability and cycling behavior. These findings may contribute to lead the way for future innovations in cathode morphology and structural design, contributing to the development of lightweight, efficient, and sustainable lithium-ion batteries.

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Carbonization of Polypropylene via Green Pretreatment: A Route to Sustainable Anode Materials for Lithium-Ion Batteries

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Waste polypropylene (PP) poses significant environmental challenges due to its non-degradability and common disposal methods such as incineration or landfilling [1]. Converting PP into carbon materials for lithium-ion battery (LIB) anodes offers a sustainable alternative [2] but typically involves harsh chemical treatments to improve thermal stability and carbon yield. This study introduces a novel, eco-friendly method that utilizes a bio-derived additive—composed of chitosan, montmorillonite, and sodium phytate—to enhance the thermal resistance of PP during carbonization. The additive, incorporated at 5 wt% through ball milling, effectively suppresses PP decomposition above 400 °C and increases residual carbon retention. The resulting carbon materials were characterized by Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), X-ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM) to investigate their structural and morphological features. Electrochemical performance was evaluated using galvanostatic charge–discharge, cyclic voltammetry, and electrochemical impedance spectroscopy, demonstrating the material's potential as a viable anode in LIBs. These findings highlight a promising pathway for sustainable plastic waste valorization through green chemistry and energy storage innovation.

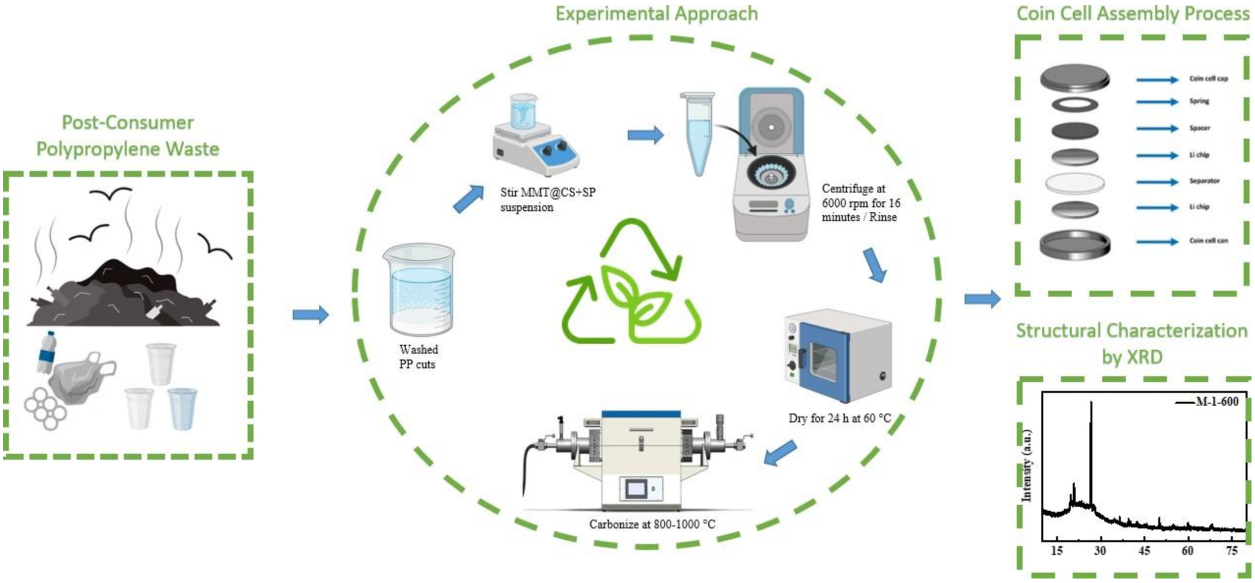

Figure 1. A schematic representation of the eco-friendly upcycling process that converts polypropylene (PP) waste into carbon anode material for lithium-ion batteries.

Keywords: Waste polypropylene, lithium-ion batteries, anode material, upcycling, plastic recycling, sustainable energy storage, carbonization.

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Cathode and Electrolyte Optimization Strategies for Room-Temperature Sodium–Sulfur Batteries

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With the rapid increase in demand for sustainable and low-cost energy storage systems, sodium–sulfur (Na–S) batteries have attracted significant attention due to the natural abundance of their components and high theoretical energy density (up to 1274 Wh kg^{-1}) [1]. Room-temperature Na–S (RT-Na/S) systems have been considered especially promising, as improved safety and reduced operational costs have been provided compared to high-temperature counterparts [2].

However, the practical implementation of RT-Na/S batteries has been hindered by several critical challenges, including low electrical conductivity of sulfur, large volume changes during cycling, dissolution and shuttle effects of polysulfides, as well as sodium dendrite growth and instability of the liquid electrolyte interphase (SEI) [3],[4]. These issues have been addressed through the development of carbon-based cathode composites, chemical immobilization of polysulfides, and electrolyte optimization [5,6]. Significant enhancement of the stability and reversibility of reactions in RT-Na/S systems has been demonstrated by these approaches, which bring these batteries closer to practical applications [7].

In this work, porous hard carbon was synthesized from biomass — buckwheat seeds — and was utilized as a matrix for sulfur composite cathodes. Both physical confinement and partial chemical binding of polysulfides have been facilitated by this structure. Electrolyte optimization was carried out based on $NaClO_4$ with the addition of $NaNO_3$ and fluoroethylene carbonate (FEC). The addition of 0.2 M $NaNO_3$ to 1 M $NaClO_4$ solution was shown to improve cycling stability and discharge capacity (up to 186.91 mAh g^{-1}), while an increase in $NaNO_3$ concentration to 0.3 M raised the initial capacity to 283.21 mAh g^{-1} but deteriorated long-term stability. Negative effects of FEC on electrode stability have been observed. This study hypothesizes that targeted electrolyte optimization enhances not only the electrochemical environment but also promotes more efficient interaction with the sulfur–carbon composite cathode, leading to a synergistic improvement in battery performance.

Despite the achieved progress, limitations in the stability and effectiveness of polysulfide binding remain. Further studies are being conducted to improve both the electrolyte composition and cathode structure.

Acknowledgements. This research was funded by the research targeted program BR21882402 “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.

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Upcycling of waste PET into nitrogen-doped hard carbon for sodium-ion battery anodes

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The growing demand for energy storage and the rising cost and limited availability of lithium have prompted the exploration of alternative battery technologies. Sodium-ion batteries (SIBs) have emerged as a promising substitute due to sodium's natural abundance, low cost, and similar chemical properties to lithium [1]. Concurrently, the global plastic crisis driven by rapidly growing polyethylene terephthalate (PET) production and consumption calls for sustainable recycling strategies. Recent studies suggest that recycled PET can serve as a viable precursor for carbon materials in SIB anodes, offering high structural stability, conductivity, and surface area [2]. However, challenges remain in optimizing synthesis processes and ensuring the long-term electrochemical performance of such materials, necessitating further innovation in material design and processing.

In this study, nitrogen-doped hard carbon (N-HC) was synthesized via direct pyrolysis of PET waste in the presence of a nitrogen source, aiming to introduce structural defects and heteroatom functionalities to enhance sodium storage capability. The resulting carbon was thoroughly characterized using Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), X- ray diffraction (XRD), Raman spectroscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM) to investigate its structural and morphological features.

Electrochemical performance was evaluated through galvanostatic charge–discharge tests and cyclic voltammetry (CV). The nitrogen doping was found to significantly improve electrical conductivity, provide additional active sites, and enhance sodium-ion intercalation behavior compared to non-doped carbon materials.

Acknowledgements. This study was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (grant No. BR24992766, grant No. AP23483880).

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Fabrication of Versatile Nanocomposite Materials for Advanced Electrochemical Applications

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The practical application of lithium sulfur batteries (LSBs) is hindered by sluggish electrochemical kinetics, severe shuttle effects caused by lithium polysulfides (LiPS), and poor cycle stability. In this study, a composite cathode architecture is proposed, where carbon nanofiber (CNF)-based electrodes are modified using catalytic materials synthesized by decorating hollow titanium dioxide nanospheres (TiO_2 HNSs) with magnetic single-atom catalyst (Ni-SAC) and the corresponding metal oxide (NiO). This decoration approach enables the formation of catalytic nanoparticles (10 – 25 nm) uniformly dispersed across the TiO_2 HNSs surface.

Comprehensive structural analysis using SEM, TEM, XRD, and EDS, along with BET surface area measurements, confirmed the uniform decoration and porous morphology of Ni- and NiO-decorated TiO_2 HNSs. Electrochemical performance, evaluated at a sulfur loading of ~1.5 mg cm-2, was systematically assessed via cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and charge-discharge testing. Preliminary results revealed that bare TiO2 HNSs delivered an initial specific capacity of 1300.8 mA h g^{-1}, which decreased by 38.9% after 100 cycles at 1.0C. In contrast, NiO-TiO_2 HNSs exhibited significantly improved stability, with only a 17.9% capacity loss under identical conditions. The outcomes of this work disclose the advantageous synergistic role of Ni and NiO nanoparticle decoration on TiO_2 HNSs as a promising strategy to achieve high-performance LSBs.

Upcycling of LDPE and HDPE into Carbon Anode Materials for Lithium-Ion Batteries: Advancing Sustainable Energy Storage Technologies

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In the context of sustainable development and the transition to a circular economy, the conversion of polymer waste into high value- added materials for energy storage systems represents an important scientific and technological challenge [1]. This study examines the transformation of low-density polyethylene (LDPE) and high-density polyethylene (HDPE) into carbon anode materials for lithium-ion batteries (LIBs) via a multistep process including sulfonation (crosslinking), pre-carbonization at 350 °C, and final carbonization at temperatures ranging from 600 to 900 °C.

The exposure to concentrated sulfuric acid (98%) initiates the sulfonation reaction, accompanied by the substitution of hydrogen atoms with sulfonic groups ($–SO_3H$). Due to its pronounced dehydrating and acidic properties, sulfuric acid facilitates the formation of a densely crosslinked polymer network [2]. Crosslinking of LDPE and HDPE at 170 °C for 4 hours results in a mass increase of up to 44.3% and 2.7%, respectively, reflecting different degrees of chemical modification owing to their distinct physicochemical properties. Following sulfonation, both polymers turn black, indicating a profound chemical transformation. HDPE retains its shape but develops macrocracks on the surface (Fig. 1g), while LDPE disintegrates into fragments (Fig. 1c) [3]. This difference is attributed to the higher crystallinity of HDPE, which restricts acid diffusion, whereas the amorphous, branched structure of LDPE promotes deeper acid penetration and facilitates the formation of sulfonate groups and C=C double bonds [4]. Final carbonization in an argon atmosphere, following intermediate pre-carbonization at 350 °C, improves the properties of the resulting carbon — increasing specific surface area and porosity, and potentially enabling heteroatom doping (Fig. 1d, h). These enhancements lead to improved electrochemical performance of the anode materials, particularly in terms of specific capacity and cycling stability [5].

The effectiveness of the proposed method is confirmed by comprehensive physicochemical characterization (FTIR, SEM-EDS, TGA, XRD, and Raman spectroscopy) and electrochemical testing (cyclic voltammetry, galvanostatic charge-discharge cycles, and performance evaluation).

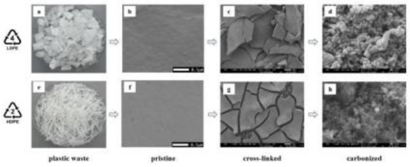

Figure 1. Photographs and SEM images of HDPE and LDPE at each stage of processing. (a) raw LDPE, (b) pristine LDPE, (c) cross- linked LDPE, (d) carbonized LDPE; (e) raw HDPE, (f) pristine HDPE, (g) cross-linked HDPE, (h) carbonized HDPE.

In conclusion, this work presents a promising strategy for the upcycling of polyethylene waste into functional carbon materials for next-generation battery technologies, offering a pathway to reduce the environmental impact of plastics and promoting the development of green energy.

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.

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Activated porous carbon from waste PET bottles as a high-performance sulfur host for lithium–sulfur batteries

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Plastic pollution is a global environmental challenge, spurring interest in sustainable waste valorization [1]. One promising approach is the upcycling of waste plastics into functional carbon materials for energy storage applications. Polyethylene terephthalate (PET) from single-use bottles is particularly attractive as a carbon precursor due to its high carbon yield and global abundance [2]. Lithium–sulfur (Li–S) batteries offer exceptional theoretical capacity (≈1675 mAh/g) and high energy density, but their practical application is hindered by rapid capacity decay caused by the polysulfide shuttle effect. Developing advanced porous carbon hosts for sulfur is therefore critical to improve Li–S battery performance and stability. In this study, we simultaneously address plastic waste valorization and Li–S performance by converting waste PET into a hierarchical porous carbon host for sulfur cathodes.

PET waste bottles were thermally converted into carbon-rich material through pyrolysis at 500 °C under a nitrogen atmosphere, followed by chemical activation using potassium hydroxide (KOH). The resulting carbon exhibited a hierarchical porous architecture, confirmed by nitrogen adsorption-desorption isotherm analysis. This porous carbon was then employed to fabricate a sulfur-carbon composite electrode via a straightforward melt-diffusion method. Electrochemical performance was evaluated in model Li–S cells using an electrolyte composed of 1 M lithium bis(trifluoromethanesulfonyl)imide (LITFSI) and 2% lithium nitrate ($LiNO_3$) dissolved in a 1:1 mixture of 1,2-dimethoxyethane (DME) and 1,3-dioxolane (DOL). The assembled Li–S cells with this composite cathode demonstrated stable cycling and high reversibility. Therefore, the activated porous carbon derived from PET waste holds significant potential as a key material for Li–S battery cathodes.

These findings highlight the significant potential of PET-derived hierarchical porous carbons as efficient sulfur hosts, providing a sustainable solution to plastic waste issues while enhancing Li-S battery performance.

Acknowledgements. This study was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (grant No. BR24992766, grant No. AP23483880).

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Solvent-assisted catalytic decomposition of PMMA into carbon anode material for lithium-ion batteries

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The sustainable transformation of polymer waste into electrochemically active carbon materials presents a promising route for lithium-ion battery (LIB) technology [1,2]. Polymethyl methacrylate (PMMA), a common acrylic plastic, was selected as a precursor due to its carbonizable backbone and industrial abundance. However, the thermal decomposition of PMMA typically results in a low carbon yield, which limits its direct application in carbon material synthesis. In this work, we present a solvent-assisted approach to enhance the carbonization efficiency of PMMA through catalytic activation, enabling its conversion into functional anode materials for LIBs.

In this work, PMMA was first dissolved in ethyl acetate (EA), propylene carbonate (PC), or dimethyl carbonate (DMC) under mild thermal agitation. Zinc chloride ($ZnCl_2$) was added in a 1:1 weight ratio as a porogen and catalytic agent. The dried mixture underwent carbonization in argon atmosphere at 750 °C, followed by acid washing and vacuum drying. The resulting carbon was used as the active material in coin cells (CR2032), assembled with lithium foil and 1 M $LiPF_6$ electrolyte in EC/DMC.

The anode material obtained using ethyl acetate (EA) demonstrated promising electrochemical performance, delivering a specific capacity of up to 420 mAh g^{-1} at a current density of 0.1 A g^{-1} (Figure 1). After 100 cycles, the electrode retained over 90% of its initial capacity, indicating excellent cycling stability.

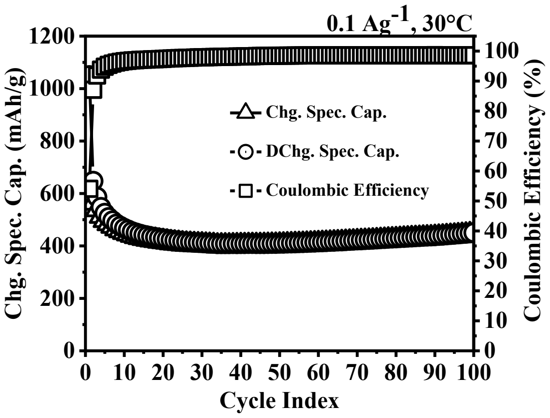

Figure 1. Cycling performance of the PMMA-derived carbon electrode at 0.1 A g^{-1} and 30 °C over 100 cycles

This study demonstrates that the use of solvent-assisted $ZnCl_2$ activation significantly enhances the carbon yield from PMMA, overcoming the typically low residue resulting from its thermal decomposition. The combination of solvent dissolution and catalytic carbonization enabled the formation of porous carbon structures suitable for lithium-ion storage. The obtained material exhibited high reversible capacity, excellent cycling stability, and favorable charge-transfer characteristics.

Acknowledgments. This study was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (grant No. BR24992766, grant No. AP23483880).

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Recycling polyethylene terephthalate (PET) waste into fibrous separators for lithium batteries

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Plastic pollution is one of the most pressing environmental issues today, yet plastics remain vital in sectors like healthcare, technology, construction, and advanced textiles due to their unique properties—such as thermal resistance, sterilizability, and mechanical strength—that are hard to replace depending on the polymer type [1]. PET is a lightweight material with excellent mechanical properties, and thus it is one of the most considered polymers for the development of flexible functional devices [2].

Plastic waste serves as a major feedstock for the production of PET, which has emerged as a promising separator material for lithium-ion batteries (LIBs) due to its outstanding thermal stability, mechanical strength, high tensile resilience, low thermal shrinkage, and excellent electrical insulation [3].

In this study, fiber-based separators for LIBs were successfully fabricated by recycling plastic cups commonly used for cold beverages. The morphology of the as-prepared separators were thoroughly investigated using scanning electron microscopy (SEM) and cross-sectional analysis to evaluate their structural integrity and suitability for electrochemical applications.

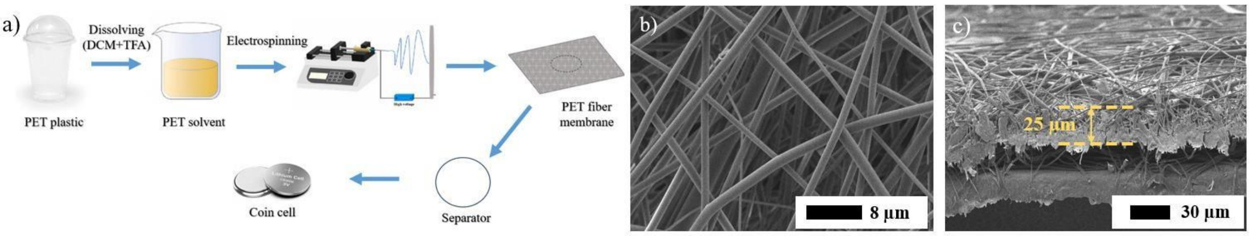

Figure 1. a) Schematic illustration of the fabrication process of fibrous separators from plastic cups; b) surface morphology of the obtained fibers characterized by scanning electron microscopy (SEM); c) cross-sectional SEM image illustrating the internal structure of the obtained fibers.

The overall preparation method and morphological characteristics of the PET-based fibrous separators are shown in Figure 1. As illustrated in Figure 1a, disposable PET plastic cups were dissolved in a suitable solvent system (trifluoroacetic acid (TFA)+dichloromethane(DCM)) and processed via electrospinning to form fibrous membranes, which were subsequently used as separators in coin cells. The surface morphology of the resulting fibers is presented in Figure 1b, revealing a uniform and interconnected network. Additionally, the cross-sectional SEM image in Figure 1c demonstrates the internal layered structure and fiber distribution throughout the membrane, which has an overall thickness of approximately 25 µm, confirming its suitability for lithium-ion battery applications.

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.

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Enhanced Biowaste-Derived Hard Carbons Enabling High-Performance Sodium-Ion Batteries For Future Energy Storage Systems

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The pursuit of sustainable and efficient energy storage solutions has spotlighted sodium-ion batteries (SIBs) as a promising alternative to lithium-ion systems. A critical challenge in advancing SIB technology lies in developing high-performance anode materials that are both cost-effective and environmentally friendly [1][2]. In this study, we present the synthesis of enhanced hard carbon (HC) anodes derived from coffee waste, a readily available biowaste resource. Utilizing a controlled synthesis approach, we optimized pre-oxidation and high-temperature pyrolysis parameters to tailor the porous architecture and reduce specific surface area, thereby promoting the formation of closed-pore structures conducive to reversible sodium storage [3]. Post-synthesis treatments, including hydrogen (H_2) reduction to eliminate surface functional groups and chemical pre-sodiation to compensate for initial sodium loss, were employed to further enhance electrochemical performance. The resulting HC anodes exhibited a remarkable initial Coulombic efficiency (ICE) exceeding 75%, a reversible capacity of 300 mAh g^{-1} at a current density of 20 mA g^{-1}, and excellent cycling stability. These findings underscore the potential of coffee waste-derived hard carbons as scalable and eco-friendly anode materials for next-generation SIBs, aligning with global efforts toward sustainable energy storage solutions.

Keywords: Sodium-ion batteries, Hard carbon, Biowaste, Coffee waste, Initial Coulombic Efficiency, Pre-sodiation, Hydrogen reduction, Surface area tuning, Sustainable energy storage.

Acknowledgments. This research was carried out under the project "Enhancement of the Initial Coulombic Efficiency of the Biowaste-derived Hard Carbon as an Anode for Sodium-ion Batteries" from Government of Republic of Kazakhstan (RK).

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Polycarbonate-Modified PTHF-based SPE for solid-state Li-SPAN cell

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Solid-state lithium-ion batteries incorporating polymer electrolytes represent a promising pathway toward the development of next-generation energy storage systems with enhanced energy density and safety. Among them, solid polymer electrolytes (SPE) are particularly attractive due to their flexibility, processability, and potential to suppress lithium dendrite growth. However, practical application remains hindered by limitations such as low ionic conductivity at room temperature, poor interfacial stability, insufficient mechanical strength, and suboptimal electrode–electrolyte contact[1][2][3].

In this work, a novel UV-curable solid polymer electrolyte film was developed based on acrylated polytetrahydrofuran (aPTHF) as the host polymer, bis(trifluoromethanesulfonyl)imide lithium salt (LiTFSI) as the lithium source, and a dual-crosslinking network formed by poly(ethylene glycol) diacrylate (PEGDA) and ethoxylated trimethylolpropane triacrylate (ETPTA). To enhance ionic mobility and electrochemical performance, propylene carbonate (PC)-based plasticizers were incorporated into the formulation. The effect of plasticizer composition on ionic conductivity and battery performance was systematically investigated.

The in situ formation of the polymer electrolyte was achieved by directly UV-photocuring the electrolyte precursor onto the surface of a SPAN (sulfur–polyacrylonitrile) cathode, ensuring intimate interfacial contact and minimizing interfacial resistance. The resulting all-solid-state Li-SPAN battery demonstrated excellent electrochemical performance, delivering an initial discharge capacity of 1242 mAh g^{-1} at 0.1C and 80 °C, confirming the high energy potential of the system.

The physicochemical characteristics of the developed SPE were thoroughly examined using thermogravimetric analysis, differential scanning calorimetry, scanning electron microscopy, electrochemical impedance spectroscopy, cyclic voltammetry, and Fourier-transform infrared spectroscopy (FTIR). FTIR analysis confirmed the successful incorporation of LiTFSI into the polymer matrix, as evidenced by distinct absorption peaks corresponding to S=O and CF_3 groups. These results demonstrate the feasibility of acrylate-based UV-crosslinked SPEs for high-performance, safe, and scalable solid-state lithium–sulfur battery applications, especially in electric vehicles and grid-scale energy storage.

Overall, this study provides valuable insight into the design of high-performance solid polymer electrolytes through UV- curing strategies and plasticizer optimization. The demonstrated approach offers a scalable and efficient route toward the practical realization of solid-state lithium–sulfur batteries with enhanced safety, energy density, and interfacial compatibility.

Acknowledgement. This research was supported by the research grants BR21882402 “Development of new technologies of materials and energy storage systems for a green economy” from the Ministry of Science and Higher Education of the Republic of Kazakhstan

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Development of a Scalable Synthesis Method for Multi-Elementn Doped Nanostructured Cathode Materials Based on LiFePO4 for Lithium-Ion Batteries

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Nowadays, the fast improvements of energy storage technologies lead to a particular attention to the development of cathode materials for lithium-ion (LIBs. Lithium iron phosphate (LFP) the most advantageous candidate for cathode materials among LIBs due to high operating voltage (~3.4 V), cycling stability, and high theoretical specific capacity (170 mAh g^{-1}) [1]. These properties are related to its olivine-type orthorhombic crystal structure. However, the electrochemical performance of LFP is hindered by low electronic conductivity (~10–9 cms^{-1}) and slow lithium-ion diffusion (10^{-13} to 10^{-16} cm^2 s^{-1}) [2], [3], [4].

To overcome these intrinsic limitations, this study utilized different techniques such as synthesis of nanoparticles using mechano- chemical activation, carbon coating and doping with supervalent cations. The synthesis method involves high-energy ball milling, which increases chemical reactivity of mixtures, leading to uniform and well-crystallized structures of LFP powder and increased both discharge potential and specific capacity by roughly 15-20% [5], [6], [7]. Similarly, carbon coating increases the electronic conductivity of LFP [8]. The LFP was doped with nickel (Ni) and zinc (Zn) at Fe site. Both dopants individually enhance electronic conductivity and lithium- ion diffusion rate of the cathode.

This research investigates effect of Ni and Zn co-doping on the improvement of electrochemical and structural characteristics. Several dopants concentrations were examined to determine an optimal sample. The results demonstrate that the LiFe0.98Ni0.01Zn0.01PO4/C shows the high cycling stability and improved specific capacities among all the doped and undoped samples. Morphology and composition of synthesized cathode materials were characterized by X-ray diffraction (XRD), inductively coupled plasma optical emission spectroscopy (ICP-OES), scanning electron microscopy (SEM) and simultaneous thermogravimetric analysis (STA).

Acknowledgments. This research was funded by the project AP19677233 "Development of a Scalable Synthesis Method for Multi-Element Doped Nanostructured Cathode Materials Based on LiFePO4 for Lithium-Ion Batteries" from the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan

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High voltage $LiMn_xFe_{1-x}PO_4$/CN cathode material for aqueous lithium ion rechargeable batteries.

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$LiFePO_4$ (LFP) is a prospective material for use in electric vehicles (EVs), but it has low energy density. One of the ways of solving this problem is adding Mn ions. Mn ions induce higher voltage for the battery material. This work examined the properties of $LiMn_xFe_{1-x}PO_4$/CN cathode material for lithium-ion batteries. Solvothermal method was utilized for synthesis of active material [1]. Three samples of x=0.8, 0.6, and 0.5 were synthesized to find the best performance by balancing the ratios of components for synthesis. For higher conductivity, carbon coating and nitrogen doping of synthesized materials was made using solutions of sucrose and sucrose-glycine to enhance electrochemical conductivity. Characterization of the $LiMn_xFe_{1-x}PO_4$/CN for a single-phase structure was made via XRD, also morphological differences were examined using SEM, SEM EDS, TGA. Moreover, electrochemical properties were checked, the results showed that nitrogen-doped samples had superior initial discharge capacity with a maximum value of 182.4 mAh/g with stable cycling performance. This work's results demonstrate glycine's potential as a carbon-nitrogen source for further research and optimization of sustainable energy storage.

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Biopolymer-based hydrogel electrodes for a flexible supercapacitor in wearable electronics

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Flexible supercapacitors are becoming increasingly important for wearable electronics, where energy storage systems must be not only lightweight and stretchable, but also safe for direct contact with skin. In this work, biopolymers-based hydrogel materials are designed to meet these requirements while aiming to improve their energy density beyond conventional limits [1].

The electrode material integrates electroactive additives with skin-compatible, biodegradable polymers, with the goal of enhancing ionic conductivity and charge storage. Particular attention is given to optimizing the internal structure and surface properties to support both mechanical flexibility and efficient electrochemical performance. While most biopolymer-based electrodes operate in the range of 1–10 Wh/kg [2], this research targets energy densities above 20 Wh/kg, even under repeated mechanical stress, to make the technology stable for real-world practical use in wearables.

The biocompatibility of the system is assessed through in vitro methods to ensure safe use on skin. The broader aim is to develop a flexible all-hydrogel supercapacitor with the potential of upscaling the fabrication process by 3D printing.

Acknowledgments. This study was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (grant No. BR24992766, grant No. AP23483880).

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Stabilizing SnO_2 thin film anodes through artificial solid electrolyte interphase modification

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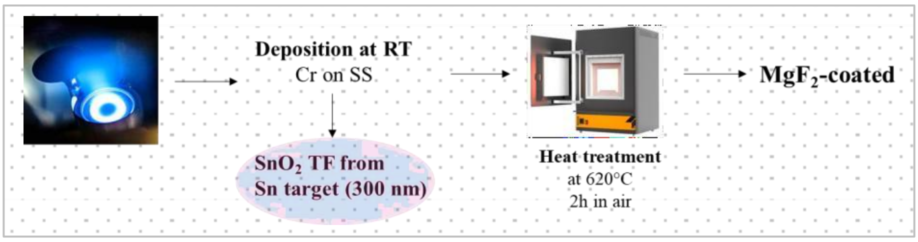
Tin oxide (SnO_2) has a high theoretical capacity (1494 $mAhg^{-1}$), but rapidly loses capacity due to strong volumetric changes during cycling. The MgF_2 coating helps to stabilize the electrode: during the first lithiation, it is converted into LiF and Li–Mg alloy. LiF improves ionic conductivity and forms a stable SEI, and Li–Mg increases mechanical strength and electronic conductivity. As a result, the cycling stability and electrochemical efficiency of the anode are improved [1–3]. In addition, MgF_2 reduces the degree of destruction of the active material and minimizes side reactions at the electrode–electrolyte interface, ensuring a longer cell lifetime. This strategy may also be effective for other anodes with unstable interfaces.

In this study, SnO_2 thin films were deposited by RF magnetron sputtering on stainless steel substrates and subsequently annealed to enhance crystallinity. To improve SEI stability and cycling performance, the films were modified with MgF_2 coating, as illustrated in Figure 1. The structural and morphological properties were analyzed by XRD and SEM, while the electrochemical performance was evaluated by cyclic voltammetry and charge-discharge testing.



The electrochemical performance of the thin-film anodes reveals that SnO_2 coated with MgF2 exhibits high capacity and excellent cycling stability, approaching the theoretical capacity of SnO2 (1494 mAhg-1). This improvement is attributed to enhanced electrical conductivity and structural stability, as evidenced by XRD and SEM analyses, which demonstrate well-defined crystallinity and a uniform, crack-free surface morphology.

This study presents a highly efficient tin oxide thin film anode for lithium-ion battery applications. The developed material exhibits outstanding capacity retention and cycling stability, highlighting its potential for use in future energy storage systems.

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Nickel-rich concentration-gradient thin film NCM cathode by SILAR for lithium-ion battery

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The intensifying demand for high-energy-density lithium-ion batteries (LIBs) has driven the exploration for better cathode materials. Among them, nickel-rich NCM-type layered oxides possess high specific capacities but poor structural and thermal stability, especially at elevated nickel contents. To overcome these shortcomings, concentration-gradient thin-film design has emerged as a viable option where a high-performance Ni-rich core is flanked by a Mn/Co-rich surface layer, thus both structural stability and electrochemical activity are enhanced. Moreover, the thin-film architecture provides improved ion transport kinetics. This article critically examines the viability of employing the Successive Ionic Layer Adsorption and Reaction (SILAR) process for preparing such gradient-structured cathode materials [1]. SILAR is particularly well-suited to this purpose due to its advantages, including layer-by-layer compositional modulation with high accuracy, low-cost processing, and ambient pressure operation [2]. Perhaps most importantly, SILAR possesses a clear synergistic role of controlled Ni-rich concentration-gradient thin film deposition, which efficiently overcomes the inherent disadvantage of conventional NCM systems. The review reflects on the current advancements in the area to justify the efficiency and potential of SILAR-synthesized Ni-rich gradient NCM cathodes as future LIB technology contenders.

Keywords: Nickel-rich NCM cathode, SILAR method, Lithium-ion batteries.

Acknowledgements. This research has been funded by the Nazarbayev University Research grant (SEDS2025008).

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Enhanced SnO_2 thin film anode material for Li-ion batteries

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Lithium-ion batteries (LIBs) are versatile energy storage systems known for their high energy density, durable cycling performance and efficiency, making them indispensable for a variety of applications, from electric vehicles to portable electronics [1-2]. Tin dioxide (SnO_2) is a very promising anode material for LIBs due to its exceptional theoretical capacity of 1494 $mAhg^{-1}$, which significantly exceeds the capacity of traditional graphite-based anodes. Moreover, SnO_2 is abundant in nature, cost-effective, and environmentally benign, rendering it an attractive alternative for the development of eco-friendly battery technologies [3].

In this study, SnO_2 thin film anodes were obtained by RF magnetron sputtering method, followed by thermal treatment to improve crystallinity and surface morphology. To enhance interfacial stability, the electrolyte was modified with a VC additive, and a carbon coating was applied to the film surface. The synthesized SnO_2 thin film was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM) to elucidate its structural and morphological properties. Electrochemical testing was performed using cyclic voltammetry (CV) and galvanostatic charge–discharge cycling with a multichannel battery testing system (Neware BTS).

A comparative study was conducted to evaluate the electrochemical performance of C-coated SnO_2 anodes in two electrolyte systems: $LiPF_6$ in EC:DEC:EMC (1:1:1 by volume) and $LiPF_6$ in EC:DEC:EMC with 5 wt.% vinylene carbonate (VC) additive. The results indicate that the electrolyte composition significantly influences the anode performance.

This research introduces a high-performance thin-film anodes based on SnO_2 for use in LIBs. The material shows excellent capacity retention and stability, making it a strong candidate for future energy storage technologies.

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3D-structured nanoporous SnO_2 thin-film anodes for lithium-ion microbatteries

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Lithium-ion batteries (LIBs) are evolving to meet increasing energy demands, particularly for micro- and nano-scale devices. A major challenge is the limited utilization of active materials and poor electrode stability caused by simple 2D structures. To address this, 3D-structured anodes based on tin oxide (SnO_2) were fabricated using self-assembled polystyrene microspheres as sacrificial templates. The resulting porous framework increases active surface area, facilitates lithium-ion transport, and improves electrolyte accessibility.

SnO_2 thin films were deposited by RF magnetron sputtering onto the polystyrene templates, followed by thermal annealing to remove the polymer and form an interconnected porous architecture. XPS analysis confirmed the complete removal of polystyrene and the formation of a clean tin oxide surface. Electrochemical testing demonstrated that the 3D-structured anodes exhibit significantly improved performance over planar electrodes. At a current density of 0.1C, the specific capacity stabilized around 300 mAh g^{-1} after 40 cycles, while at 0.5C, the anodes maintained approximately 400 mAh g^{-1} even after 600 cycles, indicating excellent long-term cycling stability. Cyclic voltammetry (CV) showed distinct redox peaks associated with reversible conversion and alloying reactions of SnO_2.

The 3D-structured electrodes exhibited higher current responses and better electrochemical reversibility compared to flat electrodes, confirming improved lithium-ion transport and electrolyte diffusion. These results highlight the effectiveness of 3D porous anode design and its strong potential for next-generation high-performance microbattery applications.

Acknowledgments. This research was funded by the research project AP19680567 “Advanced nanocomposite 3D thin film electrodes for lithium-ion batteries” from the Ministry of Science and Higher Education of the Republic of Kazakhstan.

PTHF-based solid polymer electrolyte through UV cross-linking for Li-ion battery

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The development of lithium-ion batteries (LIBs) has become increasingly important in recent years due to growing demand for sustainable energy solutions, smaller smart electronics, wearable devices, and the expanding portable electronics market. Efforts have focused on improving the electrochemical performance and safety of LIBs. Safety concerns such as leakage, flammability, and toxicity, often associated with liquid electrolytes, underscore the necessity for secure solid-state batteries utilizing solvent-free electrolytes [1]. In this study, we present a thermally stable SPE fabricated by UV-induced cross-linking of acrylated PTHF (a-PTHF), poly(ethyleneglycol) diacrylate (PEGDA), trimethilolpropane ethoxylate triacrylate (ETPTA), and lithium bis(trifluoromethanesulfonyl)imide salt (LiTFSI), exploring various ratios of EO:Li. To fabricate solid polymer electrolyte films, polytetrahydrofuran's terminal groups were modified by incorporating acrylate-groups, known for their photosensitivity in cross-linking processes . The completeness of the acrylation was confirmed by observing peaks corresponding to acrylic (C=C) and C=O bends at 1636 and 1724 cm^{-1}, respectively, in the FTIR spectrum of the product.

Subsequently, cross-linked flexible polymer films were prepared by UV irradiation of a polymer blend comprising a-PTHF, PEGDA, and ETPTA at various EO ratios. The disappearance of peaks at 1636 and 750 cm^{-1}, attributed to C=C and =C-H bends, indicated successful cross-linking process. These solid polymer electrolytes, based on acrylated polytetrahydrofuran, produced flexible and transparent films. SEM analysis confirmed that the lithium salt was fully dissolved in the polymer, resulting in smooth SEM images.

The outstanding mechanical strength and flexibility of these solid polymer electrolytes enabled the production of thin films, measuring 60 microns in thickness. Ionic conductivity studies revealed that the obtained solid polymer electrolytes using a-PTHF exhibited moderate ionic conductivity. Notably, among the polymer films, those with EO ratios of 6 and 8 demonstrated ionic conductivities of 1.1·10-5 $S \cdot cm^{-1}$ and $1.65 \cdot 10^{-5}$ $S \cdot cm^{-1}$ at 80 °C, respectively.

When incorporated into all-solid-state LFP battery, aPEP SPEs demonstrate a specific capacity of 100 mAh g^{-1} at 0.1 C at 80 °C. In addition, the further research on Li|aPEP4|LFP pouch cells was conducted to assess the commercial viability of aPEP electrolyte. The voltage of the pouch cell with aPEP4 SPE showed 2.46 V. These results represent a significant achievement for all-solid-state lithium-ion batteries utilizing polymer electrolytes. Produced highly flexible electrolytes are promising candidates to be applied in LIBs for powering flexible electronic devices.

Acknowledgement. This research was supported by the research grants BR21882402 "Development of new technologies of materials and energy storage systems for a green economy" from the Ministry of Science and Higher Education of the Republic of Kazakhstan

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Three-Dimensional Zn/ZnO-C Composite Electrode for High-Performance Lithium-Ion Batteries

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Lithium-ion batteries (LIBs), as the most advanced type of rechargeable batteries, have attracted significant attention over the past few decades. Currently, they serve as the predominant mobile power source for portable electronic devices such as mobile phones and laptops. LIBs are considered a key driver of the personal digital electronics revolution, which began approximately twenty years ago with their introduction to the commercial market. [1].

One of the main limitations of conventional two-dimensional (2D) LIBs lies in their restricted areal energy density and inefficient space utilization, which stem from their planar electrode architecture. This configuration limits the loading of active materials and elongates ion and electron transport pathways, resulting in reduced electrochemical performance and slower charge/discharge rates to overcome these challenges, the development of three- dimensional (3D) structured electrodes has emerged as a promising solution. The 3D architecture offers a high surface area, enhanced active material loading, and shortened diffusion paths, leading to improved rate capability and overall energy storage efficiency. Incorporating 3D designs into LIB systems paves the way for next-generation high- performance energy storage devices suitable for compact and demanding applications [2].

Metal foam-based 3D structures offer significant advantages as current collectors and scaffolds in LIB electrodes. Their highly porous and interconnected architecture provides a large surface area, which facilitates uniform distribution of active materials and enhances electron transport pathways. The open-cell structure allows for efficient electrolyte penetration, reducing ion diffusion resistance and improving electrochemical kinetics. Moreover, metal foams such as Zn or Ni exhibit good mechanical strength and electrical conductivity, making them ideal for supporting high mass loading without compromising structural integrity. These properties collectively contribute to improved areal capacity, rate performance, and cycling stability in advanced battery designs.

To address the issue of volume expansion commonly observed in metal oxide-based electrodes during repeated lithiation/delithiation cycles, polymer coating followed by carbonization presents an effective strategy. Coating metal oxides with a polymer such as polyethylene oxide (PEO) forms a conformal layer that acts as a mechanical buffer, accommodating stress and suppressing particle pulverization. Subsequent carbonization of the polymer under inert atmosphere converts the layer into a conductive carbon shell, which enhances electronic conductivity and further stabilizes the electrode structure. This carbon coating not only improves the integrity of the active material during cycling but also contributes to improved electrochemical performance by facilitating faster charge transfer and mitigating capacity fading the goal of this study was to improve the electrochemical performance of pure Zn/ZnO foam through the carbonization of a polymer coating. SEM-EDS analysis confirmed that carbon was uniformly deposited on the ZnO surface. Electrochemical tests revealed that, after 100 cycles, the polymer-coated Zn/ZnO foam maintained a specific capacity of approximately 260 mAh/g, whereas the uncoated Zn/ZnO foam retained only about 100 mAh/g. The carbon layer enhanced the stability of the Zn/ZnO foam by improving electronic conductivity and protecting the ZnO layer from mechanical degradation during cycling.

Acknowledgments. This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP19578472)

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Investigating the influence of obtaining technique on ionic conductivity

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Lithium-sulfur batteries (LSBs) are among the most promising next-generation energy storage systems due to the abundance of sulfur, high theoretical energy density capacity of 1675 mAh /g and theoretical energy density of 2600 Wh/kg, which exceeds that of traditional lithium-ion batteries [1]. However, typical liquid electrolytes (LEs) have significant polysulfide dissolving, dendrite development, leakage, and safety issues. All-solid-state electrolytes (SSEs), on the other hand, provide improved stability and safety but are frequently constrained by low ionic conductivity and high interfacial resistance. The focus of this work is on quasi-solid-state electrolytes (QSSEs), which integrate a little amount of liquid into a polymer matrix to combine the advantages of both LEs and SSEs. While preserving good electrode-electrolyte contact, QSSEs improve lithium-ion transport, increase safety, and inhibit the polysulfide shuttle effect. This study develops QSSEs based on poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) by various three common techniques: electrospinning, solution casting and spin coating(Figure 1). PVDF-HFP offers high mechanical strength, electrochemical stability, and a high dielectric constant that facilitates lithium salt dissociation[2]. Its semi-crystalline nature balances structural integrity with ionic mobility. LiTFSI provides excellent thermal stability, a wide electrochemical window, low lattice energy for enhanced salt dissociation, and high compatibility with lithium metal anodes[3-4]. Systematic characterization using SEM-EDS, XRD, FTIR, and PEIS was conducted to evaluate morphology, crystallinity, ion-polymer interactions, and electrochemical performance. The study identified 5 wt.% LiTFSI as the optimal salt concentration, with electrospinning yielding the highest ionic conductivity (5.55×10^{-6} S/cm at 60 °C) and improved polymer-salt interactions due to enhanced amorphous content. Despite the absence of ceramic or ionic liquid additives, electrospun QSSEs exhibited significant promise, highlighting their scalability and potential for high-performance LSBs. These findings offer valuable insights into the interplay between fabrication method and electrolyte performance, paving the way for further innovations in QSSE design.

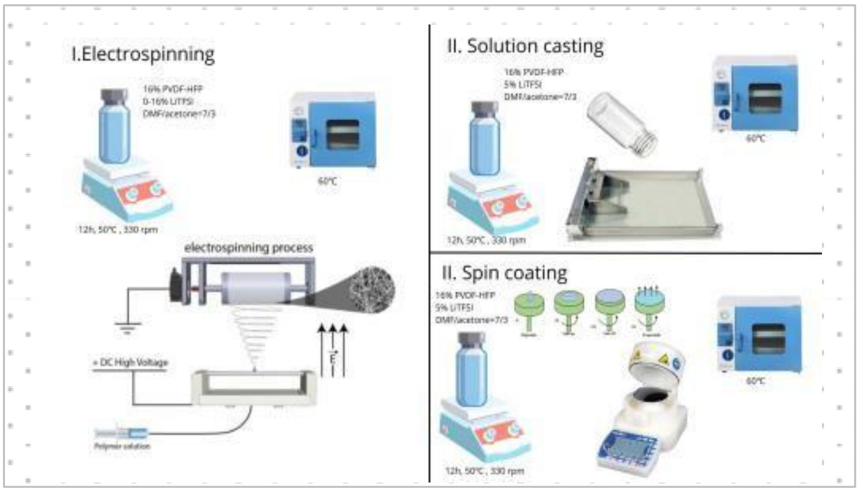

Figure 1. Methodology of obtaining QSSE via various techniques

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Optimization of Synthesis Conditions for Germanium Phosphide/Phosphate Carbon Nanofiber Anodes with Enhanced Electrochemical Performance

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Germanium (Ge) is considered a promising anode material for lithium-ion batteries (LIBs) due to its superior properties compared to other metallic anode materials with a high theoretical capacity of approximately 1600 mAh g^{-1} [1]. Among germanium-based compounds, germanium phosphides and phosphates possess unique structural and electrochemical properties that make them promising for high-performanceLIBs. Germanium phosphide features a layered structure that facilitates efficient ion transport and offers excellent electronic conductivity, while germanium phosphate provides enhanced structural stability during cycling [2]. Both materials, especially when combined with conductive carbon matrices, can effectively mitigate volume changes and improve overall battery performance [2][3].

In this study, germanium phosphide/phosphate carbon nanofibers are synthesized via electrospinning, followed by a two-step heat treatment process involving pre-oxidation and annealing. The electrospinning solution was prepared using germanium oxide, polyvinylpyrrolidone (PVP), and phosphoric acid. Electrospinning was conducted with a 1.0 mL h^{-1} flow rate, a 10 cm tip-to-collector distance, and a rotating drum collector at 100 rpm. Key synthesis parameters—including applied voltage, drying temperature, pre-oxidation temperature, and annealing temperature—are currently being optimized to achieve nanofibers with superior structural and electrochemical properties.

Preliminary X-ray diffraction (XRD) results are presented in Figure 1, comparing two samples: one processed with both pre-oxidation and annealing, and another subjected only to the annealing step. These initial findings help assess the influence of pre-oxidation on the crystalline structure of the synthesized nanofibers.

The fabricated nanofibers will be assembled into LIR2032 coin cells and evaluated to determine their electrochemical performance, with the aim of identifying optimal synthesis conditions for next-generation lithium-ion battery anodes.

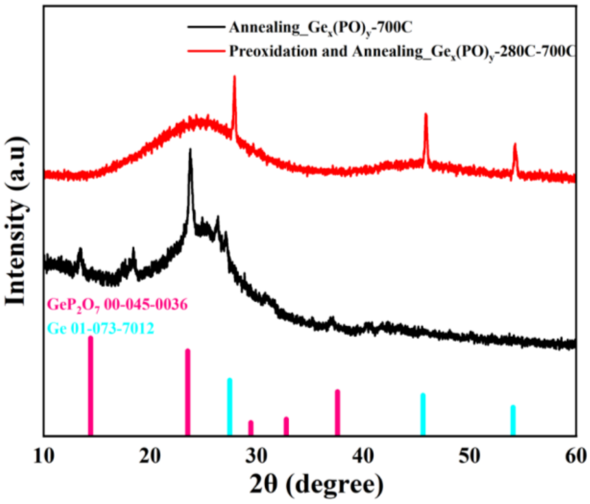

Figure 1. Preliminary XRD patterns of germanium phosphide/phosphate carbon nanofiber samples synthesized with and without the pre-oxidation step.

Acknowledgements. This research was funded by the research project AP19675260 "Development of nanofibrous electrode materials for next-generation lithium-ion batteries" from the Science Committee, Ministry of Science and Higher Education of the Republic of Kazakhstan.

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Synthesis and Electrochemical Evaluation of $LiCoPO_4$ Cathode Material via Ultrasonic Spray Pyrolysis

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The shift towards sustainable energy systems necessitates the creation of high-performance and safe electrode materials for lithium-ion batteries (LIBs), which are fundamental to the emerging circular lithium economy. Among LiMPO4-type olivine compounds (M = Fe, Co, Mn, etc.), $LiCoPO_4$ (LCP) stands out due to its high operating voltage (~4.8 V) and thermal stability, making it a promising cathode for high-energy LIBs [1]. However, its widespread application is hindered by intrinsic low electronic conductivity and electrolyte degradation at high voltages [2]. In this study, LCP was synthesized via ultrasonic spray pyrolysis (USP), a controllable technique enabling the formation of uniform spherical particles. An aqueous precursor solution containing $LiNO_3$, $Co(NO_3)_2{\cdot}6H_2O$, and H_3PO_4 was used with citric acid as a carbon source the synthesized powders were annealed and analyzed using XRD and SEM, confirming a phase-pure orthorhombic olivine structure with a spherical morphology and particle sizes of approximately 1.4 µm, consistent with literature reports. [3]. Electrochemical tests were conducted using 1M $LiPF_6$ in FEC:DMC (1:4, v/v) electrolyte with glass fiber separators. The best-performing samples (Fig.1) showed stable cycling at 0.1C and areal mass loadings up to 2.6 mg·cm^{-2}. These promising results validate the potential of USP for producing high-quality LCP cathodes and set the stage for future work focused on optimizing carbon content and exploring elemental doping to further enhance electrochemical performance.

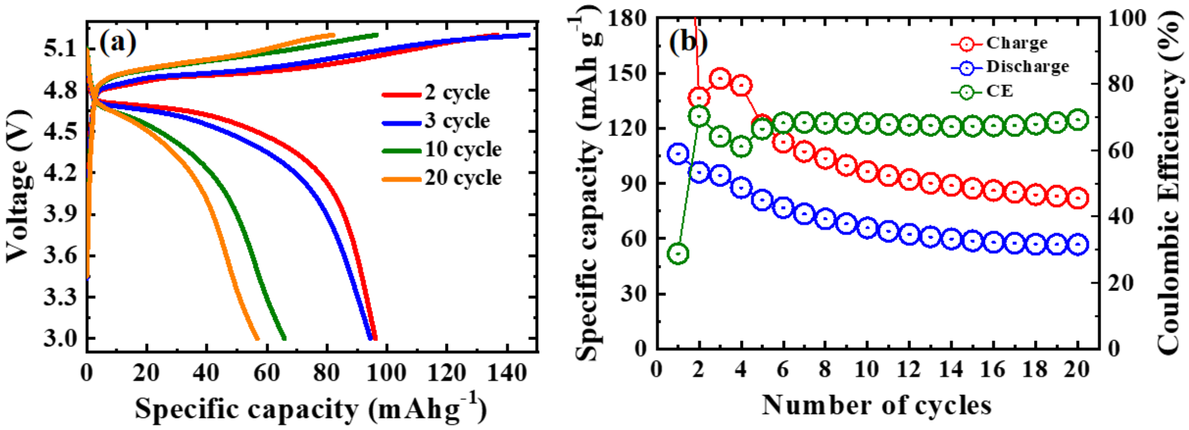

Figure 1. (a) galvanostativ charge–discharge curves and (b) cycling performance of $LiCoPO_4$ synthesized via ultrasonic spray pyrolysis.

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Freestanding TiO_2–Ni/NiO Electrode for Shuttle Suppression in Li–S Batteries

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Lithium–sulfur (Li–S) batteries are among the most promising candidates for next-generation energy storage due to their high theoretical energy density. However, their practical deployment is hindered by the shuttle effect of dissolved lithium polysulfides (LiPS), leading to rapid capacity fading and poor cycling stability. In this work, a novel freestanding TiO_2–Ni/NiO composite electrode composed of uniformly distributed nanospherical particles (15–30 nm) was developed. The active material was cast onto a conductive and flexible scaffold of carbon nanofibers (CNF) together with carbon nanotubes (CNT). TiO_2–Ni/NiO nanospheres were integrated at controlled molar ratios of 90:10, 75:25 and 50:50, effectively combining the strong chemical adsorption capability of TiO_2 with the catalytic redox activity of Ni/NiO. This dual-function architecture facilitates both the physical confinement and accelerated conversion of LiPS, thereby efficiently suppressing the shuttle effect. Comprehensive structural characterization (SEM, TEM, XRD, EDS) revealed a uniformly distributed dispersion of the nanospheres and a well-developed porous architecture, both of which are favorable for enhancing electrochemical reactivity. Electrochemical performance, tested at a sulfur loading of 2 mg cm^{-2}, was evaluated through cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge–discharge cycling. The TiO_2–Ni/NiO@CNT/CNF composite electrode demonstrated enhanced sulfur utilization, reduced polarization, and improved cycling stability, offering a promising strategy for high-performance Li–S batteries with suppressed shuttle behavior.

Controlling pore structure in templated carbons to improve Li-S battery performance

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Lithium–sulfur (Li-S) batteries are a promising energy storage system due to their high theoretical capacity and energy density. However, their practical application still requires significant improvements due to challenges such as the low conductivity of sulfur and the dissolution of lithium polysulfides. Templated carbons, with their well-controlled pore structures capable of hosting sulfur and suppressing the shuttle effect, represent a promising class of host materials. In this study, a series of hard-template-derived carbon materials (GA1-GA6) were synthesized to achieve a wide range of pore structures. The broad variation in pore size, specific surface area, and pore volume enables a comprehensive investigation of the relationship between carbon structure and electrochemical performance.

The morphological features of the carbons and their sulfur composites were characterized using BET analysis, X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM, TEM), and UV–visible spectroscopy. BET analysis confirmed the micro- and mesoporous nature of the composites and revealed distinct textural characteristics with specific surface area ranging from 414 to 3455 m^2 g^{-1}, pore size from 0.91 to 13 nm, and pore volume from 1.1 to 2.8 cm^3 g^{-1} (Figure 1 a). SEM and TEM revealed uniform particle morphology and interconnected porosity. Polysulfide adsorption studies in the UV–visible range showed that samples with smaller pores, such as GA5 and GA6, exhibited stronger polysulfide retention due to enhanced physical adsorption [1]. Cathodes were prepared by mixing the GA@S composites with acetylene black and PVDF binder in NMP to form a slurry, which was cast onto aluminum foil and dried. CR2032 coin-type cells were assembled in an argon-filled glovebox using lithium metal as the counter electrode and a liquid electrolyte containing LiTFSI and LiNO$_3$ in a DOL/DME solvent mixture. The electrochemical performance of the GA@S samples was evaluated based on their initial discharge capacity and capacity retention over 100 cycles. Among all samples, GA2@S exhibited the highest initial capacity of 1397.1 mAh g^{-1}, indicating superior sulfur utilization. However, after 100 cycles, GA1@S retained the highest capacity of 791 mAh g^{-1}, demonstrating the best stability. The highest capacity retention starting from 10th cycle was also observed for GA1@S (88.9%), followed by GA3@S (85.6%), while GA5@S (67.8%) and GA6@S (74.4%) showed the most pronounced capacity fading. Thus, higher pore size and volume ensures a more stable electrode structure and improved sulfur confinement, making GA1 material the most promising candidate for long-term lithium-sulfur battery applications.

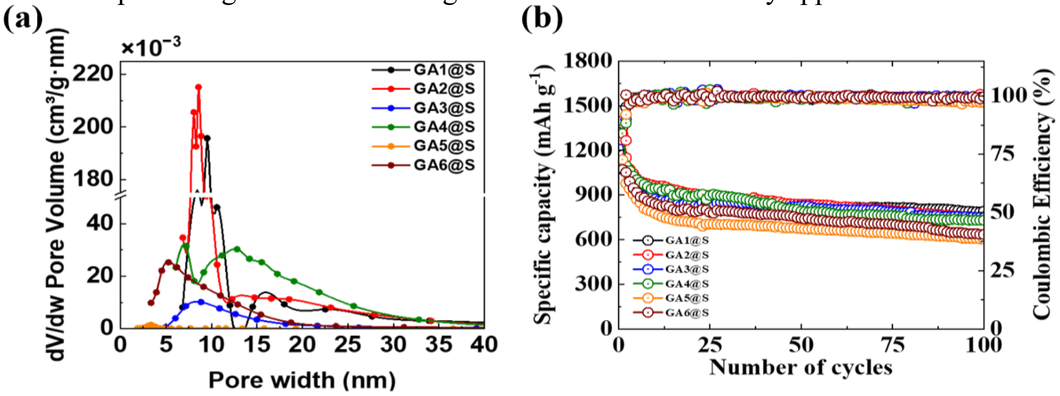

Figure 1. (a) Low temperature N2 adsorption/desorption isotherms and (b) discharge capacity values at 0.2 C current rate of the GA@S cathode composites

Acknowledgements. This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP13067625)

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Improvement of Initial Coulombic Efficiency in Biomass Briquette-Derived Hard Carbon Using Dual Inert Atmosphere Synthesis

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The increasing demand for sustainable and cost-effective energy storage technologies has led to growing interest in sodium-ion batteries (SIBs) as promising alternatives to lithium-ion batteries (LIBs). Due to the abundance and low cost of sodium resources, SIBs are particularly attractive for large-scale energy storage applications [1]. However, one of the main challenges hindering their commercial viability is the limited performance of anode materials, particularly in terms of low initial Coulombic efficiency (ICE).

The development of cost-effective and environmentally friendly anode materials is vital for advancing sodium-ion battery (SIB) technology. In this work, hard carbon was synthesized from biomass briquettes via a pyrolysis process conducted under two different inert atmospheres—argon and nitrogen. The dual-atmosphere approach was employed to investigate its effect on the microstructure and electrochemical performance of the resulting hard carbon. Structural characterization revealed that the synthesis atmosphere significantly influenced the porosity and surface chemistry of the material, which are key factors affecting sodium storage behavior. Electrochemical testing demonstrated a notable improvement in the initial Coulombic efficiency (ICE) of the samples treated under optimized inert conditions. The findings highlight the potential of using biomass-derived carbon and controlled synthesis environments to produce high-performance anode materials for sustainable energy storage applications [2].

Hard carbon has emerged as a leading candidate for SIB anodes due to its disordered structure and ability to accommodate large sodium ions. Among various sources for hard carbon, biowaste-derived materials offer a sustainable and eco-friendly approach, reducing both environmental impact and production cost. Despite these advantages, biowaste-derived hard carbon often suffers from poor ICE, primarily due to irreversible reactions with the electrolyte and the formation of solid electrolyte interphase (SEI) layers.

In this work, hard carbon derived from briquette under argon atmosphere showed that the sample treated with a 1:1 KOH ratio exhibited an initial discharge capacity of 325 mAh/g, stabilizing at ~290 mAh/g after 10 cycles. The sample treated with a 1:4 KOH ratio demonstrated a slightly higher initial capacity of 326 mAh/g but stabilized at ~265 mAh/g. Both samples retained more than 90% of their capacity after 50 cycles, indicating strong structural integrity.

In contrast, there are also some reports on the preparation of hard carbon under nitrogen atmosphere. The sample treated with a 1:1 KOH ratio exhibited an initial discharge capacity of 301 mAh/g, stabilizing at ~227 mAh/g, after 10 cycles. Thus, it is inferred that high—performance hard carbon can be obtained under argon atmosphere.

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Modification of $NaTi_2(PO_4)_3$ anode material with stearic acid to enhance its performance stability in aqueous sodium-ion batteries

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Today, lithium-ion batteries (LIBs) remain a key component in modern electronic devices, electric vehicles, and stationary energy storage systems. However, the high cost of lithium, its limited reserves, and the potential risks associated with organic electrolytes (flammability, explosion) are driving the search for alternative energy storage technologies [1]. Aqueous sodium-ion batteries (ASIBs) represent a promising alternative to LIBs due to the use of environmentally friendly aqueous electrolytes, low cost, the abundance of sodium, and high safety [2].

Among various anode materials for sodium-ion batteries, $NaTi_2(PO_4)_3$ (NTP) with a NASICON-type structure is recognized as one of the most promising due to its high sodium-ion conductivity, a significant theoretical capacity of 133 $mAh \cdot g^{-1}$, low cost, and environmental friendliness [3]. However, the practical application of NTP in aqueous sodium-ion batteries is limited by several issues: electrochemical side reactions between NTP and dissolved oxygen in the electrolyte, and the electrochemical decomposition of water on the electrode material's surface, which leads to the evolution of hydrogen and hydroxyl anions [4]. In its charged state, NTP can react with oxygen or water, leading to its gradual self-discharge according to equations 1 and 2, which is a critical issue for its use.

$$2Na_3Ti_2(PO_4)_3 + O_2 + 2H_2O = NaTi_2(PO_4)_3 + 4Na^+ + 4OH^- \quad (1)$$

$$Na_3Ti_2(PO_4)_3 + 2H_2O = NaTi_2(PO_4)_3 + 2Na^+ + H_2 + 2OH^- \quad (2)$$

In this work, we propose an approach to modify the NTP surface with stearic acid ($C_{17}H_{35}COOH$) to create a hydrophobic layer, limiting the access of water and dissolved oxygen to the electrode surface. Stearic acid was chosen as a modifier due to its availability, low cost, and ability to form hydrophobic coatings. The aim of this work is to study the effect of stearic acid on the electrochemical characteristics of the modified electrodes.

To modify the NTP powder surface, 0.5 g of the active material was used with prepared solutions of 1%, 2%, and 3% (wt.) stearic acid dissolved in ethanol. The NTP powder was added to the resulting solution and dried at 70–80°C with constant stirring until the solvent completely evaporated.

XRD, SEM, and IR spectroscopy were used to confirm the successful fabrication of the modified $NaTi_2(PO_4)_3/C_{18}H_{36}O_2$ electrode. Modification with stearic acid significantly enhanced the hydrophobicity of the electrode surface, increasing its contact angle from 69° to 145°. The addition of stearic acid to the electrode coating led to a decrease in the material's specific capacity by 10 mAh/g; however, the presence of stearic acid improved the Coulombic efficiency to 99%, indicating stable process reversibility. It was determined that the modified electrode increases the self-discharge time, which points to the positive impact of the powder modification on the electrode material's stability.

Thus, it was established that the modification of the electrode with stearic acid should effectively prevent side electrochemical reactions on the NTP surface and ensure stable electrode performance in an aqueous electrolyte. The presence of stearic acid provides sufficient hydrophobicity to protect against parasitic reactions and enhances Coulombic efficiency, while maintaining good accessibility of the active sites for electrochemical processes. Furthermore, the uniform distribution of stearic acid prevents particle agglomeration, which contributes to better utilization of the active material.

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$LaNi_5$/MXene Composites for Enhanced Electrochemical Performance of Nickel-Metal Hydride Anode

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Nickel-metal hydride (Ni-MH) batteries retain a strategic importance in sustainable energy due to their safety, environmental friendliness, and tolerance to overcharging, finding application in hybrid electric vehicles, stationary storage systems, and portable electronics. However, their development is hindered by key drawbacks of the anode materials, specifically, the degradation and sluggish electrochemical kinetics of hydrogen processes inherent to hydrogen-storage alloys.

This work presents an approach to improve Ni-MH battery anodes through the use of the two-dimensional titanium carbide $Ti_3C_2T_x$ (MXene), whose application for classical hydrogen-storage alloys in Ni-MH systems has not been previously investigated. MXenes possess a unique combination of properties: high metallic conductivity, mechanical robustness, hydrophilicity, and tunable surface chemistry. It is expected that due to these properties, MXene can simultaneously function as a conductive matrix and an effective binder, ensuring the stability and high electrochemical activity of the anode.

Nanostructured $LaNi_5$ particles were synthesized via a two-step oxide reduction method and were subsequently used to fabricate composite $LaNi_5$/MXene electrodes by vacuum filtration. The electrochemical performance of the $LaNi_5$/MXene composite was compared with that of traditional electrodes based on a PTFE binder.

Morphological analysis showed that MXene forms a layered architecture and a conductive network, encapsulating the $LaNi_5$ particles. This improves the electrical contact between them and enhances electrolyte accessibility, in contrast to PTFE, which acts as an insulator and limits the full utilization of the active material. The optimal composition ($LaNi_5$:MXene = 80:20) exhibited a discharge capacity of 225 mAh/g at 0.5C and 207 mAh/g at 10C. After 100 cycles at 1C, 43% of the initial capacity was retained (from 235 to 100 mAh/g), whereas the PTFE-based analogue, which demonstrated significant capacity fading even at increased discharge rates, retained only 12% after 100 cycles (from 214 to 25 mAh/g). Electrochemical impedance spectroscopy analysis confirmed a reduced charge-transfer resistance and an increased exchange current density for the hybrid $LaNi_5$/MXene electrodes relative to their PTFE-binder-based analogues. Despite the significant improvement in electrochemical performance, the electrode's stability is still limited by the degradation of the $LaNi_5$ phase itself, whereas the MXene component, in contrast, demonstrated high electrochemical stability under the same conditions.

The obtained results demonstrate the potential of MXene-metal hydride systems and confirm the multifunctional role of MXene as a binder, a conductive additive, and an active capacitive component. This opens a pathway for the development of high-performance and reliable aqueous batteries, especially when combining MXene with more stable, next-generation hydrogen-storage alloys.

Public environmental responsibility and End-of-Life Battery Colllection Rates: A Case Study of Almaty

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The active growth in the popularity of chemical current sources (CCS) of various types has intensified the issue of their safe and environmentally friendly disposal. One of the key stages in this process is organizing the effective collection of used CCS, which is particularly challenging for small-sized batteries (SSBs) such as AA, AAA, D, C, and others. A significant barrier remains the low level of environmental responsibility among the population and insufficient awareness about both the harm caused by improper battery disposal and the existing collection infrastructure.

As part of this study, a sociological survey was conducted among residents of Almaty (Kazakhstan) to assess their awareness of the harm caused by SSBs, current disposal practices, and willingness to change them. Statistical data analysis was performed using the Pearson chi-square test and Cramér's V coefficient.

The study results revealed a "vaue-action gap" paradox. Despite a high awareness level of 89.1 percent, only 30.7 percent of respondents regularly use battery collection points (BCPs). Three main barriers were identified: insufficient infrastructure, lack of information, and behavioral inertia. Socio-demographic characteristics showed a weak correlation with disposal practices, while the availability of infrastructure was a determining factor. Strong support for technological solutions was confirmed, with 93 percent of participants responding positively to the introduction of vending machines for automated collection of used batteries.

Based on the findings, it is proposed to prioritize the expansion of accessible BCP networks, with an emphasis on implementing automated and digital solutions, as part of environmental policy. The presented results address the lack of empirical data in post-Soviet countries and can serve as a foundation for developing more effective strategies for managing used SSBs.

Peroxodisulfuric acid as an alternative leaching agent for the extraction of valuable metals in the processing of electrode mass from spent batteries

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In recent years, the use of lithium-ion batteries has sharply increased, leading to a rise in their waste volume. Their disposal of household waste poses an environmental threat, as the heavy metals they contain (Co, Li, Cu, Fe) can contaminate soil and water systems. This necessitates the development of effective recycling methods to prevent negative environmental impacts. In this context, it is important to develop effective methods for processing black mass valuable components of spent lithium-ion batteries (LIBs) [1]. The objective of this work is to evaluate the effectiveness of peroxoacid systems for leaching metals from electrode mass. In practice, sulfuric acid (H_2SO_4) is widely used, and the extraction rate for many metals in it does not exceed 50% (Co, Ni, Mn, Li, Fe) [2]. However, when combined with hydrogen peroxide (H_2O_2), its efficiency increases significantly. In this system, hydrogen peroxide acts as a reducing agent, which helps to increase the extraction efficiency of valuable elements. Specifically, this is due to the reduction of higher valence states of metals, such as $Co^{3+} \rightarrow Co^{2+}$ and $Mn^{4+} \rightarrow Mn^{2+}$, which increases the solubility of the corresponding compounds and facilitates their transfer into the solution [3].

$$10Li(Ni_{0,8}Co_{0,1}Mn_{0,1})O_2(s)+20H^{+}+5H_2O_2(aq)\rightarrow 10Li^{+}(aq)+8Ni^{2+}(aq)+1Co^{2+}(aq)+1Mn^{2+}(aq)+10O_2(gas)+20H_2O(liq)$$

The main advantage of using H_2O_2 is its environmental safety, as its decomposition produces only water and oxygen. This makes H_2O_2 a comparatively cleaner reagent compared to other leaching agents. The initial hypothesis of our research was based on the idea that peroxodisulfuric acid ($H_2S_2O_8$) could be an effective alternative to the standardly used mixture ($H_2SO_4 + H_2O_2$) in the leaching processes of electrode mass from lithium-ion batteries. This assumption was based on several theoretical premises:

1) the possibility of direct synthesis of peroxodisulfuric acid from sulfuric acid by an electrochemical method;

2) the economic efficiency of its production;

3) its decomposition does not form by-products that could hinder the extraction of target metals, similar to hydrogen peroxide [4-5]. It was hypothesized that the decomposition of peroxodisulfuric acid forms sulfuric acid and hydrogen peroxide, which are the main leaching components. Based on the methodology developed in our previous work, we synthesized peroxodisulfuric acid with a concentration of 150–170 g/l over an electrolysis time of 2 hours. The electrolysis was carried out in a two-chamber electrochemical cell with a platinum anode and a lead cathode, separated by a porous separator. 4M H_2SO_4 was poured into the cathode space, and a solution of 4M H_2SO_4 with the addition of ammonium thiocyanate (1 g/dm^3) was poured into the anode space to stabilize and catalyze the anodic processes. Leaching of the LIB electrode mass was carried out using the obtained $H_2S_2O_8$ (2 M) under the action of ultrasound at 70°C for 1 hour. After dispersion by ultrasound, 25 ml of distilled water was added, and the suspension was stirred on a magnetic stirrer (300–350 rpm, 12–14 h) with a liquid-to-solid mass ratio of 10/1. The study showed significant differences in the efficiency of metal extraction by different leaching agents. When using the $H_2S_2O_8$ system, the extraction rates were: Li — 4%, Ni — 21%, Co — 2%, Mn — 0.02%. For example, the use of the standard $H_2SO_4 + H_2O_2$ system demonstrated significantly higher efficiency: Li — 5.01%, Ni — 25.6%, Co — 3.95%, Mn — 0.4%. Peroxodisulfuric acid ($H_2S_2O_8$) showed intermediate extraction efficiency, which indicates its limited applicability as an alternative leaching agent. The obtained results indicate incomplete dissolution of the electrode mass components when using $H_2S_2O_8$, which makes this reagent less preferable for the extraction of valuable metals from the electrode mass of lithium-ion batteries.

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Graphene Oxide-Modified Polycarbonate Track-Etched Membranes Grafted with Polyacrylic Acid as Gel Polymer Electrolytes for Supercapacitors

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All-solid-state gel polymer electrolytes (GPEs) were developed by combining polycarbonate track-etched membranes (PC-TeMs) with graphene oxide (GO) and grafted polyacrylic acid (PAA) via UV-initiated RAFT polymerization [1]. PC-TeMs doped with 0–1 wt % GO were irradiated and chemically etched to yield uniform nanochannels (~270 nm diameter). Subsequent RAFT-mediated grafting of PAA—optimized through solvent selection, monomer concentration, and irradiation time—produced composite membranes with channels narrowed to ~150 nm while maintaining open porosity. SEM and AFM analyses confirmed thorough functionalization throughout the nanochannel network. BET measurements indicated a maximum Langmuir surface area of 11.4 m²/g for the PC-GO-g-PAA membranes, evidencing preserved high surface area and pore accessibility.

When impregnated with $EMIMBF_4$ ionic liquid and assembled into symmetric carbon-based coin cells, PC-GO-g-PAA GPEs demonstrated significantly enhanced ion transport ($\sigma \approx 2.28\times10^{-5}$ S cm^{-1}), higher specific capacitance (4.33 F g^{-1} at 5 mV s^{-1}), reduced series resistance ($R_s \approx 43.6\ \Omega$), and increased double-layer capacitance (Cdl ≈ 3.4×10^{-5} F) compared to pristine PC- TeMs.These performance gains arise from the synergistic roles of GO as an ion-conduction promoter and controlled PAA grafting within the nanochannels. The robust mechanical flexibility and superior electrochemical behavior of these composite membranes make them promising electrolytes for next-generation solid-state supercapacitors, particularly in wearable and flexible electronic applications.

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

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Optimization Of the Electrochemical Discharge of Cylindrical Spent LIBs Using $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$ Red/Ox Electrolyte

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Within the decarbonization strategy of the global economy, lithium-ion batteries (LIBs) have found widespread application in power grid systems, as well as energy sources for electric transport (including electric vehicles, electric buses, electric scooters, etc.). However, along with the rapid growth in the number of batteries produced, the quantity of spent devices is also increasing, posing a significant threat to the environment if improperly disposed of. Furthermore, spent LIBs are a valuable source of metals such as Li, Co, Mn, and others. Thus, the development and implementation of advanced methods for recycling spent LIBs is a critically important stage in the economy's decarbonization strategy. One of the key stages in recycling spent LIBs is the discharge step, which is necessary to prevent thermal runaway during the shredding of the batteries. The main methods for discharging LIBs are physical and electrochemical. The physical method involves controlled short-circuiting of the batteries by connecting them to a load or immersing them in conductive powders (most often Cu, Fe, or graphite). The electrochemical method is based on the electrochemical decomposition of water in aqueous electrolyte solutions.

The electrochemical discharge method has been recognized as the most promising for large-scale application. However, despite the extensive coverage of various electrolytes for discharge in scientific literature, the electrochemical discharge method for batteries requires optimization to achieve minimal financial and time costs for the process and to reduce the environmental damage during discharge, which is associated with the potential contamination of the discharge solution by internal battery components and the release of toxic gases.

Of particular interest is a redox electrolyte based on $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$. Its use is associated with a low corrosive impact on the battery terminal material, high environmental friendliness of the process (related to preventing breaches of the battery casing and subsequent leakage of toxic organic electrolyte into the solution), and the discharge of batteries to a near- zero potential thanks to the Fe^{2+}/Fe^{3+} redox reaction at the battery poles. However, despite numerous advantages, the time required to discharge batteries in a $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$ solution is significantly longer than the time taken for discharge in solutions of salts such as NaCl, $FeSO_4$, Na_2SO_4, etc. As shown by the research of Yang W. et al. [1] and Nembhard N. [2] conducted with other electrolytes, this problem can be solved by varying the electrolyte concentration, solution temperature, and ultrasonic power.

The present study is dedicated to the systematic optimization of the electrochemical discharge process for cylindrical spent LIBs using a $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$ redox electrolyte. The main objective of the work is to study the influence of parameters such as electrolyte concentration (2.5–20 wt%), temperature (20–70 °C), and ultrasound power (0–100 W) on the discharge efficiency. The results of the study will allow for the development of a more effective and environmentally safe discharge method, capable of reducing the time and financial costs required for the process, as well as ensuring a high degree of safety during subsequent stages of LIB recycling.

In this study, Response Surface Methodology (RSM) with a rotatable central composite design is used to determine the degree of influence of factors such as electrolyte concentration (2.5–20 wt%), temperature (20–70 °C), and ultrasonic power (0–100 W) on the discharge efficiency of cylindrical 18650 LIBs. The optimization work is aimed at minimizing the total electrical resistance of the system, which includes the solution resistance, the ohmic resistance created by gas bubbles on the electrode surfaces, and the resistance from the corrosion layer, by varying the investigated parameters. It is expected that the results of this optimization will provide a reliable model for a significantly faster and more efficient discharge process using the K3[Fe(CN)6]/K4[Fe(CN)6] electrolyte. The developed improved, environmentally friendly discharge method is expected to reduce the time and financial costs associated with LIB recycling, thereby enhancing the overall safety and efficiency of the LIB recycling process.

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Electrochemical Properties of Nanostructured $LaNi_5$ Anodes for Nickel-Metal Hydride Batteries

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Nickel-metal hydride (Ni-MH) batteries remain relevant in portable electronics and electric vehicles due to their high specific energy, wide operating temperature range, environmental safety, and recyclability [1–3]. A key element determining the performance of these batteries is the anode material, which must provide efficient and reversible hydrogen storage. Among various material types, AB5-type intermetallic compounds are the most common, with $LaNi_5$ being one of the most studied representatives. Despite a high theoretical capacity (~372 mAh/g for $LaNi_5H_6$), the practical capacity of commercial materials is usually limited to 150–200 mAh/g due to thermodynamic and kinetic limitations of hydrogen absorption, as well as technological aspects of powder preparation [4,5]. Traditional synthesis of $LaNi_5$ involves high-temperature melting (>2000 °C) in an inert atmosphere followed by energy-intensive mechanical grinding, which makes it difficult to obtain submicron particles without accumulating performance-degrading structural defects [6,7]. Reducing the anode particle size is a key factor in improving the kinetics of electrochemical processes, as it increases the specific surface area and shortens hydrogen diffusion paths. However, this approach faces serious challenges: intensive mechanical grinding to obtain fine fractions leads to the accumulation of defects that degrade the material's properties, and the $LaNi_5$ intermetallic itself is prone to significant degradation and capacity loss during long-term cycling. These factors highlight the potential of direct synthesis of $LaNi_5$ in nanocrystalline form, which avoids prolonged grinding and its associated structural defects. Therefore, the key objective of this work was to conduct a detailed electrochemical evaluation of nanostructured $LaNi_5$, produced by the sol-gel method, and to compare it directly with a standard commercial analogue to identify the practical trade-offs between enhanced kinetics and cycling stability.

Structural and electrochemical investigations revealed significant differences between the synthesized and commercial materials. The $LaNi_5$ nanomaterial was characterized by primary particles of 300–700 nm in size (forming agglomerates of ~5.9 µm), whereas the commercial sample, after grinding, contained particles of 1–5 µm (forming agglomerates of ~8.4 µm). X-ray diffraction analysis revealed the pure phase of $LaNi_5$ in both cases; however, the commercial sample exhibited peak broadening, indicating the accumulation of defects. These structural features were directly reflected in the electrochemical behavior: cyclic voltammetry and electrochemical impedance spectroscopy showed that the nanostructured material exhibited significantly higher process kinetics and activated more efficiently. However, long-term testing revealed its insufficient stability: after rapid activation and reaching a maximum specific capacity of ~180 mAh/g by the 5th cycle, it decreased to 130 mAh/g by the 50th cycle. In contrast, the microcrystalline commercial $LaNi_5$ demonstrated gradual activation and reached a stable capacity of ~185 mAh/g till the same 50th cycle.

Thus, nanostructured $LaNi_5$ exhibits better kinetic characteristics but shows inferior cycling stability. This is attributed to the high density of grain boundaries, which are susceptible to mechanical and corrosive damage during cycling. For the successful application of such materials, measures to enhance their stability are necessary, including doping, composite formation, or the application of protective coatings.

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Understanding high-voltage aqueous electrolytes through water activity

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Aqueous electrolytes offer exceptional safety, environmental compatibility, and high ionic conductivity for next-generation energy storage systems. However, their practical application is severely limited by the narrow thermodynamic stability window of water (1.23 V). The electrochemical stability window (ESW) represents the potential range between hydrogen evolution reaction at the cathode and oxygen evolution reaction at the anode, beyond which water undergoes electrochemical decomposition. The most intuitive approach to expand this window is reducing water content in the electrolyte. From a thermodynamic perspective, according to the Nernst equation, decreasing water concentration shifts the equilibrium potentials of water decomposition reactions - less water means higher energy is required to initiate its decomposition since water appears in the reaction quotient. From a kinetic standpoint, reduced water content decreases the probability of water molecules reaching the electrode surface and undergoing electron transfer. Following this approach of reducing water content through extreme salt addition, Suo et al. in 2015 introduced the "water-in-salt" concept using 21 mol/kg LiTFSI1, where the molar ratio of salt to water reached 1:2.6, expanding the ESW to 3.0 V and spawning a wave of research in this field.

In this work, we demonstrate the critical importance of water activity - a measurable parameter characterizing the effective concentration of water available for electrochemical processes. For highly concentrated systems, water activity differs significantly from the total water concentration due to extensive ion-water interactions. Our theoretical analysis using the Nernst equation reveals that thermodynamic contributions from reduced water activity become substantial only at trace water concentrations, which would no longer constitute an aqueous electrolyte. Through systematic Tafel analysis of LiTFSI electrolytes (1-21 mol/kg), we show that ESW expansion is primarily kinetically driven, with oxygen evolution being disproportionately affected - exchange current densities decrease logarithmically with water activity while hydrogen evolution remains largely unchanged.

Our study examines three primary strategies for water activity reduction: increasing salt concentration, introducing organic additives, and incorporating co-solvents. Importantly, we demonstrate that different electrolyte components achieve the same water activity at vastly different water concentrations - ions with high charge density (kosmotropic ions) maintain higher water content while achieving lower water activity compared to non-ionic components or chaotropic ions. The critical finding reveals that the electrochemical stability window correlates directly with water activity rather than total water molar concentration, establishing water activity as the true governing parameter for ESW expansion.While these approaches successfully expand the ESW, they impose severe penalties on transport properties critical for battery operation. Highly concentrated LiTFSI systems exhibit conductivity levels comparable to organic electrolytes coupled with dramatically increased viscosity. Our novel 13m LiTFSI in sucrose/H_2O system, despite achieving exceptionally low water activity, suffers from both prohibitive viscosity and poor conductivity. Such compromised transport properties result in significant ohmic losses and mass transfer limitations, rendering these electrolytes impractical for real battery applications. This study establishes water activity as a unifying parameter for predicting and comparing ESW across diverse aqueous electrolyte systems, providing fundamental insights for rational electrolyte design. We conclude that future development should focus on optimizing the balance between ESW, conductivity, and viscosity rather than pursuing maximum stability windows at the expense of practical performance.

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Low-temperature properties of the sodium-ion liquid electrolyte systems based on mixtures of EC, DEC, DMC solvents

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Sodium-ion batteries (SIB) are a promising class of secondary power sources that can replace some of the lithium-ion, lead–acid, and other types of batteries in large-scale applications. This fields imply SIBs use in a wide temperature range, including down to -40°C and below. However, it is generally considered that the acceptable operating temperature range for metal-ion batteries is from -20°C to +60°C, and the optimal is +15°C ~ +35°C [1]. The use of SIB below this span may be unsafe and is associated with a significant decrease in the capacity and Coulombic efficiency of the device. It is well-known that the low-temperature properties of metal-ion batteries significantly depend on the electrolyte system type and composition [2]. In the case of liquid carbonate electrolyte systems, phase transitions are possible as the temperature decreases. Therefore, from the point of view of SIB practical application, the cooling process is of the greatest interest.

Low-temperature properties of liquid electrolyte systems based on NaPF6 solutions of various concentrations in solvent mixtures EC:DEC:DMC = 1:1:0, 1:0:1, 1:1:1, 2:1:1 (by volume) were studied. Data on phase transitions obtained during visual experiments and DSC studies were compared with the results of electrochemical impedance spectroscopy in steel-steel, NVP-NVP (NVP means NASICON-type active material electrode $Na_3V_2(PO_4)_3$), Na-Na and NVP-Na cells, and with galvanostatic chronopotentiometry in NVP-NVP, Na-Na and NVP-Na cells.

It was demonstrated that the electrochemical properties of Na-ion electrolytes at low temperature do not align precisely with their thermodynamic characteristics. Yet, there is some relationship between the DSC peaks (Fig.1a-d) and the dynamics of specific conductivity changes (Fig.1e) upon cooling. In addition, the relationship between the individual properties of solvents and the electrochemical properties of solutions does not appear to be direct either.

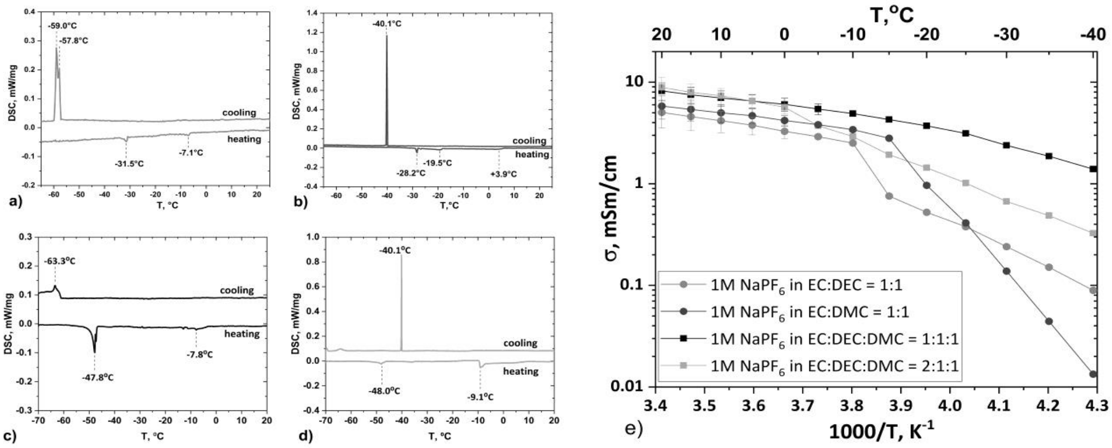

Figure 1. DSC curves for 1 M NaPF6 in (a) EC:DEC=1:1, (b) EC:DMC=1:1, EC:DEC:DMC=1:1:1, EC:DEC:DMC=2:1:1; e) Specific conductivity of $NaPF_6$ solutions.

It has been found that among the studied liquid electrolyte systems the specific conductivity of three-component solvent at low temperature is higher than that of two-component ones, and for 1M NaPF6 in EC:DEC:DMC = 1:1:1 it exceeds 1 mSm/cm at -40°C. This work was supported by the Russian Science Foundation (grant No. 25-43-00007).

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High-capacity Li-rich Mn-based cathode for lithium-ion batteries

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The global urgency to transition toward sustainable energy solutions is intensifying in response to accelerating climate change. Lithium-ion batteries (LIBs) have become the dominant energy storage technology for electric vehicles due to their high energy density, long cycle life, and cost-effectiveness. Among various cathode materials, lithium-rich manganese-based oxides (Li-rich Mn- based cathodes) exhibit exceptional specific capacity, yet suffer from voltage and capacity degradation, limiting their commercial viability. In this study, Li-rich Mn-based cathode materials were synthesized using sol-gel and co-precipitation methods, followed by lithiation with $LiOH\cdot H_2O$. Structural analysis via X-ray diffraction (XRD) confirmed phase-pure materials, while scanning electron microscopy (SEM) revealed that co-precipitation yields more uniform morphology. Electrochemical testing demonstrated promising capacity values, comparable to literature benchmarks, with performance dependent on C-rate and active material mass. While the synthesized materials show high potential, future work will focus on surface modifications, such as doping or coating, to enhance structural stability and cycling performance.

Solvothermal synthesis of Li(Fe,Mn)PO_4 cathode materials using iron and manganese oxides

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Cathode materials based on transition metals-lithium phosphates are widely used in rechargeable power supplies and make trend to the production of sustainable energy storage systems. Such materials as $LiFePO_4$, $LiFe_{1-x}Mn_xPO_4$ offer significant advantages as extended cycle life, lower production costs, and greater environmental friendliness compared to cobalt-containing cathodes. Developing or optimizing industrial-scale synthesis methods for lithium metal phosphates is necessary.

Solvothermal synthesis is widely regarded as one of the most promising approaches for producing phosphate-based materials. Its key advantage lies in the broad range of adjustable parameters – such as temperature, pressure, and solvent composition – which enable precise control over crystal structure, particle size, and morphology. This flexibility has led to the development of numerous synthesis techniques tailored to specific material properties. However, despite its versatility, the economic feasibility and resource efficiency of solvothermal methods remain unresolved challenges, limiting their large-scale industrial adoption.

Conventional hydro- or solvothermal synthesis of phosphate based cathode materials typically involves the use of water-soluble salts ($FeSO_4 \cdot 8H_2O$, $MnSO_4 \cdot H_2O$) as precursors. However, their variable water content, aging and impurity formation may cause some problems for a large scale production. Abudant in nature and industry transition metal oxides (e.g., Fe_2O_3, MnO_2) present a promising alternative to simplify and reduce the costs of synthesis.

Our scientific report adress the use of d-cation oxides as metal-containing reagents for solvothermal synthesis of $LiFePO_4$ and $LiFe_{0.5}Mn_{0.5}PO_4$ by several approaches. Various phase transformations, morphology of particles and electrochemical properties depending on the synthesis conditoins and routes have been studied, emphasizing the issues of crystal structure imperfections and ways to evaluate them. The obtained results indicate the promise of approaches associated with the use of poorly soluble iron and manganese compounds in the solvothermal synthesis of cathode materials and can be used to scale up their production technology.

Acknowledgment. The work was carried out with the financial support of the Russian Science Foundation, grant 24-13-00107.

Exploring Magnetic Field Effects on Sodium-Based Battery Systems for Enhanced Electrochemical Behavior

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External fields are gaining attention as a promising, non-invasive strategy for enhancing the performance of metal-ion batteries. Previously, magnetic fields (MF) have been explored as a way to enhance diffusion of lithium and zinc ions by promoting ionic transport through magnetohydrodynamic effect (MHD)[1,2]. This effect enhances ion diffusion and minimizes concentration gradients, effectively reducing dendritic growth and related safety concerns. Similarly, our work investigates the application of magnetic fileds to sodium-based systems with a goal of improving electrochemical performance and mitigating dendrite performance.

Initially sodium symmetrical cells were assembled and galvanostatically cycled with MF of varying strengths. The potential response of these cells were studied to determine the influence of magnetic field on ion transport, polarization and interfacial resistance. A significant reduction in potential hysterisis was observed to indicate the improvement of transport. For 100 cycels, the polarisation remained higher in the control cells without magnetic field. Simultaneously, the electrochemical impedance spectra obtained from these cells after every 20 cycles suggest the reduction of charge-transfer resistance with the help of MF. Increasing the magnetic field strength did not linearly correlate with the reduction in charge-transfer resistance or polarization, 250 mT yielded the most pronounced improvements.

Given the positive impact of MF on sodium metal systems, the study was extended to more complex chemistries than symmetrical cells to explore the influence of MF on redox behaviour and reaction intermediates. For this reason, both sodium sulphur cells and sulfurised polyacrylonitrile were electrochemically tested[3]. Lithium–sulphur and sodium–sulphur batteries suffer from the polysulfide shuttle effect, which has previously been mitigated using ferromagnetic additives under an applied magnetic field [4]. In this work, the effect of MF without the additives were checked to observe the unhindered perfromance of magnetic influence. To isolate and evaluate the direct impact of MF on battery performance, the cells were tested without any additives that might catalyse the reaction. As a result, although capacity fading was inevitable, the cells cycled with MF showed consistently higher capacities throughout the 100 cycles. Furthermore, signs of partial shuttle effect suppression and slower SDPAN breakdown were observed upon postmortem analysis with scanning electron microscopy and energy dispersive x-ray spectroscopy, indicating a positive influence of magnetic fields on electrode stability.

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Customized spray pyrolysis method for synthesis of doped NCM811 Cathode Material with High Nickel Content

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The development of high-energy-density cathode materials is critical for the advancement of next-generation lithium-ion batteries (LIBs). Among these, LiNi0.8Mn0.1Co0.1O2 (NCM811) has emerged as a promising candidate due to its high nickel content, offering superior capacity and lower cobalt dependency. However, challenges such as structural degradation, cation mixing, and poor cycling stability remain. This study investigates a scalable and cost-effective customized spray pyrolysis (cSP) method for synthesizing doped NCM811 cathodes, aiming to enhance structural integrity and electrochemical performance. The cSP process enables the formation of spherical, homogeneous precursor particles with controlled morphology and uniform dopant distribution. This study explores the spray pyrolysis synthesis of doped NCM811 cathode material with high nickel content. To enhance electronic conductivity, novel carbon-containing additives such as citric acid or urine were also tested as surface modifiers or internal carbon sources. The NCM811 powders were calcined at 720 °C under O2 atmosphere and characterized using XRD, SEM analyses. The XRD analysis confirmed the presence of NCM811. This indicates that the material meets the standard reference ICDD 00-068-0117 in terms of high crystallinity and the desired layered structure following sintering. The SEM illustrations of the synthesized powders revealed a wrinkled and contracted spherical morphology, closely resembling the structure described in the study by Dai et al. [1]. These findings highlight the complexity of incorporating organic additives and the critical role of controlled calcination. The results serve as a foundation for optimizing carbon-assisted NCM811 synthesis toward stable, high- capacity lithium-ion battery cathodes.

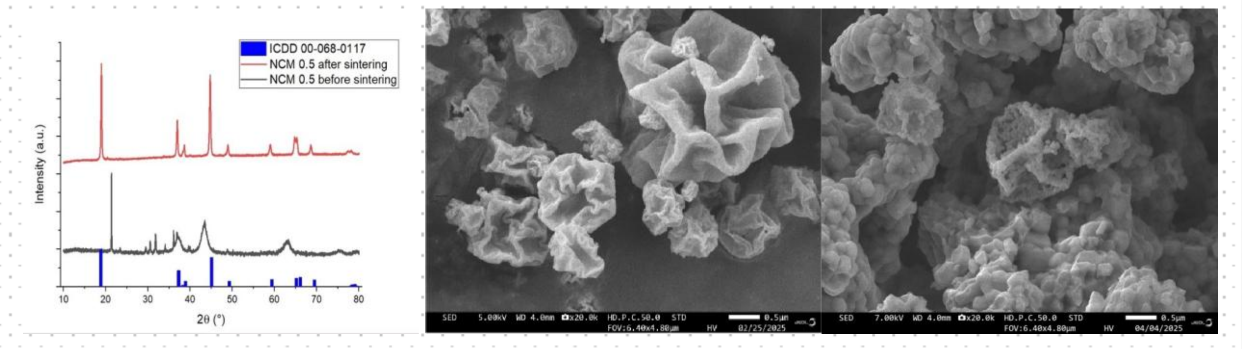

Figure 1. XRD of synthesized NCM811 with 0.5M Tmax=600°C before and after sintering and SEM images of synthesized material with concentration of 0.5 M at 600°C before sintering under 10.0K and 20.0K magnification

Acknowledgements. This research has been funded by the Committee of Science of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. BR21882402).

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The microstructural descriptors of carbon anode materials for sodium-ion batteries

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The demand for energy storage systems is increasing growing every year. Sodium-ion batteries, or SIBs, can be used as a promising and cheaper alternative to lithium-ion batteries (LIBs) [1]. However, the key challenge in commercializing this technology is finding suitable electrode materials with good electrochemical properties. Graphite, an anode material used in lithium-ion batteries, is not a suitable electrode material for SIBs. This is because sodium ions do not intercalate between the graphite layers. This limits the potential for SIBs development.

Hard carbon and soft carbon, as other sp2-hybridized carbon materials, can be promising anode materials for SIBs [2]. However, the exact relationship between the microstructure and the charge storage mechanism remains unclear. This study aims to investigate the microstructural features of these materials, including microporosity and defectiveness, as well as the mechanism of sodium ion insertion.

We obtained and compared hard carbon and soft carbon materials, based on different precursors and synthetics methods. Hard carbon materials were obtained from different sources (glucose, phenol-formaldehyde resin) and using different synthesis methods (hydrothermal and air pretreatment), soft carbon materials were obtained from petroleum pitch and synthetic polymers. The microstructural features of the materials were studied using powder X-ray diffraction, low-temperature gas adsorption, Raman spectroscopy and small angle X-ray scattering techniques. The materials demonstrated the initial Coulombic efficiency of up to 90% and a reversible capacity of up to 400 mAh g-1.

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Entropy Profile and SOC Estimation of Lithium-Thionyl Chloride Batteries

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The accurate and reliable estimation of battery state-of-charge (SOC) remains critical for the performance and safety of lithium-based batteries. In this research, the entropy profile of lithium-thionyl chloride ($Li/SOCl_2$) batteries were investigated at various states of charge. The experimental entropy data revealed significant and abrupt variations corresponding closely with changes in the electrolyte composition during the discharge process [1, 2]. Additionally, this work evaluates the applicability of Yazami's universal law for SOC estimation on $Li/SOCl_2$ battery systems [3]. Contrary to the behavior observed in lithium-ion batteries, our findings demonstrate that Yazami's universal law does not accurately predict the state parameters for lithium-thionyl chloride batteries. The deviations observed underscore fundamental differences in thermodynamic and electrochemical behavior between $Li/SOCl_2$ and conventional lithium-ion chemistries. The insights provided by entropy profile analysis and the limitations of existing universal models emphasize the need for customized modeling approaches specific to lithium-thionyl chloride systems. This study lays the groundwork for further research into tailored thermodynamic and electrochemical models that can enhance the accuracy of battery management systems (BMS) for $Li/SOCl_2$ technologies.

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Electrochemical generation of peroxydisulfuric acid using a flow electrolyzer

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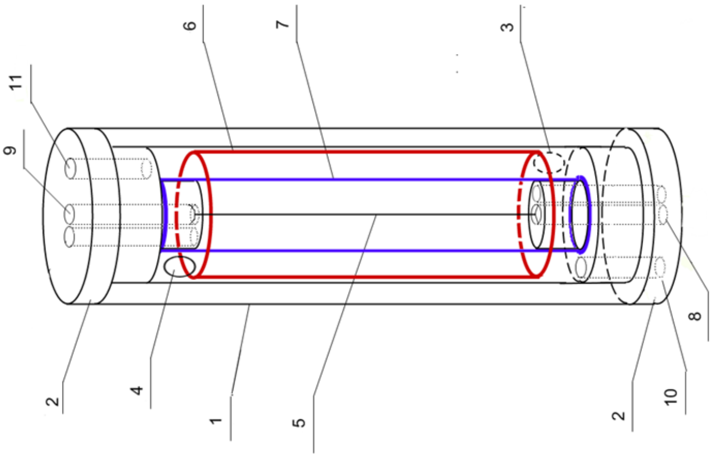
Hydrogen peroxodisulfuric acid ($H_2S_2O_8$) or persulfuric acid, is a strong oxidizing agent due to the presence of a peroxo bridge(-O-O-) between two sulfur atoms that can even oxidize Cr^{3+} to $Cr_2O_7^{2-}$ or Mn^{2+} to MnO^{4-} or other compounds. One of the essential applications of $H_2S_2O_8$ is the synthesis of hydrogen peroxide (by $H_2S_2O_8$ hydrolysis), which has better purity compared to other H_2O_2 synthesis methods. $H_2S_2O_8$ itself is usually synthesized by anodization of H_2SO_4 in a platinum (or other inert catalytic electrodes) electrode at specific electrochemical conditions. In this work, we present the electrochemical generation of peroxydisulfuric acid using a flow electrolyzer and the optimization of the process by varying different parameters, such as current density, electrolyte flow rate, and electrolyte temperature, that affect the generation yield. The flow electrolyzer for optimizing the process of peroxydisulfuric acid generation was made of teflon and has a cylindrical shape. The electrolyzer diagram is shown in Figure 1. The membrane is a cylinder separating the cathode and anode parts. The material used as a membrane is the same as the separators in lead-acid batteries. A platinum anode (5), membrane (7) and lead cathode (6) are coaxially located inside the teflon cylinder (1). The membrane is tightly fixed on teflon stops (2). Outside the membrane, in the cathode area, there are cooling tubes (10,11). Current supply for the anode is carried out through the opening for feeding the anolyte (8), and the cathode current supply is carried out through the opening for introducing the catholyte (3).



1 – electrolyzer corps; 2 – teflon stoppers; 3 – feeding catholyte hole; 4 – hole for removal of catholyte electrolysis products; 5 – anode (platinum wire); 6 – cathode (lead plate in the form of a cylinder); 7 – membrane; 8 – hole feeding; 9 – hole for removal of electrolysis products; 10,11 – inlet and outlet of the cooling system

Figure 1 – Schematic diagram of a flow electrolyzer for $H_2S_2O_8$ generation

To select the starting point for optimizing the process of peroxydisulfuric acid generation in a flow electrolyzer, we used data obtained in previous studies in a stationary electrolyzer. From these data, it is known that the main significant indicators for optimizing peroxydisulfuric acid generation are the current yield of the final product, its concentration, and energy consumption per unit mass of the product.

In the electrochemical process of generation of H2S2O8 in a flow electrolyzer, optimized in terms of energy consumption and productivity, the final solution contains on average 600 g/dm3 of H2SO4 and 180 g/dm3 of H2S2O8. This solution can be used as an independent oxidizer (wastewater treatment, black mass leaching, disposal of organic waste) or for the following production of H2O2.

Acknowledgment. This work is funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. BR27198753).

Analysis of heavy metal detection technology in water

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Water is an important resource of life and vital to humans and ecosystems. However, with the development of industrialization and the increase of human activities， the water environment is suffering from increasingly serious pollution. Among them, heavy metal pollution in water is a global environmental problem that poses a serious threat to ecosystems and human health. Therefore it is of great significance to develop efficient and accurate heavy metal detection technologies in water.

Heavy metals are metal elements with high density, high relative atomic mass and high toxicity. Heavy metals can enter the water environment through various channels, including industrial wastewater discharge, use of pesticides and fertilizers, mineral mining and coal burning. Once heavy metals enter the water body, they will be enriched in the water for a long time, causing serious pollution to the water environment.

Methods for heavy metal detection in water: Traditional analysis methods (atomic absorption spectrometry, inductively coupled plasma mass spectrometry), electrochemical sensor detection method, detection method based on biosensor, detection methods based on nanotechnology.

Heavy metal pollution in water poses a serious threat to humans and the ecological environment. The research on heavy metal detection technology in water has important scientific significance and practical value. As a water quality analyst, you need to master various detection technologies, select the most appropriate detection method according to different water environment pollution conditions, improve the accuracy and reliability of detection data, and provide strong technical support for water resource protection.

Acknowledgments. This study was funded by the Scientific Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (AP19676917 "Preparation of sensor by electrochemical methods for the determination of pesticides)

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Photocatalytic optimization of ZnO-Ga2O3 composite thin films for PEC water splitting: effects of thickness, environment, and annealing temperature

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This study reports a systematic investigation into the photoelectrochemical (PEC) performance of Ga_2O_3/ZnO (GZO) composite thin films fabricated via RF magnetron sputtering. GZO films were deposited on FTO/Glass and titanium (Ti) foil substrates, with key fabrication parameters - namely deposition time, annealing gas atmosphere, and annealing temperature - systematically varied to optimize photocatalytic activity. Surface morphology and crystallinity were evaluated using SEM and XRD, respectively, revealing that both deposition time and annealing conditions significantly influence grain structure and crystallinity, which in turn affect PEC performance. Among the tested conditions, films deposited for 25 minutes and annealed in air exhibited optimal performance, with annealing at 600 °C on Ti foil substrates yielding the highest photocurrent density of 1.7×10^{-4} A/cm^2 at 1.23 V vs. RHE. Electrochemical impedance spectroscopy (EIS) confirmed improved charge transfer properties at this temperature, although stability testing indicated potential trade-offs between performance and long-term durability. These findings highlight the critical role of thermal and atmospheric control during post-deposition treatment in tailoring the structural and electronic properties of GZO thin films. The optimized GZO photoanodes demonstrate strong potential for low-cost, efficient, and scalable solar hydrogen production, contributing to the advancement of sustainable energy technologies.

Feasibility Study of a Modular Wind-Solar Hybrid System for Low Wind Regions

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In many rural and isolated locations, there is still limited availability to a stable source of electricity, especially in conditions of low wind activity. This makes it urgent to search for new solutions in the field of autonomous energy. In my research, I am considering the possibility of creating a simple, inexpensive and easily assembled modular installation that combines wind and solar energy. Such a system could work both in open areas and in rooms where there is a natural air flow, for example, in building corridors.

At the moment, I am at the initial stage of work — collecting and analyzing information on existing hybrid systems, their advantages and limitations. I pay special attention to projects designed for low winds and those that can be assembled without complex equipment. I am interested in how effectively this approach can be used in developing or remote areas.

The purpose of my work is to form the concept of an installation that is suitable for minimal but stable power supply in difficult conditions. In the next step, I plan to move on to modeling, prototyping, and experimentally testing the idea.

Findings from this research may aid in making sustainable energy more affordable and accessible.

Keywords: Modular wind-solar unit, Low wind speed, Hybrid energy, Rural electrification, Alternative energy sources

First-Principles Investigation of Hydrogen Storage Potential in Boron-Doped and Lithium-Functionalized Graphene Structures

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Using first-principles density functional theory (DFT) simulations, we examine the potential of graphene-based materials—including pristine graphene, defect-engineered graphene, and boron-doped graphene decorated with lithium atoms—as candidates for hydrogen storage. Multiple configurations of boron substitution were analyzed to evaluate their structural integrity and electronic characteristics. To suppress lithium clustering and optimize hydrogen uptake, Li atoms were strategically positioned on the graphene surface. Among the materials studied, a boron-doped graphene structure featuring a single carbon vacancy and lithium decoration demonstrated the most promising hydrogen adsorption behavior. Adsorption energy calculations for up to eight hydrogen molecules revealed strong initial binding (approximately 0.73 eV for the first H_2 molecule), followed by moderate interactions for subsequent molecules—indicating potential for efficient and reversible hydrogen storage.

This investigation extends our earlier work on hydrogen adsorption in pristine and modified graphene (Myrzakhmetov et al., International Journal of Hydrogen Energy, 126, 413–428, https://doi.org/10.1016/j.ijhydene.2025.04.083), which addressed the effects of defects, nitrogen doping, and lithium decoration. The current study focuses specifically on the role of boron doping in tuning graphene's adsorption capabilities, offering further insights into designing advanced materials for hydrogen storage technologies.

Hydrogen Adsorption in Graphene Slit Pores: A GCMC Study of Pore Size and Temperature Effects

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Hydrogen storage is a central challenge in advancing clean energy systems, and nanoporous carbon materials—particularly graphene- based structures—offer promise due to their high surface area and tunable pore geometry. Prior density functional theory (DFT) studies have demonstrated that introducing defects, heteroatom doping, and metal decoration can locally enhance hydrogen binding energies by modifying the electronic structure and adsorption potential landscape [1]. In particular, lithium decoration within slit- shaped pores has been predicted to increase uptake via charge-induced polarization effects [2].

In this preliminary study, we perform Grand Canonical Monte Carlo (GCMC) simulations to systematically explore hydrogen adsorption in graphene slit pores with widths ranging from 0.4 to 4.0 nm. Six classical forcefields (COMPASS-I, COMPASS-II, COMPASS-III, PCFF, CVFF, and DREIDING) are evaluated to quantify variability in uptake predictions due to differences in interatomic interaction models. Simulations using the COMPASS-II forcefield were carried out at 77 K, 87 K, 98 K, 195 K, and 298 K to quantify temperature effects. Our results highlight the significant influence of pore width and temperature on hydrogen uptake, with lower temperatures substantially enhancing adsorption capacities, as shown in Figure 1. On the effect of pore width, while total hydrogen uptake generally increases with pore width due to greater pore volume, excess adsorption, a measure of adsorptive efficiency, exhibits a distinct optimal pore width range. This optimal range corresponds to the regime where the overlap of adsorption potentials from opposing walls maximizes hydrogen binding. At higher temperatures, adsorption is suppressed by thermal motion, but lithium decoration consistently enhances uptake across all pore widths due to stronger H_2–Li interactions.

These results underscore the dual importance of optimizing pore geometry and accurately modeling adsorption energetics. Future simulations will incorporate DFT-calibrated potentials and additional chemical functionalization of graphene systems to enhance the reliability and predictive accuracy of hydrogen adsorption modeling.

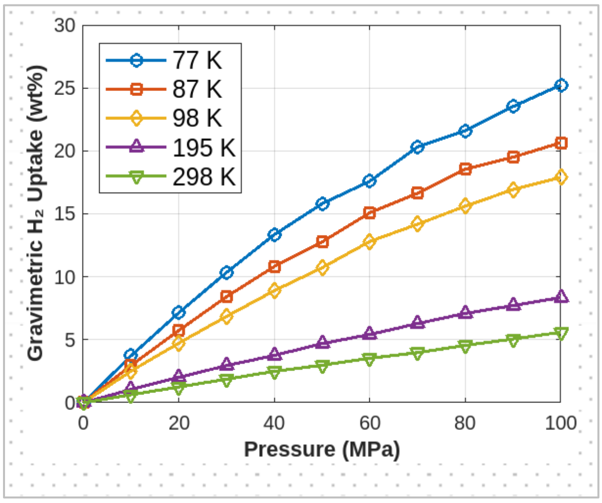

Figure 1. Hydrogen adsorption isotherms (wt%) for 1.0 nm pore at different temperatures (77–298 K).

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Predicting electronic properties of strongly correlated materials using the ACBN0 pseudo-hybrid density functional in the FHI-aims software package

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Density Functional Theory (DFT) is a powerful tool for electronic structure calculations, but it often fails to accurately describe strongly correlated systems. The DFT+U method addresses these limitations by introducing an on-site Coulomb repulsion term (Hubbard U) that improves the description of electron localization. This approach is particularly effective for transition-metal oxides, rare-earth compounds, and other materials where strong electron correlations play a crucial role, leading to more accurate predictions of band gaps, magnetic properties, and structural stability. By balancing computational efficiency with improved accuracy, DFT+U serves as a practical and reliable method for studying strongly correlated systems. However, the value of the Hubbard correction U should be determibed either empirically or ab initio using some additional approaches.

The ACBN0 pseudo-hybrid density functional [1] is one of the most promising approach for Hubbard U calculation from the first principles. Unlike other ab initio methods (cRPA[2], linear response[3]), the ACBN0 has a relatevely low computational cost, which makes possible to use it in high-throughput calculations for materials discovery. In this work, the ACBN0 method was implemented in the FHI-aims package [4], an all-electron code for electronic structure calculations based on numerical atom-centered orbitals. The advantage of using this package over plane-wave basis set codes, for which the ACBN0 method was originally implemented, lies in the availability of a localized basis set, which allows for modeling of localized states naturally. The implemented code was tested on bulk transition metal oxides (same as in the original paper [1]) —TiO_2 (rutile), MnO, NiO, and ZnO (wurtzite) — demonstrating improved predictions of their band structures compared to PBE (see Table 1).

	TiO_2	MnO		NiO		ZnO
	direct	direct	indirect	direct	indirect	direct
Experimental	3.03 [5]	4.1[6]		4.0 [6]		3.3 [7]
PBE	1.83	1.40	0.85	1.11	0.97	0.75
ACBN0 (FHI-aims)	2.74	2.86	2.31	4.69	4.11	2.68
ACBN0 (QE) [1]	2.83	2.83	2.31	4.29	3.80	2.91

Table 1. Band gap (in eV) for different transition metal oxides.

As a more complex structure, the double perovskite Ba_2CoNbO_6 electronic structure was studied with different functionals and the band structure was compared (see Table 2). Since there are no experimental data for band gap value for this material, it was compared with the reliable HSE06 hybrid funcional. One can see a significant improvement with respect to the PBE result, but still far from the HSE06 one. However, as it was shown in the work [8], for such materials the hybrid functional can overestimate the band gap.

	PBE	ACBN0 (FHI-aims)	ACBN0 (QE)	SCAN[8]	HSE06 [8]
Band gap, eV	0.53	1.83	1.76	0.60	3.05

Table 2. Band gap (in eV) for Ba2CoNbO6 calculated with DFT using different potentials.

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Investigation of ion migration and hysteresis effects in perovskite solar cells via drift-diffusion simulation

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Hybrid organic–inorganic perovskites, particularly methylammonium lead iodide ($MAPbI_3$), have attracted considerable interest due to their exceptional photoelectric properties, making them promising candidates for next-generation solar cells [1,2]. However, despite these advantages, $MAPbI_3$-based perovskites are susceptible to ion migration, during which dissociation into methylammonium (MA^+) and iodide (I^-) ions occurs [3]. This phenomenon leads to instability in device performance, including the emergence of hysteresis in current–voltage (J–V) characteristics.

In this study, drift–diffusion modeling is employed to analyze these effects. This approach enables a detailed investigation of hysteresis behavior and allows for the assessment of how scan rate, carrier lifetime, and charge carrier mobility influence the shape of the J–V curves in perovskite solar cells [4].

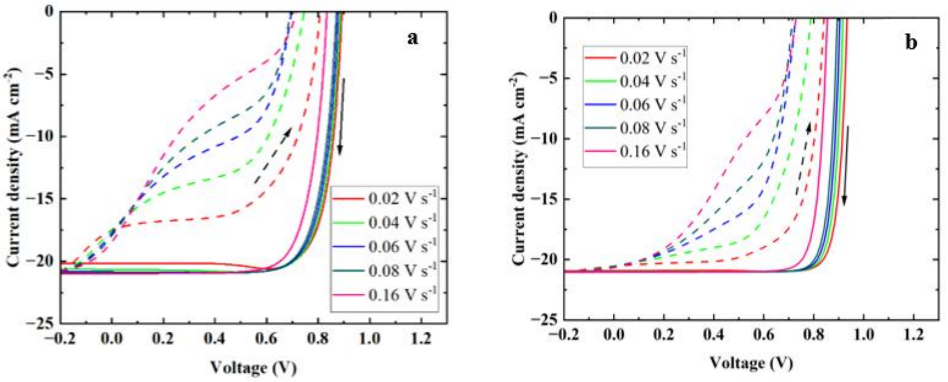

Figure 1. J–V characteristics of $MAPbI_3$ under varying ion mobilities: (a) symmetrical changes in both anion and cation mobilities; (b) varying anion mobility while fixing cation mobility at 10^{-12} cm^2/V·s.

Figure 1a illustrates the case where the mobilities of cations and anions are equal ($\mu_a = \mu c$). At high mobility (10^{-8} cm^2/V·s), the J–V curve appears symmetric with minimal hysteresis, indicating rapid ion redistribution and efficient compensation of the internal electric field. In contrast, Figure 1b shows in which cation mobility is fixed at 10^{-12} cm^2/V·s, while anion mobility varies from 10^{-8} to 10^{-12} cm^2/V·s. As anion mobility decreases, hysteresis progressively intensifies: at the lowest value ($\mu_a = 10^{-12}$ cm^2/V·s), the reverse J–V curve exhibits a pronounced shift, indicating significant distortion in charge transport processes.

Acknowledgments. This work was supported by the Grant No. AP27508227 of the Ministry of Science and Higher Education of the Republic of Kazakhstan

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Performance optimisation of $CH_3NH_3SnI_3$ based perovskite solar cells via drift-diffusion simulation

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Methylammonium tin iodide ($CH_3NH_3SnI_3$) has attracted significant attention in recent years as a promising lead-free material for perovskite solar cells (PSCs), offering an environmentally friendly alternative to traditional lead-based compounds. With a direct band gap of approximately 1.3 eV, high hole mobility, and favorable charge transport properties, $CH_3NH_3SnI_3$ possesses strong theoretical potential for high-efficiency solar energy conversion [1-3].

However, further development of devices based on this material is limited by several fundamental challenges, most notably the pronounced hysteresis in current–voltage (J–V) characteristics. This behavior is associated with slow internal dynamic processes, including ion migration and interfacial charge relaxation [4].

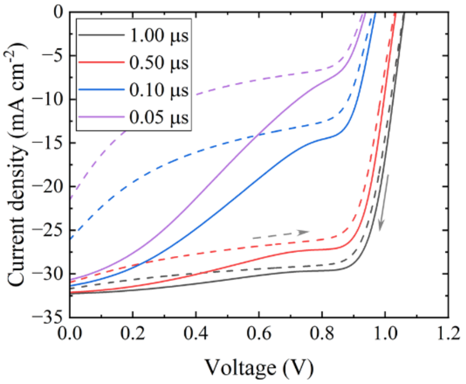

Figure 1. Numerical simulation results demonstrating the influence of charge carrier lifetimes (τ_n, τ_p) on the performance of $CH_3NH_3SnI_3$-based PSCs.

In this study, numerical simulations based on the drift-diffusion model were conducted to investigate the role of ion-mediated recombination and ionic mobility in the formation of hysteresis in $CH_3NH_3SnI_3$-based devices. Particular attention was paid to the influence of carrier lifetime (τ), a key parameter governing the efficiency of photogenerated carrier generation, transport, and extraction (see Fig. 1). The simulation results show that increasing τ significantly reduces bulk and interfacial recombination losses, minimizes the hysteresis index (HI), enhances the short-circuit current density ($J_{sc} = 31.62$ mA/cm^2), and improves the operational stability of the device under both forward and reverse scan directions. Analysis of the J–V characteristics as a function of carrier lifetime confirmed that longer lifetimes lead to improved photovoltaic performance, reduced impact of ion migration, and enhanced output stability. Thus, this study highlights the critical importance of precise control over carrier lifetime and ionic mobility in improving the efficiency and long-term stability of $CH_3NH_3SnI_3$-based PSCs. It also demonstrates the potential of numerical modeling as an effective tool for the engineering optimization of perovskite photovoltaic devices.

Acknowledgments. This work was supported by the Grant No. AP19174728 of the Ministry of Science and Higher Education of the Republic of Kazakhstan

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Some role of ^{9}Be liner's impurities in MagLIF device fuel

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One of the problems of Magnetized Liner Inertial Fusion (MagLIF) type fusion devices [1, 2] to solve is an appropriate selection of material of liner, which is the wall of this type of fusion reactor. When the liner walls melt due to high current and are compressed by its magnetic field, it will create impurities in the fuel of the device, initially loaded into the liner's cavity. This will affect the nature and parameters of thermonuclear burning, launched by the inertial field due to laser ignition.

The electron component of impurity creates additional radiation losses. Therefore, using a material with a low Z allows them to be reduced. However, the ionic component can actively participate in energy delivery by interacting with fuel particles. This affects the burning efficiency with depend on the temperature of the fuel burning area. Then, it is available to select the liner material most suitable for certain tasks. As example, the prospect MagLIF liner material is stable beryllium (9Be) [3]. This element under the given conditions has a metallic form and can be used as a material for the liner. In the main channel beryllium splits into 2 alpha particles, which actively participate in the exothermic reaction, and a neutron.

Up to a certain value of the impurity ratio, the burning of MagLIF thermonuclear fuel can stay self-sustaining. Therefore, one of the issues to keep in mind when tuning the parameters of such magneto-inertial fusion devices is the permissible values of impurity in the fuel.

In this paper, based on the modelled burning pattern of the MagLIF device in work [3], an assessment of the instantaneous threshold values of the liner impurity for efficient burning is made. This instantaneous indicator shows what maximum proportion of the fuel the liner impurity can make up at a certain time moment to maintain the growth of the burning region temperature with "contaminated" fuel. It was found that the most energy-efficient type of fuel DT allows the presence of beryllium liner impurities in the fuel up to values of several tens of percent. Other types of fuel DD and D3He are also considered.

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Computational Analysis of Bi_2S_3 Crystal Morphology and Hydrogen Adsorption Behavior

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Bismuth sulfide (Bi_2S_3) is a low-cost, non-toxic semiconductor with potential applications in photocatalytic hydrogen production. In this study, we performed a comprehensive first-principles investigation of the surface stability and hydrogen adsorption characteristics of Bi_2S_3 using density functional theory (DFT). Surface energies were calculated for all possible cleaved facets corresponding to the (100), (101), (001), and (010) orientations. The lowest-energy facet for each orientation was identified, with surface energies of 1.41, 1.55, 1.58, and 0.81 $J \cdot m^{-2}$ for the (100), (101), (001), and (010) surfaces, respectively, indicating that the (010) surface is the most stable. Using the Wulff construction, we predicted the equilibrium crystal morphology of Bi_2S_3 (Figure 1). To assess the potential for hydrogen evolution reactions (HER), the free energy of hydrogen adsorption was calculated on each surface, identifying the most catalytically active facet (Figure 2).

Computational Details: All calculations were carried out using the Vienna Ab initio Simulation Package (VASP). The projector augmented-wave (PAW) method was employed to describe the interaction between ions and electrons, and the Perdew–Burke–Ernzerhof (PBE) form of the generalized gradient approximation (GGA) was used for the exchange–correlation functional. A plane-wave energy cutoff of 500 eV was used and verified to ensure total energy convergence. Geometry optimizations were performed using the conjugate gradient method until the forces on all atoms were less than 0.02 eV/Å and the electronic self-consistent field (SCF) cycles converged to within 10^{-5} eV. To account for long-range dispersion interactions, van der Waals corrections were included via the DFT-D3 method with the Becke–Johnson damping scheme.

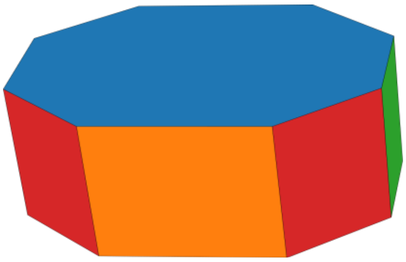

Figure 1. Calculated crystal structure of Bi_2S_3 using the Wulff construction method.

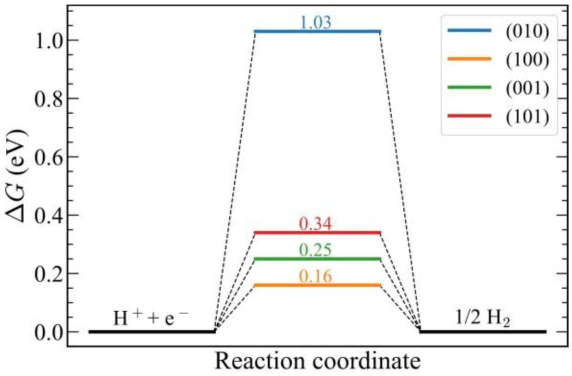

Figure 2. Calculated Free energy for each considered side of Bi_2S.

DFT Study of Pristine 6FDA and Bisimidazolium-Br Crosslinked Polyimide Triboelectric Layers

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Triboelectric nanogenerators (TENGs) harvest mechanical energy through contact electrification, and polymeric dielectric films, particularly those bearing strongly electron-withdrawing substituents, are widely employed as the negative friction layers [1]. In particular, fluorinated 6FDA-based polyimides (with $–CF_3$ groups) have been developed as tribo-negative films, yielding significantly enhanced output compared to non-fluorinated analogs [2]. The bulky $–CF_3$ units in 6FDA increase backbone rigidity and electronegativity (restricting chain packing), which underpins their high negative affinity. In this study, we introduce a novel ionic crosslinked variant of 6FDA polyimide, synthesized using a bisimidazolium bromide linker, and conduct a comprehensive density functional theory (DFT) investigation to compare its electronic structure and triboelectric potential with pristine 6FDA polyimide. First-principles DFT calculations were performed using Gaussian 16 (B3LYP/6-311++G) for isolated molecular models and Quantum ESPRESSO (PBE plane-wave basis) for periodic structures. Both polymers were fully optimized and analyzed for frontier molecular orbitals, natural bond orbital (NBO) charge distributions, and electrostatic potential (ESP) surfaces. To assess triboelectric compatibility with common electrode materials, we also calculated the work functions of Al(111) and Cu(111) slabs as representative tribo-positive layers. Comparisons of HOMO–LUMO levels, NBO charges, and area-vs-ESP plots (generated using Multiwfn) revealed distinct electronic behavior between the pristine and crosslinked polymers, particularly in terms of surface charge localization. The results offer atomic-level insight into how ionic crosslinking modulates charge distribution and electron affinity in fluorinated polymers, providing a rational basis for designing high-performance TENG materials via molecular-level modifications such as selective fluorination and ionic functionalization.

Keywords: 6FDA polymer, bisimidazolium Br crosslinked, Tribonegative, DFT

Acknowledgments. This research was supported by the research projects AP23486880 from the Ministry of Higher Education and Science of the Republic of Kazakhstan and 111024CRP2010, 20122022FD4135 from Nazarbayev University.

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Development of a Freestanding and Flexible Sensing Material for Methane Gas Monitoring

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Nowadays, flexible and wearable gas sensors have attracted increasing attention for real-time, low-power environmental monitoring. However, many conventional sensors suffer from poor flexibility, low methane selectivity, and limited sensitivity at room temperature. To address these challenges, composites based on conductive polymers and carbon materials have emerged as promising alternatives due to their flexibility, tunable conductivity, and ease of fabrication [1]. In this study, a flexible and wearable gas sensor was developed using a poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) composite which was deposited onto flexible interdigitated electrodes. The primary objective was to create a methane-selective sensor with low power consumption and high sensitivity. Morphological characterization via SEM and EDS confirmed a uniform distribution of components within the composite, while TGA analysis indicated thermal degradation beginning above 150 °C. FTIR spectroscopy verified the presence of key functional groups in the polymer matrix. Electrical properties evaluated through Hall effect measurements revealed a strong temperature dependence of charge carrier mobility and sheet resistance, with optimal mobility observed at 110 °C correlating with the maximum sensing response. Gas detection tests performed at 110 °C for 100 ppm concentrations of NH3, CO, CO2, CH4, and NO showed the highest response of 7% for CH4, confirming excellent methane selectivity. The sensor also exhibited stable electrical conductivity, supporting its suitability for low-voltage operation. These results highlight the potential of the developed composite sensing material for cost-effective, scalable, and high-performance methane sensing in flexible and wearable electronic applications.

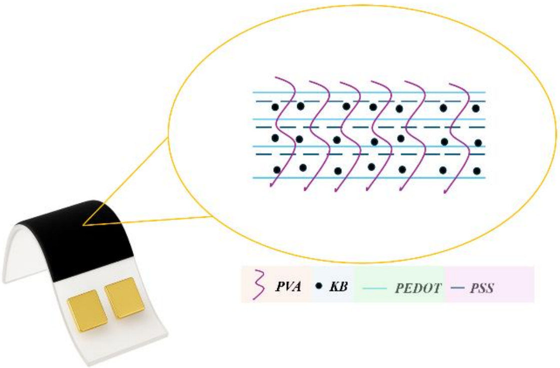

Figure 1. Structure and Composition of the Wearable Gas Sensor Based on KB/PVA/PEDOT:PSS.

Acknowledgments. This research has been funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP23489498, Development of advanced polymer-based sensor containing biowaste-derived carbon for detection of NH3).

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Conductive polymer-coated electrospun nanofibers for chemoresistive gas sensing

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Chemoresistive gas sensors based on electrospun nanofiber coatings are of growing interest due to their high surface area, interconnected porosity and efficient interaction with gas molecules. A flexible platform for creating nanostructured sensing layers is provided by electrospinning, where the polymer selection has a significant impact on the fiber's morphology, stability and functionality. By adding functional nanomaterials into the electrospun nanofibers, chemoresistive sensor performance can be further improved [1]. Among them, metal oxide semiconductors (MOS) with their semiconductive nature, presence of oxygen vacancies and surface reactivity, and carbon-based materials, which have high electrical conductivity and many active sites. To further impart conductivity and amplify resistance-based signal variation, electrospun nanofibers are coated with intrinsically conductive polymers [2]. In this context, polyaniline (PANI) and polypyrrole (PPy) are extensively researched because of their tunable electrical characteristics, resilience to environmental changes and sensitivity to redox-active gases.

In this study, polyvinylpyrrolidone (PVP) and polyvinylidene fluoride (PVDF) were selected as matrix polymers for the obtaining of nanofibers via the electrospinning technique. PVDF has greater chemical resistance and mechanical properties, while PVP has an advantage for processing, fiber homogeneity and compatibility with different dopants. Obtained nanofibers were successfully coated with a conductive polymer. In addition, MOS and carbon-base material were incorporated into the structure to improve sensing performance through enhanced selectivity, conductivity and gas adsorption. Gas sensing performance was evaluated by resistance changes when the material was exposed to target gases at different concentrations and thermal conditions.

Acknowledgments. This research was funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan, AP23488260 "Anionic Sulfonic Polyamides as Conductive Polymers and Gas Sensor Materials".

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

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Air pollution continues to be a major global challenge, threatening both human health and the environment. Addressing this issue requires the development of advanced gas sensors capable of detecting harmful gases and monitoring air quality effectively [1,2]. Metal oxide semiconductor (MOS)-based sensors have gained significant interest due to their promising sensing properties. Among these, ZnO@NiO@C core-shell nanofibers demonstrate superior gas sensing performance, thanks to their high surface area, excellent sensitivity, and selectivity. Notably, unlike traditional MOS sensors that typically require high operating temperatures, ZnO@NiO@C sensors operate efficiently at room temperature, resulting in lower energy use and improved safety [3,4].

This study introduces a novel approach for synthesizing ZnO@NiO@C core-shell nanofibers through a combination of electrospinning and the Successive Ionic Layer Adsorption and Reaction (SILAR) method. The fabricated nanostructures exhibit enhanced gas response, fast recovery times, and low-temperature operation, positioning them as promising candidates for future gas sensing technologies.

Acknowledgements. This research has been funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP22785922, Development and production of heterostructure thin films with unique properties for highly effective detection of hazardous gases).

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Ab initio studies on ZnO-based gas sensors for detecting VOCs.

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Monitoring volatile organic compounds (VOCs) released during food spoilage is essential for ensuring food safety during storage and transport. VOCs act as indicators of microbial growth and chemical degradation, making them key targets for gas-sensing technologies. Metal oxides and polymer-based composites are widely studied sensing materials due to their high sensitivity and selectivity [1]. However, sensor performance is highly dependent on surface characteristics and gas adsorption behavior. To explore these interactions, Density Functional Theory (DFT) was used to model VOC adsorption on the ZnO (100) surface, focusing on how surface properties influence detection.

The ZnO (100) surface was structurally optimized, yielding lattice constants of a = 3.263 Å and c = 5.235 Å, with a unit cell volume of 48.30 Å^3. Among the tested VOCs, ethanol exhibited the strongest adsorption with an energy of –1.028 eV, forming a strong chemisorption bond through its hydroxyl group, which withdraws +1.27e from the ZnO surface. Acetone also showed strong interaction with an adsorption energy of –0.947 eV. These strong bindings suggest high sensitivity but may limit desorption at room temperature.

Other toxic gases, including NO2 (–0.511 eV), formaldehyde (–0.357 eV), NO (–0.264 eV), and CO (–0.260 eV), exhibited weaker interactions. This trend highlights ZnO’s selectivity toward ethanol and acetone.

To reduce desorption challenges and improve sensor efficiency, ZnO can be integrated with CuO to form a heterostructure. Prior calculations showed that ethanol adsorbs onto the CuO (111) surface with a moderate energy of –1.75 eV, allowing for better sensing at lower temperatures. These findings demonstrate the potential of theoretical modeling to guide the design of VOC sensors with improved performance and lower energy demands [2].

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Zinc Oxide decorated carbon nanofibers for room temperature gas sensing applications

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Chemiresistive gas sensors gained much attention and the most popular active materials made of metal oxide semiconductors (MOS). ZnO is under active research for gas sensing due to good response toward toxic gases such as CO, NO, NH3. However, ZnO suffers with low electrical conductivity and high resistance at room temperature (RT). Therefore ZnO based chemiresistive gas sensors operate at high tempratures which leads to the safety concerns and additional energy input is costly. The electrospun nanofibers possess high surface area while carbon nanofibers (CNF) has good electrical conductivity at room temperature which is very beneficial for gas sensing applications due to more active sites to interact with target gases.

In this research, ZnO was synthesized via sol gel method which subsequently used for the electrospinning with PAN, which is precursor for the CNF, in the DMF solvent. The electrospun nanofibers were treated with 2 steps of annealing processes called stabilization and carbonization. The obtained free-standing ZnO/CNF composite material is the active material for gas sensing. The obtained sample demonstrates ohmic behaviour at the RT therefore can be utilized for the chemiresistive gas measurement. The sample shows dynamic respone for the CO_2 from 10 to 500 ppm in a linear manner (Figure 1a).

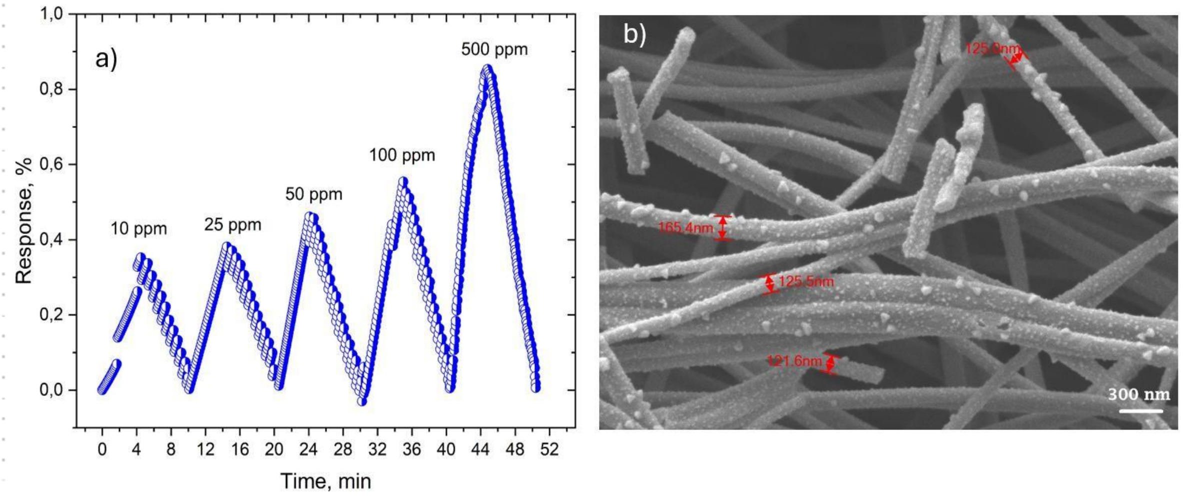

Figure 1. a) dynamic respose of the sample for the CO_2, b) the SEM image of the ZnO decorated CNF which clearly indicates that the ZnO particles are on the surface of CNF.

Acknowledgments. This research was funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan, AP23488260 " Anionic Sulfonic Polyamides as Conductive Polymers and Gas Sensor Materials".

Characterization of Co-Doped ZnO Thin Films Synthesized via RF Magnetron Sputtering for Enhanced Gas Sensing Applications

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Chemoresistive gas sensors often utilize metal oxides because of their superior physicochemical characteristics. Zinc oxide (ZnO) has emerged as a highly promising gas sensing material due to its chemical stability, abundance, and a large bandgap energy of 3.37 eV. Nonetheless, pristine ZnO exhibits low selectivity and elevated working temperatures, which constrain its practical sensing uses. This study examines cobalt (Co) doping as a method to enhance the structural and optical characteristics of ZnO thin films and augment their gas sensing capabilities [1].

Co-doped ZnO (CZO) thin films were synthesized via RF magnetron sputtering on glass substrates. The films were analyzed utilizing X-ray diffraction (XRD), UV-Vis spectroscopy, and energy-dispersive X-ray spectroscopy (EDS). XRD examination verified the retention of the hexagonal wurtzite structure of ZnO, including a predominant peak associated with the (101) plane. Doping caused peak shifts and broadening, signifying lattice strain and a decrease in grain size. The crystallite size of 3 wt% CZO was determined to be 51.5 nm, with a lattice strain of 0.00225, in contrast to 57.8 nm and 0.00200 for undoped ZnO. The results indicate heightened lattice distortion resulting from the integration of smaller Co^{2+} ions into the ZnO lattice. UV-Vis research indicated a modest reduction in bandgap energy following Co doping, which may improve visible light absorption and electrical conductivity—attributes advantageous for gas sensor performance. EDS validated the homogeneous distribution of cobalt within the ZnO matrix, confirming effective doping. The structural and optical alterations resulting from Co doping are anticipated to enhance the gas sensing efficacy of ZnO-based thin films, positioning CZO as a viable choice for next-generation chemoresistive gas sensors.

Acknowledgments. This research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP13067814) and Nazarbayev University under the Collaborative Research Program (Grant No. 111024CRP2008).

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Biomass-derived Co-modified carbon-paste electrode for electroanalytical sensing

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This research investigates various applications and methods for utilising carbon nanomaterials within the field of electrochemical science, aiming to establish a foundation for cost-effective identification technologies that can transition from academic exploration to commercial use. There is a growing interest in real-time analysis facilitated by electrochemical sensors. A chemical sensor is an analytical tool designed to provide data about a particular component in a sample continuously. Carbon-paste electrodes (CPEs) are versatile devices capable of detecting a wide range of substances [1]. Additionally, potentiometric measurements using CPEs offer simplicity, speed, and cost-effectiveness advantages compared to other electrochemical techniques [2]. Noteworthy benefits of CPEs include their stable response and low ohmic resistance, especially in contrast to membrane electrodes that have been modified for renewability. Furthermore, CPE sensors do not require the use of internal solutions.

This study examines the feasibility of transforming agricultural biomass waste into carbon-rich materials suitable for fabricating carbon-paste electrodes. Material characterisation indicates that the resultant carbonaceous material primarily comprises aromatic graphitic-like structures, with hydrogen-to-carbon and oxygen-to-carbon ratios measuring 0.006 and 0.18, respectively. The SEM-EDS analysis demonstrates uniform elemental distribution across the surface. It is confirmed that activated carbon, derived from thermally treated waste wheat and chemically modified with Co(II, III) ions, can function effectively as a carbon-paste sensor in direct potentiometry and potentiometric (acid-base and redox) titration. In the permanganometry tests conducted to measure hydrogen peroxide levels (n=3), 3.00% was introduced, 2.97% was detected, yielding an absolute error of 0.02%, a relative error of 0.78%, and a precision rating of 99.23% (as depicted in the titration curves shown in Figure 1). This electrode is chemically stable and gives reproducible results with a practical lifetime of 12 weeks, with a fast response time (□10 s).

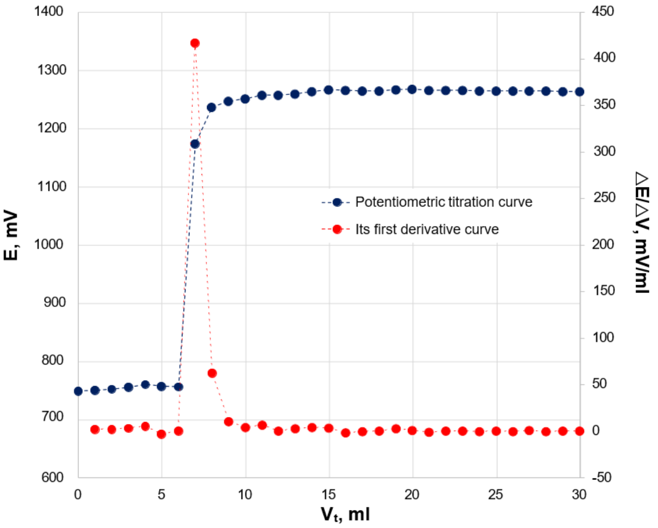

Figure 1. Permanganometry titration curves recorded using Co-modified carbon-paste electrode

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Electroanalytical Sensor Based on Ni-Modified Carbon Paste Electrode from Renewable Biomass Precursors

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This study presents a Ni-modified carbon paste electrode (Ni-CPE) made from activated biochar derived from wheat straw, a cost-effective and renewable agricultural by-product. The development of these electrodes is timely due to the increasing demand for affordable and environmentally friendly sensors in analytical chemistry [1]. With easily accessible raw materials and a straightforward preparation process, the electrode boasts low production costs, simple modification, and quick adaptability for various analytical applications [2].

The study has demonstrated that two-step carbonisation of wheat straw-derived biochar resulted in carbonaceous material with a reduced H/C atomic ratio of 0.01 and decreased polarity, indicating a high degree of aromatisation and enhanced hydrophobicity (Figure 1). Raman spectroscopy confirmed the formation of a partially graphitised structure with detectable defects. XRD analysis revealed the presence of graphite, graphene oxide, and nickel crystalline phases, while SEM-EDX mapping showed a uniform distribution of elements, ensuring structural homogeneity and stability. These physicochemical properties contributed to the high electrochemical activity, stable potential response, and sensitivity of the nickel-modified carbon paste electrode towards acid-base titration.

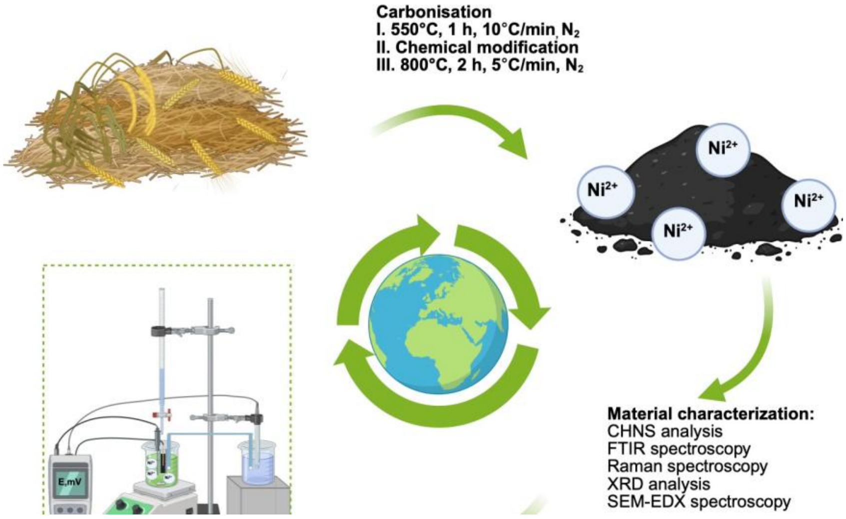

Figure 1. The graphical abstract reflecting this study

Potentiometric titration of nitric acid with sodium hydroxide confirmed the high accuracy, reproducibility, and reliability of the determination of the equivalence point, demonstrating the potential of the developed material for applications in analytical chemistry and electroanalytical sensors.

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Advanced Nanostructured Conducting Polymer Sensors for Ultralow-Level Hydrogen Detection

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The rapid advancement of the hydrogen economy demands novel sensor technologies capable of detecting trace levels of hydrogen gas (H_2) with high sensitivity, stability, and rapid response. In this study, we present an integrated approach combining intrinsic morphology-tuned polyaniline (PANI) structures [1] and hybrid p-toluenesulfonic acid (p-TS) doped vanadium pentoxide/polypyrrole (V_2O_5/PPY) composites to develop next-generation sensors for ultralow-concentration hydrogen monitoring at ambient conditions.

We systematically designed and fabricated three types of PANI-based nanostructures: hollow nanotubes, thin films, and nanofibers to evaluate structure-property relationships in hydrogen (H_2) sensing [2]. The PANI hollow nanotube sensor demonstrated outstanding performance with 1 ppm detection limit, 29% sensitivity, and ultrafast response/recovery times of 15 s and 17 s, respectively. Its superior electrical properties, including conductivity (9.15 S/cm) and hole mobility (~100 cm^2/Vs), were found to be strongly correlated with its one-dimensional morphology and high carrier concentration (2.68×10^7 cm^{-3}).

Complementary to this, we employed a facile intercalation-polymerization strategy to synthesize VOH-PPY/p-TS films [3]. The introduction of p-TS dopant enhanced crystallinity and charge transport by increasing interlayer spacing, enabling efficient polaron formation. These films achieved a sensitivity of 32.4% at 250 ppm H_2, with improved response/recovery times (43 s and 37 s) compared to undoped composites. Hall effect measurements confirmed significant increases in carrier mobility (14 cm^2/Vs 4.76 cm^2/Vs), further validating the morphological and electronic benefits conferred by sulfonic acid doping.

Combined, these two approaches represent a dual-innovation strategy: the first rooted in intrinsic nanostructuring of conducting polymers, and the second leveraging hybridization with redox-active metal oxides and advanced doping chemistry. This work provides comprehensive insights into the interplay of morphology, doping, and nanocomposite architecture on sensor performance, establishing a scalable pathway toward robust, low-cost, and highly selective hydrogen sensors for industrial safety and clean energy infrastructure.

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Green-Synthesized Ag Nanoparticles incorporated into the high-performance Triboelectric Wearable Sensors

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Triboelectric nanogenerators (TENGs) are gaining increasing attention as sustainable power sources and self-powered sensors, particularly for wearable electronics. In this study, we report the green synthesis of silver nanoparticles (Ag NPs) [1], using garlic (Allium sativum) extract as a reducing and stabilizing agent, aiming to enhance the triboelectric output performance of an Ecoflex-based TENG [2]. The garlic extract was first prepared through aqueous extraction, followed by the reduction of silver nitrate ($AgNO_3$) under ambient conditions. Transmission electron microscopy (TEM) revealed spherical Ag nanoparticles with an average diameter of approximately 5 nm, demonstrating uniform dispersion.

These biosynthesized Ag NPs were incorporated into an Ecoflex matrix at various weight percentages (0, 0.03, 0.04, 0.05 wt%) to fabricate tribo-negative films. The performance of each TENG was evaluated and compared to that of a pristine Ecoflex-based device. Notably, the sample containing 0.03 wt% Ag-garlic nanocomposite exhibited the most significant enhancement, delivering a ~17% and 12% increase in output voltage and current, respectively, which we attribute to improved surface charge density and dielectric properties introduced by the conductive nanofillers.

Following this optimization, the 0.03 wt% Ag-garlic nanocomposite was selected for further development. The material was processed for micro-patterning with the goal of integrating it into wearable glove-based sensors for real-time detection of hand and finger movements. This design paves the way for cost-effective, biocompatible, and flexible TENG-based sensors with potential applications in human–machine interfaces, gesture recognition, and healthcare monitoring.

Keywords: Triboelectric nanogenerators (TENGs), silver NPs, green synthesis, garlic, sensor, micropatterns

Acknowledgments. This research was supported by the research projects AP23486880 from the Ministry of Higher Education and Science of the Republic of Kazakhstan and 111024CRP2010, 20122022FD4135 from Nazarbayev University.

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Heat-Resistant, Flexible Self-Powered Triboelectric Nanogenerator Sensor for High-Temperature Sensing

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Compared with conventional rigid, energy-intensive sensors, self-powered flexible sensors offer compelling advantages, but most lose functionality at elevated temperatures, limiting their use in harsh environments. To overcome this challenge, we have developed a novel heat-resistant, self-powered triboelectric nanogenerator sensor. Its electrode is fabricated by Direct-Ink-Writing (DIW) printing method from a proprietary silver-nanoparticle based conductive ink. It incorporates spherical silver nanoparticles synthesized via a wet-chemical polyol method and formulated with a cellulose-based additive to ensure optimal printability on a polyimide (Kapton) substrate. The polyimide (Kapton) substrate thereby operates as the negatively charged triboelectric layer, while the aluminum foil functions as the positively charged counterpart. The sensor exhibits excellent thermal stability, maintaining its electrical conductivity and mechanical integrity thanks to the inherent heat resistance of the polyimide (Kapton) substrate and the thermal robustness of the silver-nanoparticle ink. Under dynamic contact–separation cycling against the aluminum foil layer at 3 N, the device produces a peak open-circuit voltage of ≈120 V at 1 Hz, which rises to ≈310 V at 8 Hz, alongside a corresponding short-circuit current density increase from 4 μA to 26 μA. Notably, these output levels remain stable over 172800 cycles. The electrode's adhesion to the polyimide (Kapton) substrate shows no signs of delamination or cracking even after extended durability tests. Building on its demonstrated electrical and mechanical robustness, temperature-dependent performance evaluations are now planned to fully characterize the sensor's operating window. Future work will involve systematic measurements of electrical output at temperature ranges up to 250 °C under the same 3 N, 8 Hz. These tests will assess the stability of output over time and thermal cycling and confirm the adhesion stability of the printed silver nanoparticle electrode under elevated temperature. The outcomes will validate this triboelectric nanogenerator sensor as a truly heat-resistant, self-powered device for flexible sensing in high-temperature environments, such as oil and gas wells, airplane's engines, automobile exhaust pipes, thermal power filed, ceramic and glass manufacturing.

Keywords: Self-Powered Triboelectric Nanogenerator (TENG) sensor, conductive ink, printed flexible electrode, polyimide (Kapton).

Acknowledgments. This research was supported by the research projects AP23486880 from the Ministry of Higher Education and Science of the Republic of Kazakhstan and 111024CRP2010, 20122022FD4135 from Nazarbayev University.

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Smart Gripper with Triboelectric Sensors and Data-Driven Machine Learning for Object Classification

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Efficient waste sorting remains a critical challenge in recycling systems, often relying on expensive, vision-based technologies. This project presents a smart robotic gripper integrated with triboelectric nanogenerator (TENG) sensors and a data-driven machine learning algorithm for object classification, specifically designed to enhance automated waste sorting processes. Triboelectric nanogenerators (TENGs) are devices that harvest energy from mechanical motions, and when embedded into the gripper, they generate electrical signals during contact, enabling a self-powered mechanism for capturing tactile information such as the material type and texture. These tactile signals will serve as the input for supervised machine learning algorithms aimed at distinguishing between common categories of waste such as plastic, metal, paper, and organic materials. By learning from these interactions, the system aspires to facilitate intelligent decision-making during the sorting process, increasing the sorting accuracy. This approach is expected to reduce the reliance on manual labor and vision-based systems while enhancing the precision, scalability, and energy efficiency of automated recycling operations. By combining low-power sensing with intelligent data-driven classification, this work contributes a novel solution to the automation of waste sorting in recycling and environmental management industries. Furthermore, this technology promises significant cost reductions and improved operational efficiency, offering a sustainable alternative that aligns with global environmental conservation efforts.

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Implementation of PVDF-SnO_2 Fiber TENG Sensor onto Continuum Manipulator for Collison Detection

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Contact sensing is a necessary feature to prevent in-pipe manipulators stretching through contact with the environment to prevent collisions and obtain safe navigation in pipe inspection. Traditional in-pipe robots are not equipped with effective tactile sensors, thus, it is necessary to incorporate flexible tactile sensing for real-time collision detection. In this work, we proposed a self-powered sensing solution by using a PVDF-SnO_2 triboelectric nanogenerator (TENG) fiber sensor mounted on a continuum manipulator. The piezoelectric polymer matrix is furnished by polyvinylidene fluoride (PVDF), and locally stronger electrostatic field and output of the composite fiber are attributed to the incorporated tin oxide (SnO_2) nanofillers. The obtained TENG sensor is a kind of ultrasoft fiber for mechanical energy harvesting and an output electrical signal generation upon contact, working as a self-powered touch sensor. It is worth mentioning that TRIboelectric sensors can have response times in the ms range (ms.CompareTo this) which makes them suitable for real-time detection of the collision. We embedded the PVDF-SnO2 TENG fiber into the body of a cables driven with continuum manipulator for in-pipe inspection. When the manipulator makes contact with the pipe wall or an obstruction, the sensor directly generates a unique voltage spike for immediate contact detection. The sensor output was between 0 V (zero contact) and several tens of volts at maximum deformation during its calibration, leaving a clear electrical signature for collisions. A basic signal processing routine including a threshold (0.5 V) and a low-pass filter was used to get rid of noise and small vibrations, so that only real contacts are able to trigger the alert. The control system of the manipulator was programmed to exploit TENG sensor feedback for reactive actions so that, for instance, the robot would automatically halt or move backwards upon collision detection. Experimental verification was performed in a partially-penetrating pipe through the tested sensor system. The PVDF-SnO_2 TENG sensor could also detect contacts in real time, which contributed to quick reaction to the collisions as well as to avoiding possible jamming for the robot. We found reliable voltage spikes that correspond to contact events, and the robot would stop or back away within 350 ms of collision detection. The continuum robot was successfully navigated through a curved pipe section and could sense and react to unanticipated obstacles. These results reveal that the TENG fiber sensor has been used to allow real-time collision detection at absence of external power supply, which will greatly promote the autonomy and safety of continuum robot. This strategy of integration of TENG sensors into soft robots provides a novel way for advanced sensing in restricted or vulnerable surroundings. The method is not limited to pipeline inspection, instead it could be applied to other continuum robotic systems where real-time contact feedback is beneficial, for example, in hazardous environment inspection or even in medial continuum robots for minimally invasive surgery. In the future, we will investigate improving the sensitivity and spatial distribution of the sensor through incorporation of multiple TENG fibers along the manipulator as well as the development of contact (location, force) detection systems with more precision. Future work will also address the use of advanced signal processing methods and machine learning algorithms to identify the different contact conditions or materials, with the ultimate goal of smarter and more autonomous pipeline in-line inspection systems.

Keywords: PVDF-SnO_2 fiber, triboelectric nanogenerator, self-powered tactile sensor, continuum manipulator, collision detection, pipeline inspection.

Acknowledgments. The authors gratefully acknowledge UNAM – National Nanotechnology Research Center, Bilkent University (Ankara, Türkiye) for providing the PVDF-SnO_2 fiber sensors used in this study.

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Fabrication of an Electrochemical Sensor Array Using Functionalized Carbon Dots as the Sensing Elements

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Airborne particulate matter (PM) constitutes a complex mixture of varying chemical species originating from different sources [1]. PM10 particles classified as those particles with an aerodynamic diameter of less than 10 µm are considered inhalable particles with the tendency to reach and penetrate the bronchi of the lungs [2] Inhalable atmospheric particulate matter (PM10) originates from many different anthropogenic activities, such as combustion, processing industries, traffic emissions, and urban construction activities. These sources as well as natural sources are the most environmental concerns battling some major megacities globally [3], since they impact air quality, ecosystems, and human health [4]. Exposure to airborne particulates has been linked to many negative health effects including increasing respiratory issues, lung dysfunction, asthma, cough, sore throat, and cardiac arrhythmias [5,6].

This study presents the development of an electrochemical sensor array utilizing functionalized carbon dots (CDs) for the selective detection of chromium species, Cr(III) and Cr(VI). Chromium, existing primarily in trivalent [Cr(III)] and hexavalent [Cr(VI)] forms, poses distinct environmental and health risks, making its accurate detection critical. Carbon dots were synthesized and functionalized with specific surface groups to enhance their electrochemical responsiveness to Cr(III) and Cr(VI) ions. The sensor array was fabricated cost-efficiently and demonstrated excellent selectivity and sensitivity for the two chromium species. Electrochemical techniques were employed to evaluate sensor performance, including cyclic voltammetry and differential pulse voltammetry. The functionalized carbon dots exhibited strong electron transfer properties, allowing for rapid and sensitive detection with a clear distinction between Cr(III) and Cr(VI) in aqueous solutions. The sensor array achieved low detection limits, high reproducibility, and good stability across a range of concentrations. This platform holds promise for applications in environmental monitoring and industrial wastewater management, providing an efficient tool for real-time chromium speciation analysis. This project directly addresses a pressing environmental issue specific to Kazakhstan.

Our study on the development of electrochemical sensors for chromium ion detection (Figure 1) demonstrates significant potential for environmental monitoring. Nitrogen and sulfur co-doped fluorescent carbon dots (N,S-CDs) were successfully synthesized and employed as sensitive probes by modifying screen-printed carbon electrodes (SPCEs). The resulting electropolymerized CD-modified SPCEs exhibited a remarkably low limit of detection for both Cr(VI) and Cr(III) ions, enabling rapid and reliable analysis. The sensor's performance was validated using real water samples, achieving favorable recovery rates. Furthermore, the prepared CD-modified SPCEs show promising applicability for detecting chromium contamination in both aqueous and airborne environments, highlighting their potential for real-world environmental sensing applications.

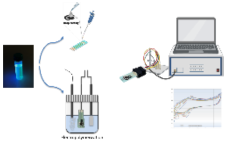

Figure 1. Application of a new class of nanomaterials, for enhancing sensitivity and selectivity in heavy metal (Cr) detection in electrochemical approach.

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Optimization of photocatalytic degradation of microplastics using silver chloride under simulated sunlight

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Microplastics (MPs), defined as plastic particles ranging in size from 1 μm to 5 mm, have become a serious environmental problem. Due to their large surface area and durability, MPs can absorb and accumulate toxic pollutants, creating a potential risks to marine organisms and human health when exposed. According to World Wildlife Fund (WWF) in average people consume 5 g of MPs everyweek, and was estimated that the highest distribution is from bottled water [1]. There are two main types of MPs. The first type is used as abrasives in daily skin products and as plastic resin pellets. The majority of MPs, however, are the secondary type, which are produced from the breakdown of larger plastics as a result of human activity [2]. These particles enter wastewater, which becomes one of the major potential sources of MPs contamination spreading through the rivers to other aquatic environments. Conventional removal methods such as filtration and sedimentation, which used for Waste Water Treatment (WWT), are often ineffective for MPs due to their small size and buoyancy. Consequently, advanced oxidation processes (AOPs) are becoming promising method. Among them, photocatalysis is one of the most efficient and environmentally friendly methods, since it utilizes solar energy as the driving force.

This study presents the results of an investigation into the optimization of the photocatalytic degradation of MPs using silver chloride (AgCl) as a photocatalyst. AgCl has been widely recognized for its effectiveness in the degradation of organic dyes and exhibits outstanding photocatalytic activity under visible light irradiation [3–5]. In this work, MP samples of various compositions, both with and without the presence of AgCl, were exposed to simulated sunlight to evaluate the degradation efficiency. To better understand the factors influencing this process, various parameters were systematically tested in order to determine the optimal conditions for the photocatalytic degradation of MPs.

The extent of degradation was systematically assessed using a combination of advanced characterization techniques, including Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), and thermogravimetric analysis coupled with differential scanning calorimetry (TGA-DSC). These analyses provided comprehensive information on the chemical, morphological, and thermal changes occurring in the MPs as a result of photocatalytic treatment.

The findings of this study offer valuable insights into the degradation mechanisms of MPs facilitated by AgCl and highlight critical parameters that influence photocatalytic efficiency. This work contributes to the ongoing development and refinement of photocatalyst materials and offers a foundation for future research aimed at enhancing the environmental remediation of MP pollution.

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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Ti_3C_2/TiO_2-coated nickel foam as a promising catalyst for hydrogen evolution reaction

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Layered (2D) materials have attracted significant attention due to their high specific surface area, enabling their use as freestanding catalysts or as coatings for other materials, thanks to their lubricating nature [1]. Among them, MXenes — transition metal carbides and nitrides — stand out for their tunable surface chemistry and multifunctionality [1,2]. These materials are typically synthesized by selectively etching the A-element from MAX phases (M — transition metal, A — p-element (Al, Si), X — C or N), resulting in thin flakes with surface terminations such as F, O, OH, or Cl depending on the etchant used [2]. Titanium carbide MXene ($Ti_3C_2T_x$) has been widely studied as a catalyst for the hydrogen evolution reaction (HER). However, in its pristine form, it exhibits relatively high overpotentials [3], prompting efforts to enhance its catalytic performance through surface functionalization or nanoparticle incorporation.

Titanium dioxide (TiO_2) has been investigated as a modifier for HER electrodes. As an example, TiO_2-coated cobalt hydroxycarbonate on carbon paper exhibited an overpotential of 75 mV at 10 mA/cm^2 after 25 activation cycles [4]. A more promising result was achieved using a Ni-TiO_2 composite on nickel foam (NF), where the optimal Ni:TiO_2 ratio of 3:1 provided an overpotential of just 46 mV [5]. This suggests TiO_2 could enhance MXene-based electrodes. However, many existing synthesis approaches are limited to producing full electrodes rather than dispersible additives compatible with MXene modification. $Ti_3C_2T_x$ can be oxidated partially by oxygen in air or by interaction with oxidizing agent forming TiO_2 as the oxidation product [6].

In this work, TiO_2-modified MXene was prepared by controlled oxidation of MXene suspension, on a sand bath at 35°C and stirring. Samples were taken after 1, 2, 3, 6 and 8 days by 5-fold immersion of a nickel foam strip (working area - 2.68 cm^2) in the suspension with following drying . Obtained composite, MXene/TiO_2/NF, fixed in a special holder, was used as the working electrode (cathode). The glass-graphite beaker and saturated calomel electrode were the auxiliary and reference electrodes, respectively. The electrolyte was 1 M KOH. Linear voltammetry (LV) was performed on a Biologic SP-300 potentiostat at a scan rate of 5 mV/s.

According to the appearance of the obtained electrodes (figure 1a,b), the coatings were thin, uniform, and firmly held on the surface of NF. Since the LV curves obtained in this experiment are very close to each other, to demonstrate more clearly the influence of the oxidation degree of MXene on its catalytic activity, a graph of this dependence was plotted (figure 1c), which clearly shows that MXene exhibits the lowest HER overpotential of -301 mV after 3 days of oxidation.

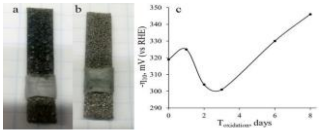

Figure 1. Nickel foam coated with the pristine MXene suspension (a) and oxidized for 3 days (b), and (c) overpotential dependence of the HER process on MXene/TiO_2/NF on the oxidation time of the MXene suspension

Based on the obtained results, composite material MXene/TiO2/NF is a promising catalyst for hydrogen evolution from alkaline electrolytes. Nevertheless, there's still a need for further studies to achieve even higher efficiency.

Acknowledgment. This work is funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. BR21882200).

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Photocatalytic degradation of microplastics using AgBr under solar light: investigation and optimization

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Microplastics (MPs), defined as plastic particles ranging from 0.1 mm to 5 mm, are of particular concern due to their high mobility in water and ability to adsorb harmful chemicals [1]. Their resistance to biological, chemical, and physical degradation allows them to accumulate in soil, marine environments, and food chains, threatening both ecosystem stability and human health. [2] Photocatalysis has become a promising tool for the degradation of MPs due to the low costs of the process, environmentally safe byproducts, and relatively high efficiency [3]. Silver bromide (AgBr) was chosen as a photocatalyst due to its high photocatalytic activity and stability for the degradation of organic pollutants [4]. Although the photocatalytic degradation of MPs has been studied for a considerable period, there remains a significant lack of standardized knowledge regarding the design of experiments in this area. Each study conducted in this field tends to be highly individualized, incorporating numerous specific parameters and experimental conditions.

The present study focuses on the investigation and optimization of the photocatalytic degradation of MPs under solar light irradiation. Various factors influencing the photocatalytic process were examined, including light intensity, irradiation duration, type and size of polymeric MPs, and the dosage of the photocatalyst. Based on the experimental results, optimal conditions were identified for the efficient degradation of MPs using AgBr as a photocatalyst. The degradation efficiency of MPs was assessed using several instrumental techniques, including Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), energy- dispersive X-ray spectroscopy (SEM-EDS), and thermogravimetric analysis with differential scanning calorimetry (TGA-DSC).

This study makes a valuable contribution to the advancement of photocatalytic degradation of MPs and provides practical insights for future research and environmental applications in this field.

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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Exploring and Optimizing Ag_3PO_4-Driven Photocatalytic Degradation of Microplastics Under Sunlight

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Environmental pollution remains a significant concern, with microplastics (MPs) identified as one of the most persistent and harmful contaminants. MPs are plastic particles smaller than 5 mm [1]. Their small size, chemical stability, and widespread distribution complicate efforts to manage their impact. MPs have been detected across various ecosystems, including marine and terrestrial environments, as well as in plants, the atmosphere, and living organisms. Photocatalysis represents a viable method for the degradation of MPs, offering an environmentally benign, accessible, and efficient approach. The silver phosphate (Ag_3PO_4) photocatalyst demonstrated excellent photocatalytic activity for water oxidation (oxygen evolution) and photodegradation of organic pollutants in aqueous solution under visible light irradiation [2]. Despite the extensive study of photocatalytic degradation of MPs, standardized approaches are still lacking in this field, as most studies are conducted with varying parameters and experimental conditions.

This study investigates and optimizes the photocatalytic degradation of MPs under solar irradiation. Various factors influencing the photocatalytic process such as light intensity, photocatalyst dosage, and others were systematically examined. The degradation efficiency was assessed using multiple analytical techniques: scanning electron microscopy (SEM) to evaluate surface and morphological changes; Fourier-transform infrared spectroscopy (FTIR) to detect the presence or absence of specific functional groups; thermogravimetric analysis combined with differential scanning calorimetry (TGA-DSC) to analyze thermal stability and transitions such as glass transition or melting behavior; and energy-dispersive X-ray spectroscopy (EDS) coupled with SEM to determine the elemental composition of MP surfaces. The findings enhance the understanding of the photocatalytic degradation process of MPs using Ag_3PO_4 in aqueous media and highlight the potential of this method for addressing plastic pollution in the environment.

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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A Green Photocatalytic Strategy for Persistent Antibiotics: Mechanochemical Synthesis of AgX (Cl, Br, I, PO_4) Nanomaterials for Nitrofurazone and Furagin Degradation

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The environmental persistence of nitrofuran antibiotics, particularly Nitrofurazone ($C_6H_6N_4O_4$) and Furagin ($C_{10}H_8N_4O_5$), poses a serious threat to aquatic ecosystems due to their bioactivity, chemical stability, and resistance to conventional treatment (Fig.1). In this study, we report the first mechanochemical synthesis of silver-based photocatalysts: AgCl, AgBr, AgI, and Ag_3PO_4 and evaluate their visible light driven degradation performance toward NFZ and FUR. The catalysts were characterized using XRD, Raman, SEM, TEM, and UV-Vis to determine structural and optical properties. All materials exhibited photocatalytic activity under visible light, with Ag_3PO_4 and AgCl showing the highest degradation efficiencies: ~95% for NFZ and ~99% for FUR within 90 minutes. Kinetic analysis confirmed pseudo-first-order behavior, with rate constants up to 0.05891 min-1 for FUR (AgCl) and 0.03468 min^{-1} for NFZ (Ag_3PO_4). The enhanced activity was attributed to efficient charge separation, visible light absorption, and reactive oxygen species (•OH, $•O^-$), which promoted oxidative cleavage of nitro and furan groups. A compound specific reactivity trend was observed. This study introduces a green, scalable approach for synthesizing silver based photocatalysts and demonstrates, for the first time, their efficacy in degrading nitrofuran antibiotics. The findings offer insight into structure function relationships and highlight a promising strategy for solar driven pharmaceutical pollutant removal.

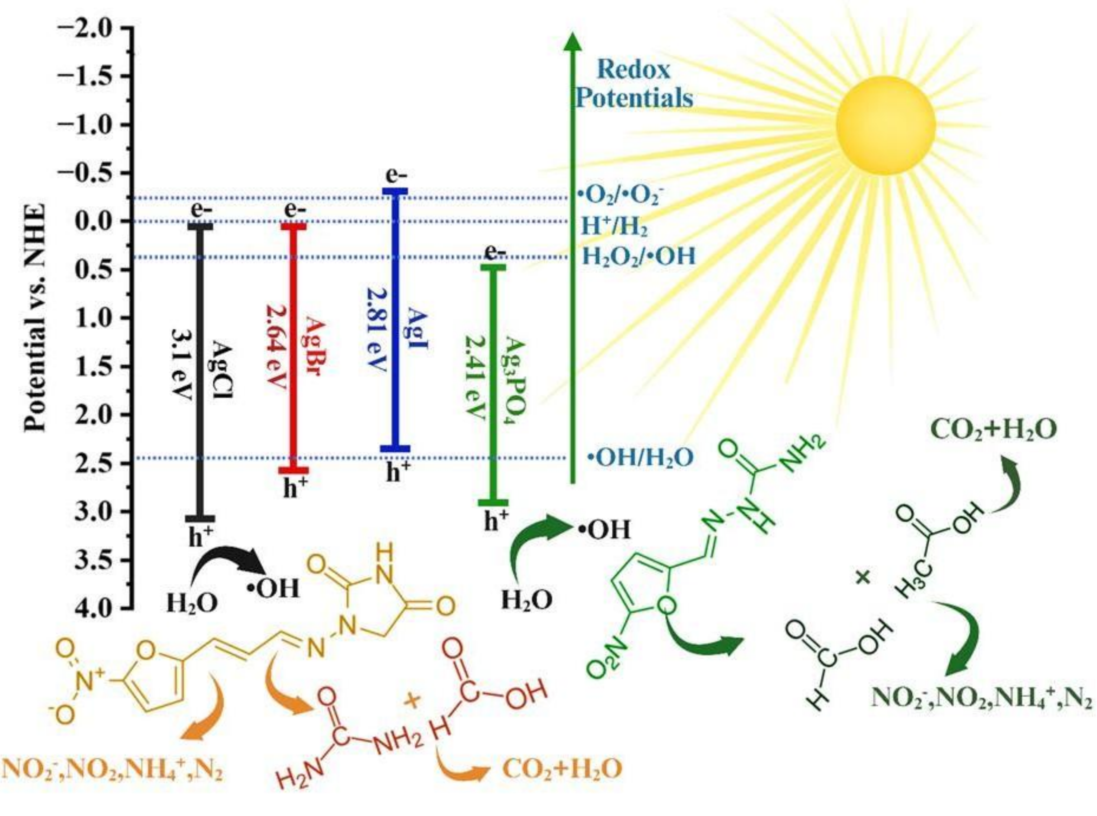

Figure 1. Schematic illustration band edge positions and hypothetical ROS-driven mineralization mechanism of nitrofuran antibiotics by AgX photocatalysts.

Magnesium Removal in Nickel Sulfide Flotation Concentrate by Mechanochemical Treatment

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The growing demand for high-purity nickel sulfate in lithium-ion battery production requires efficient removal of magnesium impurities from nickel-bearing ores. This study investigates a sustainable method for magnesium removal from nickel sulfide flotation concentrate using multi-stage dry mechanical activation followed by water leaching. XRD, SEM-EDS, TGA-DSC, and ICP- OES analyses revealed that mechanochemical treatment induces structural disorder and crystal lattice deformation in vermiculite and talc, facilitating selective magnesium leaching while preserving nickel and cobalt. Three consecutive milling-leaching cycles achieved a cumulative magnesium extraction efficiency of 74.88%, with minimal nickel and cobalt loss (<14%). The first activation stage led to 50.48% Mg removal, followed by 21.97% and 2.43% in subsequent stages (Figure 1). SEM analysis demonstrated significant particle size reduction and nanoparticle formation (~50 nm), enhancing leaching kinetics. XRD of leachates confirmed magnesium sulfate hydrate formation, while TGA-DSC-MS indicated water release due to structural breakdown. The findings highlight mechanochemical activation as a green, efficient pretreatment to reduce magnesium levels and improve downstream purification of nickel sulfates, contributing to more sustainable hydrometallurgical processing for battery materials.

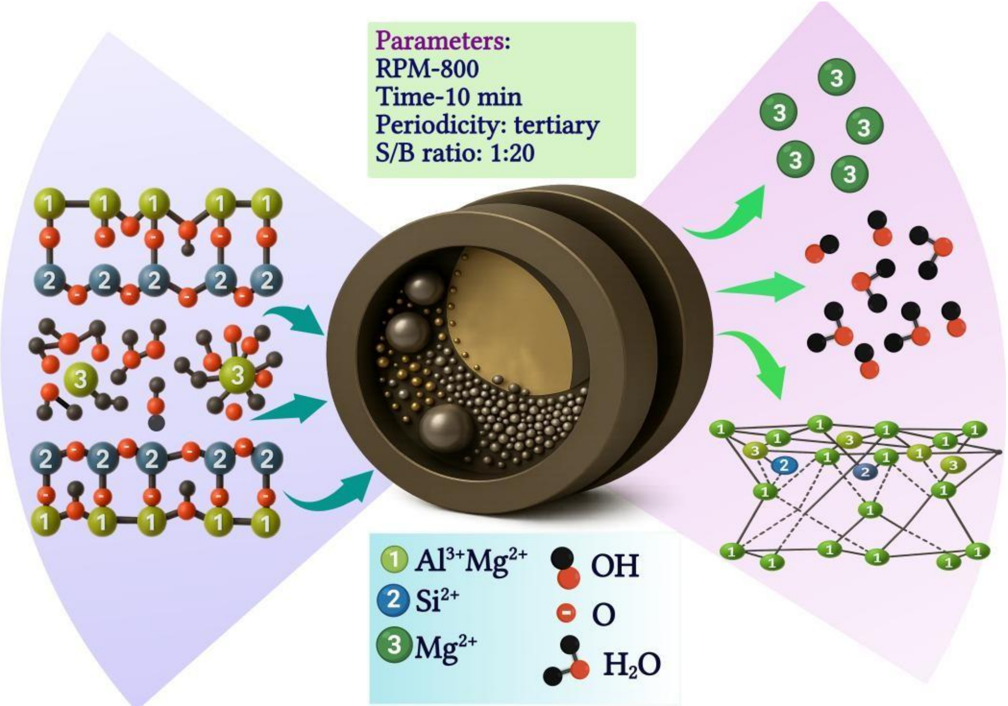

Figure 1. Schematic Illustration of the Mechanochemical Disruption of Vermiculite Structure and Magnesium Release

Investigation of the photocatalytic activity of $LaFeO_3/TiO_2$ composite

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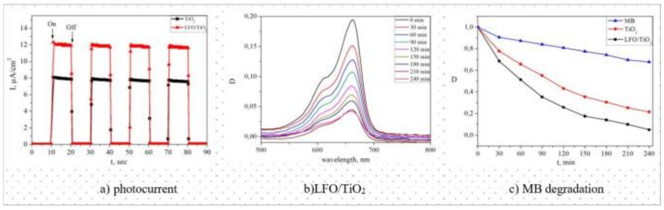
One of the effective ways of modifying TiO_2 is the formation of heterostructures with narrow-bandgap semiconductors, such as lanthanum ferrite ($LaFeO_3$) [1]. The creation of a heterojunction between TiO_2 and $LaFeO_3$ allows achieving a synergistic effect in the photoresponse of the system [2]. Synthesis method of $LaFeO_3/TiO_2$: 2 mmol TiO_2 nanoparticles were dissolved in ethanol by stirring. Then 2 mmol of perovskite $LaFeO_3$ obtained by hydrothermal synthesis was added to it and continuously stirred for 12 hours in a dark room. The result is a thick paste. The paste was then applied evenly onto the FTO glass using the Doctor Blading method. A single-channel potentiostat-galvanostat CS 350 (Corrtest Instruments, China) was used to study the photocatalytic properties. An Ag/AgCl counter electrode was used as a reference electrode. The measurements were carried out in an aqueous solution of 0.1 M NaOH. The radiation source was a xenon lamp with a power of 300 W/cm^2 (Newport, USA). The samples under study are connected to the working electrode, and the platinum electrode is opposite the electrode. The photocatalytic activity of the samples was assessed by the photocurrent response under artificial sunlight with 10-second intermittent on-off switching. Figure 1a shows the current characteristics of TiO_2 and LFO/TiO_2. The samples demonstrate excellent stability over the presented time interval. The photocurrent density is practically zero when the light is off and increases instantly when it is turned on. This phenomenon indicates that the material generates electrons and holes when exposed to light, forming photogenerated charge carriers. The photocurrent intensity for TiO_2 is relatively low, indicating its weak activity in visible light and high probability of electron recombination. It can be seen that the photocurrent density of the LFO/TiO_2 nanocomposite is 1.5 times higher than that of TiO_2. This indicates high visible light activity of LFO/TiO_2 and increased electron lifetime, i.e. slow recombination. Photocurrent density measurements showed that the LFO/TiO_2 nanocomposite responded quickly and stably to light pulses and had a high photocurrent density. This indicates that the photogenerated charge carriers are effectively separated and slowly recombined.



a) photocurrent
b)LFO/TiO_2
c) MB degradation

Figure 1. Photocatalytic activity of TiO_2 and LFO/TiO_2.

The photocatalytic activity of nanocomposite materials was assessed by the degradation of methylene blue (MB) dye. MB is used as a model dye and can serve as a source of any pollutant. The experiment was conducted by irradiating the samples with an Ossila (UK) solar simulator with a power of 1000 W/m^2. When photocatalysts placed in an aqueous solution of dye are irradiated, a decrease in the optical density of the dye is observed, which indicates that the molecules in the solution are gradually decomposed under the influence of light rays. Figure 1b shows the degradation of methylene blue dye using $LaFeO_3/TiO_2$ nanocomposite. The graph shows that as the measurement time increases, the optical density decreases. The change in optical density was observed at the characteristic absorption peak of the MB dye in the region of 662 nm (Figure 1c). According to the results obtained after 240 minutes, the degree of degradation was: for methylene blue - 32.26%, for TiO_2 nanoparticles - 78.49%, and for the $LaFeO_3/TiO_2$ nanocomposite - 94.97%. It was found that the degradation of $LaFeO_3/TiO_2$ nanocomposite was 16.48% higher than that of TiO_2 nanoparticles and 62.71% higher than that of spontaneous degradation of methylene blue. The analysis confirmed that modification of TiO_2 nanostructures using lanthanum ferrite ($LaFeO_3$) allows to significantly increase their photocatalytic activity. The extended spectral absorption and high efficiency of methylene blue degradation confirm the ability of the composite to function effectively in the visible region. Thus, LFO/TiO_2 is a promising photocatalyst for the purification of aqueous media from organic pollutants due to its improved light absorption capacity and accelerated transfer of photogenerated charges.

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Electrical transport characteristics of the $TiO_2/LaFeO_3$ nanocomposite

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TiO_2 nanotubes (TNT) have high photocatalytic activity, but are limited by a wide band gap [1]. Modification of TNT $LaFeO_3$ with a narrow band (~2.0 eV) allows the formation of a p-n heterostructure, improving charge separation, expanding absorption in the visible range and increasing photocatalytic efficiency [2]. This paper examines the effect of adding $LaFeO_3$ nanoparticles to the TNT structure on the electrical transport properties of the resulting nanocomposites, studied by impedance spectroscopy. TNT was synthesized by anodic oxidation of a titanium substrate in a fluoride-based electrolyte for 6 hours at a voltage of 60 V. Perovskite $LaFeO_3$ was synthesized using a hydrothermal method from precursors $La(NO_3)_{36}H_2O$ and $Fe(NO_3)_{39}H_2O$ with heat treatment at a temperature of 800 °C to form a perovskite structure. Figure 1 shows scanning electron microscopy images of modified TNTs coated with a layer of perovskite $LaFeO_3$. The image shows an ordered array of nanotubes, and the 100 nm scale allows one to see their surface coating with $LaFeO_3$ particles. The modification preserves the nanotube morphology and provides an increase in the active area for photocatalytic processes. The electrical properties of the samples were studied by impedance spectroscopy using a Co rrtest CS350M potentiostat-galvanostat (China). Figure 2 shows the Nyquist diagrams of TNT and TNT/LFO films.

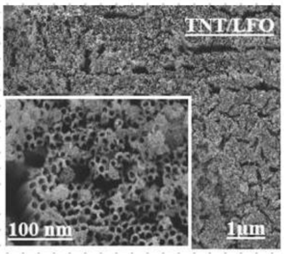

Figure 1. SEM images of TNT/LFO nanocomposite.

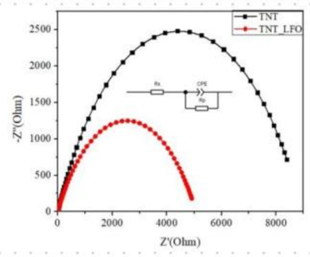

Figure 2. Nyquist diagram of TNT and TNT/LFO samples.

The calculation of the parameters of charge transfer and recombination was carried out on the basis of the model proposed by Adachi et al. [3], according to which the peak frequency of the arc on the Nyquist diagram (ω_{eff}) is directly proportional to the effective rate constant of electron recombination k_{eff}

$$k_{eff} = \omega_{eff}$$

In this case, the charge transfer resistance R_S is defined as the diameter of the high-frequency arc on the impedance diagram and reflects the total ohmic resistance of the system, including the electrolyte, conductive contacts and the surface of the photoelectrode. The analysis showed that the effective lifetime of electrons τeff is calculated as:

$$\tau_{eff} = \frac{1}{k_{eff}}$$

for the TNT/LFO composite is 0.88 s, which is almost 2.4 times higher than for pure TNT (0.37 s), indicating a slowdown in recombination processes. The minimum resistance values (R_S=2.662 Ohm, Rp=5056.3 Ohm) are observed for TNT/LFO, which confirms improved conductivity characteristics. Increased electrical conductivity and charge carrier lifetime contribute to more efficient separation of electron-hole pairs and accelerated interphase transfer, which enhances photocatalytic activity. Thus, the introduction of $LaFeO_3$ into the TiO_2 structure forms a p-n heterojunction and significantly improves electrotransport characteristics, making the TNT/LFO composite a promising material for photocatalytic applications.

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CO_2 capture using lithium-based sorbents made from construction raw materials

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Increasing atmospheric carbon dioxide concentrations is one of the major threats to climate change, affecting the sustainability of natural processes, the quality of human life, and the energy balance of our planet. In this regard, large-scale scientific research is being conducted around the world to create effective processes for capturing CO_2 from fuel gases in order to reduce anthropogenic greenhouse gas emissions [1].

One of the most promising materials for capturing CO_2 are solid sorbents based on lithium silicates, which combine the advantages of chemical selectivity with thermal stability. In this work, composite sorbents Li_4SiO_4 from construction waste such as sand and clay are synthesized in order to create low-cost, sustainable, and effective materials for capturing carbon dioxide [2,3].

The samples were synthesized using alkaline melting and mixing methods in order to increase the reactivity and structural stability of the sorbents. During the work, the properties of samples with Li:Si ratios in the range from 1.5:1 to 4:1 were analyzed, which made it possible to determine the effect of the composition on their sorption properties.

The result showed that with an increase in the process temperature from 300 °C to 500 °C, the sorption capacity of the samples for CO_2 also increased. The highest sorption capacity of 38.1% was achieved on a sample with a ratio of SiO_2:Li_2O = 1:1.5, synthesized by mixing clay with lithium nitrate. While for a sample with a ratio of SiO_2:Li_2O = 1:4, synthesized by alkaline fusion of sand with lithium hydroxide, the maximum sorption capacity reached 38.7% at a temperature of 500 °C. These data confirm the advantages of such composite sorbents in the processes of capturing CO_2 from exhaust gases. The efficiency of desorption was also thoroughly analyzed in a series of thermal exposures. The maximum degree of CO_2 desorption was achieved at a temperature of 750°C. The use of temperatures above 750°C was recognized as impractical due to thermal degradation of the Li_4SiO_4 structure, changes in the phase composition and an increase in energy costs, which affects the practical significance of the process from a technical and economic point of view.

Thus, the composite sorbents based on lithium silicates synthesized from construction waste prove to be effective, sustainable and cheap materials for capturing CO_2 from exhaust gases, which can be one of the approaches to reducing the greenhouse effect and mitigating climate change. The results obtained can be used in the development of effective systems for capturing and utilizing carbon dioxide based on lithium silicates, which helps to reduce greenhouse gas emissions and reduce the negative impact on the environment.

Acknowledgments. The work was carried out with financial support from the Ministry of Science and Higher Education of the Republic of Kazakhstan within the framework of scientific project No. BR24992935.

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Study of ethanol reforming on copper-containing catalyst

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In the context of rapid growth of energy consumption and the need to reduce carbon dioxide emissions into the atmosphere, technologies for producing hydrogen from renewable sources are becoming especially relevant [1]. One of the promising ways is ethanol reforming, which allows obtaining hydrogen and synthesis gas, which are in demand in the energy and chemical industries. Ethanol reforming includes several approaches, among which are dry reforming, steam-carbon dioxide reforming and reforming on copper-containing catalysts [2].

In this work, a catalyst 10 wt.% CuO/γ-Al_2O_3, obtained by impregnation, was developed. The catalyst was studied in reactions of thermal conversion, steam-carbon dioxide and dry reforming of ethanol in a flow mode. The study of 10 wt.% CuO/γ-Al_2O_3 in the thermal conversion reaction of ethanol in the temperature range of 250–450°C showed that ethanol is converted mainly into hydrogen, acetaldehyde and ethylene. The highest concentration of hydrogen (27 vol.%) and acetaldehyde (16 vol.%) is observed at a temperature of 350°C, and the maximum yield of ethylene (94 vol.%) is achieved at 400°C. In the reactions of steam-carbon dioxide reforming and dry reforming of ethanol in the temperature range of 500–800°C, hydrogen, carbon monoxide, ethylene and methane were found in the reaction products. The maximum concentration of ethylene (47 vol.%) is achieved at 550°C, which indicates the predominance of the ethanol dehydration reaction under these conditions. Synthesis gas with a molar ratio of H_2:CO = 1:1 is formed at a temperature of 750°C and higher in the reaction of steam-carbon dioxide reforming of ethanol, which corresponds to the optimal conditions for the further use of synthesis gas in various industrial processes.

Thus, the 10 wt.% CuO/γ-Al_2O_3 catalyst exhibits high activity and selectivity in ethanol reforming reactions, ensuring the production of hydrogen and synthesis gas in a wide temperature range. The most promising direction is the use of this catalyst for the production of synthesis gas with a given ratio of components, which opens up opportunities for its application in the power and chemical industries. Further research will be aimed at optimizing the process conditions and increasing the stability of the catalyst.

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Photocatalytic activity of hybrid g-C_3N_4/ZnO nanocomposites

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A novel in-situ mechanochemical synthesis approach for ZnO/g-C_3N_4 photocatalytic nanocomposites, characterized by simplicity, environmental friendliness, and potential for industrial scalability. The synthesized composites demonstrated high efficiency in photocatalytic degradation of the organic dye methylene blue (MB) under solar light, demonstrating their potential for use in wastewater treatment

Graphitic carbon nitride (g-C_3N_4) was synthesized via thermal polymerization of a mix of melamine and urea. The mechanochemical activation of $Zn(CH_3COO)_2·2H_2O$ and g-C_3N_4 was carried out using a planetary ball mill, followed by thermal treatment at 150 °C to convert $Zn(OH)_2$ to ZnO. Composites with different g-C_3N_4 loadings 2–20 wt% were obtained and labeled $ZOCN_2$, $ZOCN_5$, $ZOCN_{10}$ and $ZOCN_{20}$.

The morphology and structure were investigated using XRD, FT-IR, SEM, TEM, EDS, and XPS analysis. The data confirmed the formation of ZnO/g-C_3N_4 heterostructures with uniform dispersion of ZnO nanoparticles on the g-C_3N_4 layers. HR-TEM and SAED patterns revealed preserved hexagonal ZnO structure [1]. XPS analysis demostrated the formation of Zn–N bonds and revealed Zni defects that had no significant impact on the crystal structure [2].

Photocatalytic performance evaluation showed that the $ZOCN_5$ composite exhibited the highest activity, with a degradation rate constant of $k = 0.00986\ min^{-1}$, which is 4.3 times higher than that of pure g-C_3N_4 and 1.4 times higher than pure ZnO. This enhanced activity is attributed to the synergistic effect at the heterojunction structure, which facilitates charge separation and suppresses electron–hole recombination. The stability of $ZOCN_5$ was confirmed through four recycling cycles without noticeable loss of efficiency.

The synthesized ZnO/g-C_3N_4 nanocomposites present a promising solution for the development of efficient, stable, and green photocatalysts for organic water pollutant treatment.

Acknowledgements. This research has been funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP27511547).

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ACKNOWLEDGEMENTS

**The Advanced Energy Storage Systems and Functional Nanomaterials Research Group
and**

Prof. Zhumabay Bakenov would like to express our cordial thanks to all who helped make this conference a success.

**Our great pleasure to express sincere thanks to the organizers:
PI “National Laboratory Astana”, Institute of Batteries LLP, and Nazarbayev University.**

We would like to express our very special gratitude to the all Speakers,

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for excellent contribution to our event.

**Last, but not least, we would like to thank all Chairmen and Co-Chairmen of the respective sessions and all Members of the Scientific Advisory and Organizing committees.
Without their tireless efforts, the conference would not have been possible.**

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