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Selected
Oral Presentation
Abstracts

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Nickel-doped Li_2ZrCl_6 applied in all-solid-state Li-ion batteries

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All-solid-state batteries (ASSBs) incorporating inorganic solid electrolytes are widely regarded as promising candidates for next-generation energy-storage systems due to their potential to overcome key limitations of conventional liquid-electrolyte lithium-ion batteries, particularly in terms of safety and energy density. **[1]** For an electrolyte to be considered viable for ASSB applications, it must satisfy several stringent requirements, including high lithium-ion conductivity ($>10^{-3}$ S cm^{-1}), extremely low electronic conductivity ($<10^{-9}$ S cm^{-1}), and broad electrochemical stability against both high-voltage cathodes and lithium metal anodes, spanning at least 4.2 V vs. Li^+/Li. **[2]** Among the various classes of inorganic solid electrolytes, halide-based solid-state electrolytes (SSEs) have recently garnered significant attention owing to their intrinsic low electronic conductivity, favourable mechanical deformability, and the demonstration of high room-temperature ionic conductivity values in certain compositions. **[3]** Despite these advantages, numerous high-performance halide SSEs rely on rare-earth precursors such as YCl_3 or $InCl_3$, whose scarcity and high cost restrict their large-scale deployment in economically viable energy-storage devices. **[3]** In contrast, Li_2ZrCl_6 (LZC) has emerged as a promising, rare-earth-free alternative. Synthesised from $ZrCl_4$, a relatively abundant and inexpensive precursor, LZC exhibits an ionic conductivity of ~4.0×10^{-4} S cm^{-1}, an electronic conductivity on the order of 10^{-8} S cm^{-1}, and a broad electrochemical stability window spanning approximately 1.75–4.25 V vs. Li^+/Li. Although its ionic conductivity approaches the threshold for practical application, further enhancement is desirable to meet or exceed the $>10^{-3}$ S cm^{-1} benchmark, typically associated with high-performance halide SSEs. **[4]**

Aliovalent substitution has proven to be an effective strategy for improving ionic transport in halide electrolytes. **[5, 6]** Replacing Zr^{+4} with lower-valence cations introduces additional Li^+ to maintain charge neutrality, thereby increasing the concentration of mobile charge carriers. **[6]** Furthermore, such substitutions can induce structural disorder, modify halide-metal bonding environments, and potentially widen the electrochemical stability window. Motivated by these considerations, this work explores Ni-based aliovalent substitution in Li_2ZrCl_6, yielding compositions of the form $Li_{(2+x)}Zr_{(1-x)}Ni_xCl_6$ (x = 0, 0.02, 0.05, 0.10). **[5]**

The substituted materials were synthesised via mechanochemical milling followed by thermal annealing, and subsequently characterised using X-ray diffraction (XRD), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS) to elucidate structural and chemical modifications arising from Ni incorporation. Electrochemical impedance spectroscopy (EIS), chronoamperometry, linear sweep voltammetry (LSV), and cyclic voltammetry (CV) were employed to assess ionic and electronic transport properties as well as electrochemical stability. **[2, 3, 5]** The substitution strategy allowed for an improvement of the ionic conductivity from 0.40 mS cm^{-1} to 0.79 mS cm^{-1}, highlighting its potential.

To evaluate the applicability of Ni-substituted LZC in practical ASSB architectures, pellet-type solid-state cells were constructed using $LiFePO_4$ (LFP) as the cathode and lithium metal as the anode. With LZC electrolyte layers fabricated via doctor-blade coating. **[7]** An integrated fabrication approach allowed for systematic evaluation of the electrochemical performance of LZC-based electrolytes within fully assembled ASSB configurations. **[7]**

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Surface Chemistry Engineering of LLZO via Piezo-Shaker-Enabled RF-Magnetron Deposition

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Composite electrolytes have attracted considerable interest for all-solid-state lithium batteries by combining the mechanical compliance of polymers with the high ionic conductivity and electrochemical stability of ceramics **[1–3]**. Among all the possible combinations, polyethylene oxide (PEO) and garnet-type $Li_{6.25}Al_{0.25}La_3Zr_2O_{12}$ (LLZO) emerged as a promising platform for the development of next-generation composite solid-state membranes. Despite these electrolytes have been widely studied, their performance is often limited by interfacial challenges, particularly the formation of resistive lithium carbonate (Li_2CO_3) layers on LLZO surfaces and poor polymer–ceramic interfacial compatibility, which lead to increased interfacial resistance and non-uniform lithium transport **[4–5]**.

In this work, we present a surface modification strategy for LLZO that effectively promotes lithium carbonate conversion while inducing the nucleation of a lithiophilic surface layer. This engineered surface was obtained by employing RF-magnetron deposition chamber, equipped with a piezo-shaker specifically designed to deposit in a single step and using dry processes thin film on powders. An oxide thin film was deposited on LLZO applying different amounts of power (25-60 W) for different deposition times (20-80 min) and annealed at high temperature (550-750 °C) to obtain a lithiophilic surface layer. Compared with composites prepared using untreated ceramic, the modified PEO–LLZO composite electrolyte exhibits improved ceramic dispersion, higher ionic conductivity, and reduced interfacial resistance. Furthermore, Li|electrolyte|LFP cells demonstrate more stable cycling performances, attributed to the lithiophilic interphase promoting Li^+ motion and mitigating interfacial polarization.

This study highlights the importance of engineering garnet surface chemistry in polymer–ceramic composite electrolytes and provides a scalable route for improving interfacial stability and electrochemical performance in solid-state lithium batteries.

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Life cycle assessment harmonisation through collaborative cluster work – the Battery Heroes Sustainability Working Group example

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Life Cycle Assessment (LCA) is widely applied in EU-funded battery research and innovation, yet the methodological diversity across projects limits comparability, benchmarking and policy relevance. To tackle this, the Battery Heroes Sustainability Working Group was established as a collaborative platform within the European battery research landscape, aiming to promote knowledge exchange, methodological alignment, and sustainability-driven innovation across five Horizon EU-funded projects: NoVOC, GIGABAT, BatWoMan, GIGAGREEN and BATMACHINE. Comprising research institutions, industrial partners, and sustainability experts, the group facilitates cross-project discussions on topics such as LCA and regulatory compliance, particularly in the context of the new EU Battery Regulation. By fostering synergies through Horizon Europe projects, the Battery Heroes initiative supports the harmonisation of methodologies and enhances the collective impact of EU battery research.

Starting the cluster work without a clear goal in mind, the collaboration evolved with time, and the Working Group is currently in the process of submitting a joint paper with the developments and findings gathered throughout the work. The group concluded that LCA is increasingly embedded as a core environmental sustainability tool in EU battery R&I projects, often implemented iteratively, progressing from early screening assessments to full LCA/life cycle sustainability assessment (LCSA) at later project stages.

Furthermore, the group also reviewed current LCA practices across the five Horizon Europe battery projects. The analysis focused on key methodological elements that influence results, including functional units, system boundaries, end-of-life modelling and allocation, electricity modelling, background data choices, LCIA methods, and impact category coverage. The results showed emerging convergence in the use of capacity-based functional units (1 kWh), reliance on ecoinvent databases, and increasing adoption of the Environmental Footprint (EF3.1) method. The increasing convergence was partly a result of joint work and successful collaboration in the Battery Heroes Sustainability Working Group, a concept to build on for future research projects applicable to any field or expertise.

However, substantial variability persists in boundary definitions, recycling modelling approaches, electricity assumptions and reporting practices, which can significantly affect interpretation. Based on identified barriers and practitioners' experience, the group together propose practical recommendations and a minimum harmonised reporting set to improve transparency, robustness, and cross-project comparability, supporting alignment with EU regulatory frameworks such as EF/Product Environmental Footprint (PEF) and the EU Battery Regulation.

Figure 1. Battery Heroes logo.

Operando Synchrotron Techniques for Next-Generation Batteries: Probing Mechanisms Beyond Lithium

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Operando synchrotron-based methods have emerged as powerful approaches to investigate the complex processes occurring in next-generation battery systems. By allowing structural and spectroscopic measurements while the electrochemical cell is operating, these techniques provide direct insight into dynamic phenomena that are otherwise difficult to access using conventional ex situ characterization. [1] In this contribution, the concept of operando methodologies and their relevance for battery research will be introduced, emphasizing the unique capabilities of synchrotron radiation for multiscale and multimodal investigations of electrochemical materials.

Two representative case studies will be discussed. The first concerns the combined use of operando energy-dispersive X-ray diffraction (ED-XRD) and time-resolved X-ray tomography to study aluminum/graphite batteries. This approach enables the identification of staging mechanisms, spatially heterogeneous strain within the electrode, and volume changes occurring during cycling. [2] The second example focuses on a coupled operando SAXS/WAXS investigation aimed at tracking the anion intercalation process in graphite. The measurements reveal intermediate phase transitions, the evolution of staging phenomena, and the reversibility of the structural transformations, together with changes in the microporous carbon framework. [3] [4]

Together, these studies illustrate how operando synchrotron techniques can provide fundamental understanding of ion intercalation processes and interfacial phenomena in battery electrodes. Such insights are crucial for guiding the rational development of advanced energy storage technologies beyond conventional lithium-ion systems.

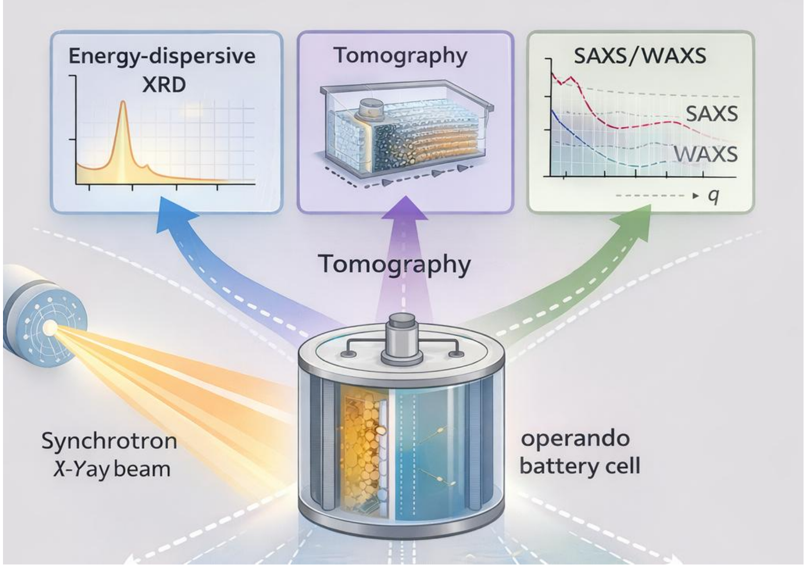

Figure 1 Multimodal operando synchrotron approach combining diffraction, tomography and scattering to probe ion intercalation, structural evolution and pore reorganization in battery electrodes during cycling.

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Nanostructured Reference Electrodes for Consistent Electrochemistry in Liquid-Phase TEM

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Electrochemical devices are central to energy conversion, storage, catalysis, and sensing, motivating the development of operando techniques such as electrochemical liquid-phase transmission electron microscopy (EC-LPTEM). However, the miniaturized electrochemical platforms used in EC-LPTEM suffer from severe geometrical constraints that limit the implementation of stable reference and counter electrodes. Conventional reference electrodes cannot be easily miniaturized, and on-chip quasi-reference electrodes often show poor potential stability due to confined volumes, changing electrolyte composition, and beam-induced effects. Counter electrodes, meanwhile, typically have limited electroactive area, leading to high polarization and parasitic reactions that hinder accurate measurements.

Here, we present a robust strategy based on molecular-template-assisted electrodeposition of metallic thin films to nanostructure both reference and counter electrodes. This approach significantly increases electroactive area without altering the electrode footprint, while maintaining compatibility with EC-LPTEM spatial constraints. The nanostructured reference electrode material choice shows dramatically increased stability and it is a true-RHE. The counter electrode exhibits improved unplarizability, enabling clearer and more reliable electrochemical measurements. Overall, this method provides stable electrochemical control in EC-LPTEM and other highly confined environments, paving the way for more reliable operando electrochemistry.

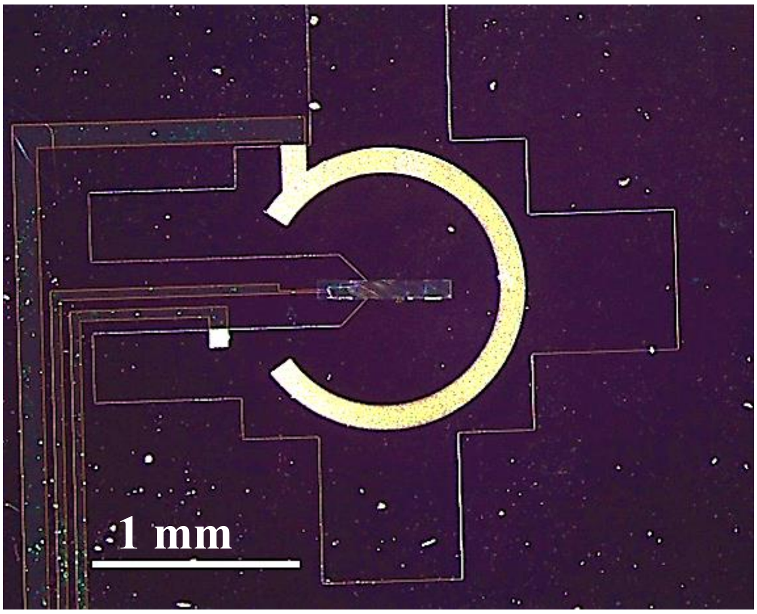

Figure 1. LP-TEM modified electrochemical three electrode cell

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Ultralong cycling of Li-metal cells enabled by aromatic diluents in localized-high concentration electrolytes

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With the maturation of the state-of-the-art lithium-ion batteries (LIBs), rechargeable Li-metal batteries (LMBs) have been regarded as the "holy grail" to achieve higher energy densities. However, the high reactivity of Li-metal leads to poor performance and safety concerns due to the instability of Li|electrolyte interface and dendrite growth during repeated Li electrodeposition/-dissolution.[1] In recent years, high-concentration electrolytes (HCEs) gained much attention because the increased salt concentration leads to higher oxidative stability of the electrolyte compared to diluted systems.[2] This allows the use of ether as solvent in the electrolyte which are known for their higher reductive stability but lower oxidative stability at concentrations ~1 M compared to carbonate-based electrolytes[3]. Furthermore, the higher reductive stability of the solvent leads to more pronounced reaction between the Li-salt and the Li metal anode resulting in an inorganic-derived solid electrolyte interphase (SEI). To overcome the drawbacks of high-concentration electrolytes such as high viscosity and high cost due to more Li salt per volume electrolyte, the concept of localized high-concentration electrolytes (LHCEs) has been introduced in the last years. In LHCEs, a non-solvating liquid, also called diluent, is added to the HCE to maintain the unique solvation structure of HCEs, *e.g.* contact ion pairs and aggregates instead of solvent-separated ion pairs.[4] Key requirements for a suitable diluent are the miscibility with the HCE, sufficient electrochemical stability and poor solvating capacity for Li^+. Several publications reported different hydrofluorinated ethers as diluent in LHCEs, however they belong to the potentially banned PFAS-chemicals and a systematic comparison about the structural influence of the diluent is rarely published.

In this work, we demonstrate the concept of LHCEs in LFP‖Li cells by directly comparing LiFSI-DME electrolytes (lithium bis(fluorosulfonyl)imide in 1,2-dimethoxy ethane) with two aromatic diluents – toluene and its fluorinated analogous *m*-fluorotoluene (mFT). Liquid FT-Raman spectroscopy confirmed the presence of contact ion pairs and aggregates in both LHCE-toluene and LHCE-mFT and the absence of uncoordinated DME molecules. An oxidative stability >4.3 V vs. Li|Li^+ successfully enables the potential use in NCM or LFP cells, however the pronounced dissolution of the Al current collector by LiFSI in NMC-based cells only allows stable cycling in LFP‖Li cells. Longterm cycling in LFP‖Li cells show outstanding capacity retention for LHCE-toluene of 81% SOH after 3000 cycles (Figure 1a). Surprisingly, the LHCE-mFT shows SOH <20% after 420 cycles which is still better than the state-of-the-art electrolyte for LIBs. Further investigations of the Li surface by scanning electron microscopy and time-of-flight secondary ion mass spectrometry (ToF-SIMS) showed minor differences between the Li electrodes cycled with LHCE-toluene or LHCE-mFT. Recovery of the electrolyte after 20 cycles and subsequent LC-MS-MS investigation revealed an electrochemically induced reaction mechanism between mFT and FSI^- leading to conductive salt depletion and cell failure (Figure 1b). With this study we successfully demonstrated that Li metal electrodes can reach up to 3000 cycles in a liquid electrolyte based on the concept of LHCE with a PFAS-free cell setup. Additionally, small structural differences of the diluents can lead to major effects on the electrochemical performance even though the diluent is often described to play a minor role on the performance.

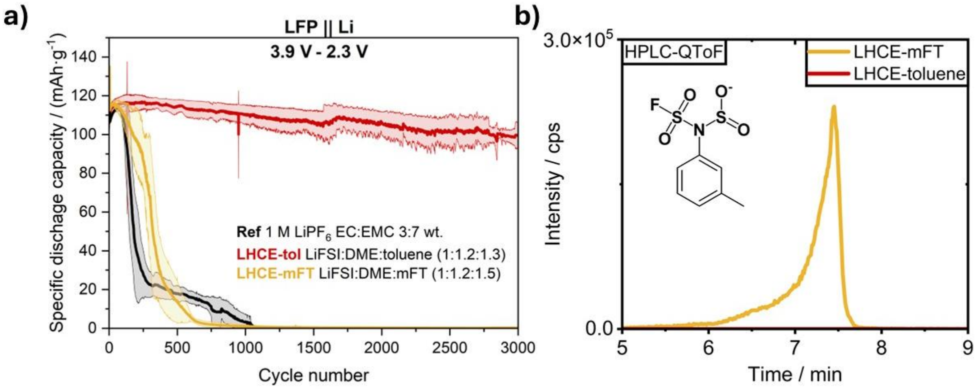

Figure 1.a) Longterm cycling of LFP‖Li cells with different electrolytes with 1C discharge and 0.5C charge with an additional constant voltage step at 3.9 V. b) Chromatogram of LHCE-mFT and LHCE-toluene after 20 cycles.

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Selected
Poster Pitch
Abstracts

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Screening novel cathode materials from the Energy-GNoME database using MACE machine learning force field and DFT

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The development of new battery materials, particularly novel cathode chemistries, is essential for enabling next-generation energy storage technologies. In this work, we employ a multi-fidelity screening protocol starting from the Energy-GNoME database **[1]** to identify promising novel intercalation cathodes for post-lithium batteries, namely Na-, K-, Mg-, and Ca-ion batteries. While density functional theory (DFT) remains the gold standard, its computational cost is prohibitive for large-scale exploration. In this work, we use foundational MACE machine learning force fields (MLFF) **[2]** as surrogate models to efficiently assess key properties, including thermodynamical stability, average voltage, and theoretical specific energy, enabling a rapid screening of candidates. We further apply physically motivated heuristic filters to retain the most plausible candidates for experimental realization. For the most promising candidates, voltage predictions are refined using DFT+U calculations. An overview of our protocol is shown in Fig. 1. This work establishes and validates a robust high-throughput screening approach for cathode materials utilizing foundational MLFFs and provides an actionable list of cathode candidates for the development of next-generation of batteries **[3]**.

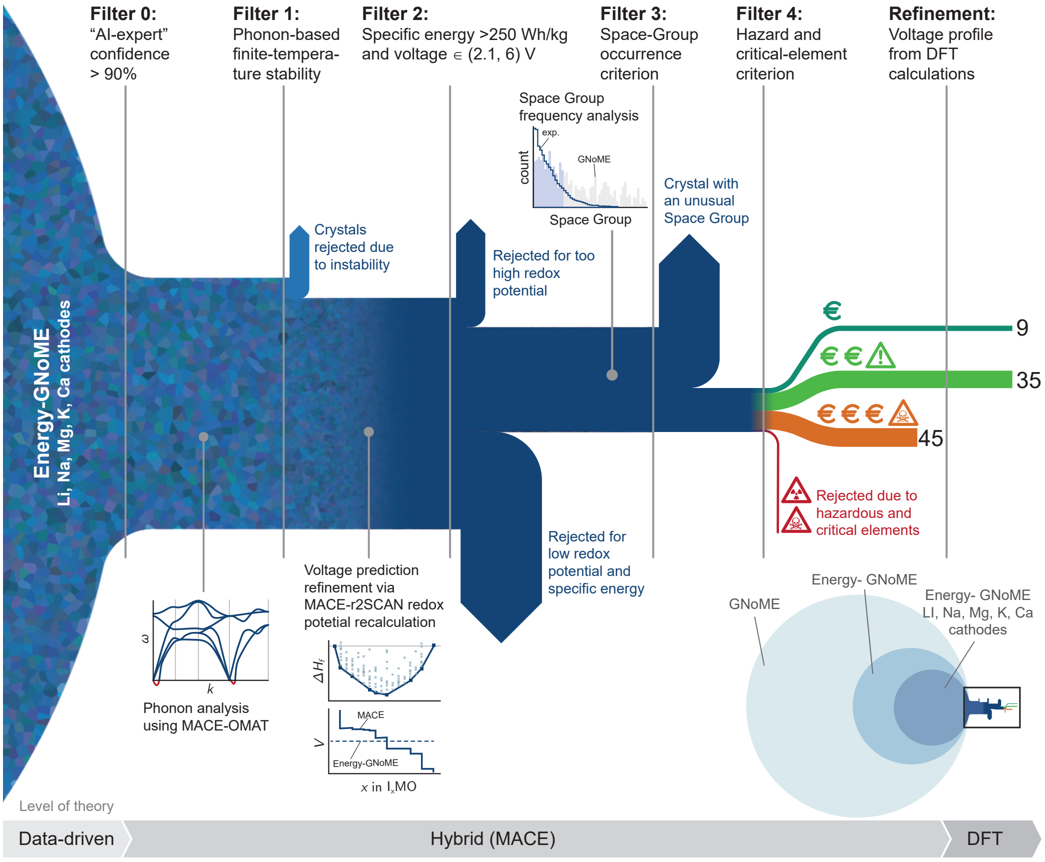

Figure 1. Overview of the screening protocol. The flow diagram shows the progressive reduction of the candidate pool across the different screening stages.

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Enhancing Interfacial Stability and Performance in PVDF-HFP-based Polymer Electrolytes: One Goal Different Routes

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Solid-state secondary batteries are emerging as the next-generation electrochemical energy storage systems, offering high performance for electric vehicles and smart grid applications. To facilitate a sustainable energy transition, the development of safe and reliable solid polymer electrolytes (SPEs) is crucial. These electrolytes not only enhance energy density and safety but also enable the use of lithium metal anodes, thereby advancing more efficient and durable battery technologies. However, the practical implementation of SPEs is hindered by intrinsic limitations, such as low ionic conductivity at room temperature and inadequate mechanical strength to prevent dendrite formation[1,2].

The SOLVE European project aims to address key challenges associated with solid polymer electrolytes (SPEs) for next-generation solid-state secondary batteries. The project focuses on the development of mechanically robust macromolecular networks incorporating specific additives or fillers to achieve high ionic conductivity and improved electrochemical stability.

In particular, lithium salt and ionic liquid (IL), together with organic additives and/or inorganic crosslinkers, are incorporated into a PVDF-HFP (polyvinylidene fluoride-co-hexafluoropropylene) polymer matrix. Solid-like polymer electrolytes are then produced through a solvent-free extrusion process, enabling efficient integration of the electrolyte component. This approach aims achieved enhanced ionic conductivity (≥ 1 mS cm^{-1}), high oxidative stability (≥ 4.6 V vs. Li^+/Li), and strong compatibility with cathode composites.

These strategies play a crucial role in the development of full solid-state cells employing NMC811 cathode materials, enabling improved rate capability and contributing to the advancement of safe, energy-efficient, and durable solid-state lithium-metal battery technologies operating at room temperature [3,4].

In summary, this work demonstrates how the integration of different materials can address the major challenges associated with PVDF-HFP/ionic liquid (IL) systems, particularly IL leakage and polymer degradation. The incorporation of ionic liquids (ILs) and alkali metal salts provides several advantages, including high ionic mobility, enhanced cycling stability, and improved safety. These benefits arise from the intrinsic properties of ILs, such as low flammability, low volatility, and high chemical stability. Currently, we are actively working on further optimizing this system to improve the long-term stability and low-temperature rate performance of PVDF-HFP/IL electrolytes.

Acknowledgements

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POLIDEMO: A Degradation Model for Irreversible Swelling and Capacity Knee-Point Prediction in Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) are well known to undergo performance degradation during operation. Accurate prediction of LIB aging is crucial for optimizing battery design and usage, as well as for enabling second-life applications and effective recycling strategies.

The primary drivers of LIB performance degradation are electrochemical and mechanical processes. During battery operation, lithium ions intercalate and deintercalate within the active material particles that form the electrode microstructure. Regions with higher lithium concentration experience greater deformation than those with lower concentration, leading to differential strain and diffusion-induced stresses. In addition, electrochemical side reactions, such as the growth of the solid electrolyte interphase (SEI) and lithium plating, continuously consume lithium ions. These mechanisms result in capacity fade, increased internal resistance, and irreversible battery swelling, a phenomenon that is often overlooked in the existing literature.

This contribution presents POLIDEMO [1], an innovative LIB degradation model that overcomes key limitations of traditional physics-based approaches by significantly reducing computational cost, improving the accuracy of parameter estimation, and providing a more comprehensive representation of degradation mechanisms.

The key strengths of POLIDEMO are two: (a) The prediction of the knee point in the capacity fade curve, thanks to and advanced fatigue law and the correlation of the resulting loss of active material with the increasing tortuosity and resistance ultimately; (b) The irreversible swelling, mainly caused by the gas generated by the SEI reaction, which is highly relevant to the mechanical design of the battery pack.

POLIDEMO is validated using aging tests performed on different battery chemistries and operating conditions, with an efficient parametrization over a limited set of data, as shown in Figure 1. Thus, POLIDEMO is a valuable tool that enhances LIBs lifetime modelling in both academic and industrial contexts.

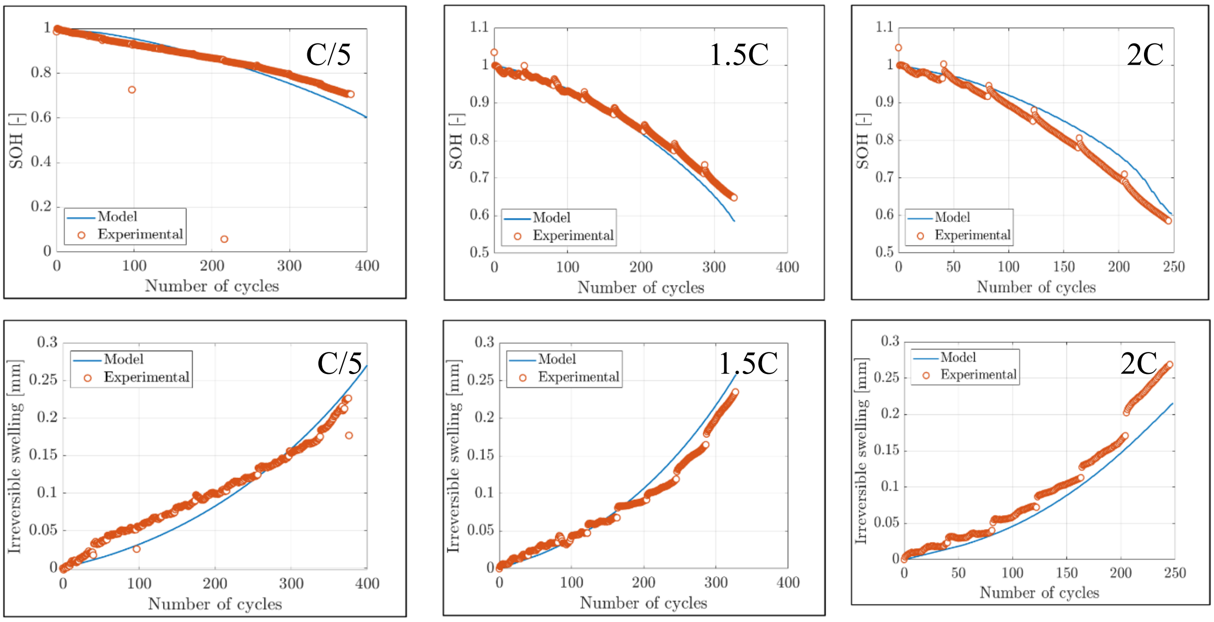

Figure 1. Validation of POLIDEMO on NMC batteries at different operating conditions. The parameter set is identified at the low current condition (C/5) and the same parameter set is applied at the other test conditions.

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An overview of recycled polymer binders/electrolytes for next-generation sustainable batteries

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Renewable energy production is inherently intermittent, necessitating large-scale implementation to enhance energy storage capacity, which presently accounts for less than 1% of global electrical energy production. The pursuit of greener, more affordable, and safer rechargeable batteries is currently recognized as strategically important in advancing electrochemical energy storage technology, addressing environmental concerns, and establishing a sustainable energy economy. Li-ion batteries (LIBs) and Na-ion batteries (NIBs) play a crucial role as energy storage devices for electric vehicles and smart grids. It is widely recognized that a detailed analysis of an electrode reveals that each component (active material, conductive carbon, current collector, and binder) contributes to the overall battery performance. It has been demonstrated that the binder, despite its relatively low content, typically a few percent of the total composition, plays a decisive role in determining the electrode performance, which is noteworthy considering its chemical and electrochemical inactivity. In addition, the transformation from liquid- to gel-/quasi-solid or fully solid-state architectures is expected to improve safety by using low-volatile, non-flammable materials and energy density of energy storage devices by enabling the use of lithium metal anodes, particularly if constraints of low ionic conductivity, low cation transport properties, and stringent processing conditions are overcome [1] .

In this context, an overview is offered of recent developments in our laboratories on the development of innovative solutions, including recycled or biosourced polymer binders/electrolytes, towards the development of sustainable, safe, high-performing post-lithium batteries. These include the possibility of repurposing in batteries the recycled polyvinyl butyral (PVB) from post-consume laminated glasses (from automotive and construction) that cannot be reused in glasses because of degraded optical properties. Three strategies were pursued: using recycled PVB as a binder in the electrode composition, transforming it into a membrane to be used as an electrolyte separator [2] , and utilizing it in advanced solid-state batteries. In the case of PVB as binder, we investigated the electrochemical and structural properties of polymer blends of PVB with standard binders, as polyacrylic acid (PAA) and poly(vinylidene fluoride) (PVDF), demonstrating its effective use in the development of various electrodes, including hard carbon (HC) anodes, and high-energy cathodes (NMC and NVP) showing full capacities even at high C-rates and stable long-term operation at ambient temperature, which pave the way to the development of more sustainable binders/separators from waste products for next-generation, sustainable energy storage. Regarding solid-state batteries, the incorporation of recycled PVB into polyethylene oxide (PEO)-based solid polymer electrolytes was investigated to address both performance and sustainability challenges. This approach enables the design of composite polymer electrolytes with improved mechanical strength, thermal stability, and electrochemical performance while promoting the use of recycled materials to reduce environmental impact.

Overall, in all cases, preliminary results are highly encouraging and pave the way to the development of more sustainable separators and binders from waste products for safe, low-cost energy storage devices.

Acknowledgments
The SUNRISE project (https://sunrise-project.eu/) has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 958243. The HIPERZAB project (https://hiperzab.eu/en) has received funding from the European Union's EIC research and innovation programme under grant agreement No 101115421.

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Non-fluorinated dual-solvent electrolyte for high-performance zinc-based energy storage

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The pursuit of fluorine-free electrolytes represents a critical step toward sustainable and environmentally benign zinc-based energy storage systems. Here, we present a novel dual-solvent electrolyte comprising a newly introduced zinc methanesulfonate (ZMS) salt, utilized for the first time in zinc-based energy storage applications. Structurally, ZMS serves as a fluorine-free analogue of the widely used zinc trifluoromethanesulfonate ($Zn(OTf)_2$), offering comparable ionic dissociation and solubility while eliminating fluorinated components that raise environmental and cost concerns. The ZMS salt was dissolved in N,N-dimethylpropyleneurea (DMPU) and triethyl phosphate (TEP), forming a highly stable electrolyte system. While the single-solvent DMPU system showed limited reversibility at 0.5 mA cm^{-2}, the introduction of TEP remarkably enhanced zinc plating/stripping stability—achieving over 1000 h cycling at 1 mA cm^{-2} and up to 2.5 mAh cm^{-2} capacity. Spectroscopic and electrochemical analyses reveal that TEP modulates the Zn^{2+} solvation environment, weakens strong DMPU–Zn^{2+} coordination, and promotes efficient desolvation at the electrode interface. Partial reduction of TEP during initial cycles forms a robust zinc phosphate-rich solid electrolyte interphase (SEI), effectively suppressing dendrite growth and parasitic side reactions. The Zn/Zn symmetric cells in the dual-solvent electrolyte delivered >1800 h stable cycling with a coulombic efficiency of 99.45%, representing a six-fold improvement over the DMPU-only electrolyte. Moreover, PANI-based full cells retained 88% capacity at 0.1 A g^{-1} and ~80% at 1 A g^{-1} over 500 cycles, while activated-carbon (AC) cells maintained 76% retention at 0.1 A g^{-1}. This entirely fluorine- and halogen-free electrolyte system demonstrates excellent compatibility across zinc-ion batteries and zinc-ion supercapacitors, underscoring its potential for high-performance, sustainable energy storage applications. Overall, the proposed mechanism highlights how the dual solvent electrolyte optimises performance through strategic solvation modulation and interfacial engineering (Figure 1).

Keywords: fluorine-free electrolytes, dual-solvent system, zinc methanesulfonate, solid electrolyte interphase, zinc-ion batteries, zinc-ion supercapacitors

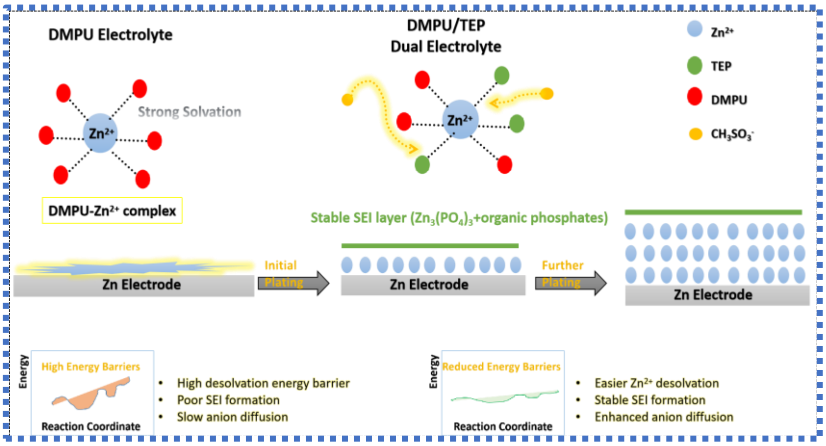

Figure 1. Schematic illustration of the molecular mechanism of the non-fluorinated electrolyte structures and interfacial behaviour in the DMPU-based (left) and the dual electrolytes (DMPU-TEP) (right).

EXPERIMENTAL AND THEORETICAL STUDIES OF BIOMASS-DERIVED CARBONS FOR Li–S BATTERIES

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Lithium-sulphur batteries are a promising alternative for energy storage, thanks to their high specific capacity, high energy density and lower environmental impact compared to lithium-ion batteries. However, their practical application is restricted by the low conductivity of sulphur and the dissolution of polysulphides in the electrolyte, phenomena that compromise stability during cycling[1]. One strategy to mitigate these limitations is the incorporation of porous carbonaceous materials in the cathodic active material, which can improve conductivity and limit polysulphide migration[2].

This work focuses on the development and optimization of cathode materials derived from coffee-waste biomass in order to improve Li–S battery performance. Particular emphasis is placed on correlating structural and electronic features with lithium polysulfide adsorption mechanisms. An integrated experimental and theoretical strategy was employed to achieve a comprehensive understanding of the system and guide material design.

Experimentally, coffee residues were subjected to controlled pyrolysis followed by activation of the resulting biochar. Comparative physicochemical and electrochemical characterisation was performed using scanning electron microscopy, X-ray diffraction, X-ray photoelectron spectroscopy, surface area analysis, and thermogravimetric analysis.

Additionally, computational simulations of amorphous carbon structures were performed to study their interaction with polysulfides. The modelling of amorphous carbon was carried out, firstly, using classical molecular dynamics (MD) simulations with LAMMPS using the ReaxFF force field, to obtain structures with densities comparable to those reported experimentally. Representative sheets were then extracted and optimised using ab initio molecular dynamics (AIMD) and density functional theory (DFT) calculations. The latter were performed using the Quantum ESPRESSO software package, employing PAW-type pseudopotentials, the PBE functional, and van der Waals dispersion corrections (Grimme-D2).

Our results clearly show that the structure of the biochar is significantly altered by the activation process, generating a porous network and increasing its surface area. The presence of micropores enhanced the electrochemical performance of the sulphur cathode, and activated samples exhibited superior cycling stability, higher specific capacity, and improved coulombic efficiency compared to non-activated materials. Notably, they retained substantial capacity even at high current densities, demonstrating excellent robustness for energy storage applications. Furthermore, this integrated approach enabled the assessment of the influence of pore size and electronic properties of the carbonaceous material on its interaction with lithium polysulphides. These findings provide valuable theoretical and experimental guidelines for the design of sustainable biomass-derived materials aimed at developing more efficient Li–S battery cathodes.

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Unraveling Solvent Co-Intercalation in Solution-Based Chemical Pre-Lithiation of Graphite for Dual-Ion Batteries

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In dual-ion batteries, irreversible side reactions at the negative electrode (*e.g.*, SEI formation) consume electrons and cations, thereby requiring compensating oxidation at the positive electrode. This results in irreversible anion intercalation, as charge neutrality of the electrolyte must be maintained. These anions cannot be recovered afterwards, resulting in irreversible capacity loss similar to traditional lithium-ion batteries. [1] One vital strategy for increasing the energy density of dual-ion batteries is to add active lithium to the existing active lithium reservoir before or during battery assembly, which is called pre-lithiation. A possible pre-lithiation strategy involves the chemical lithiation of negative electrodes in a solution containing suitable lithiation agents, which represents a fast and scalable pre-lithiation method. For negative electrodes with low operating potentials, highly reducing lithium-arene complexes (LAC) are necessary, which are formed *via* the reaction of lithium metal with biphenyl derivatives, *e.g.*, 4,4'-dimethyl biphenyl. [2]

Solution-based pre-lithiation of graphite electrodes still faces challenges, primarily due to the co-intercalation of solvent. This results in the formation of ternary graphite intercalation compounds (*t*-GICs), which are known to potentially cause exfoliation of the graphite, depending on the reducibility of the solvation shell. Solvent co-intercalation has been identified by Choi *et al*. as detrimental for multiple solvents for graphite electrodes, including glyme-based electrolytes.[3] However, this is relatively surprising, since multiple papers state reversible solvent co-intercalation with different metal-ions for glyme-based electrolytes, including lithium-ions.[4]

This work attempts to bridge the gap between two different research areas, clarify contradictions and to investigate, whether or not solvent co-intercalation is a suitable pre-lithiation strategy. Therefore, solution-based chemical pre-lithiation was performed *via* a LAC solvated in diglyme. XRD measurements demonstrated the successful lithiation of graphite with a layer distance known from typical solvent co-intercalation. Furthermore, the pre-lithiated graphite electrodes were characterised electrochemically in half-cells. However, almost no cycling was possible in a traditional carbonate-based electrolyte, which is in alignment with previous works. The failure mechanisms were further investigated using GC-MS analysis of the electrolyte, which revealed large amounts of diglyme in the carbonate-based electrolyte after cell assembly. These results suggest that, although chemical pre-lithiation involving solvent co-intercalation is stable for graphite electrodes, it faces distinct challenges when introduced to a carbonate-based electrolyte, representing a missing link in the existing literature.

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From Polymer Films to Functional Electrodes: Smart Functionalities in Silicon Anodes

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The SALAMANDER project aims to develop long-lasting lithium-ion batteries through the integration of self-healing functionalities embedded directly in electrodes, triggered by external stimuli on internal sensors. The aim is to counteract mechanical fracturing due to repeated volume changes of Si-based anodes with the integration of self-healing polymers. Self-healing properties of polymers are typically evaluated in pure polymer films, for which the ability to repair a microsized cut is tested (Figure 1). However, in batteries, only a small percentage of the electrode can consist of the polymer additive, which completely changes the playing field to test the self-healing capabilities. A common understanding on testing self-healing in batteries will help to enhance the quality, reliability and lifetime of Li-ion batteries with the use of smart functionalities. Hence, a testing matrix is needed to bridge the gap between polymer model systems and functional battery electrodes.[1]

In this project, experimentally optimized polymers have been developed with covalent adaptable networks (CANs) as self-healing functionality. The polymer is used as coating for Si nanoparticles. Hindered urea bonds allow for reversible forming of covalent bonds that may restore electrical connectivity lost during cycling.[2] Extensive structural characterization of the interaction between the Si and the polymer, as well as electrochemical characterization are ongoing to understand and optimize the effect of self-healing polymers in Si anodes for LIBs.

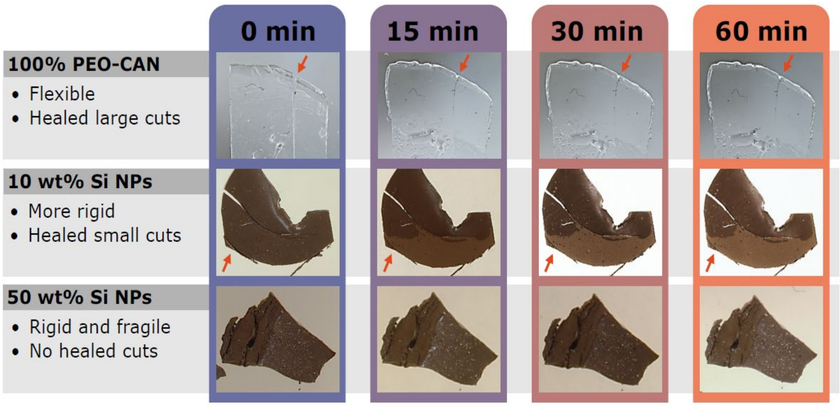

Figure 1. The integration of active materials for LIB (Si nanoparticles) affect the healing capabilities of self-healing polymers on the microscale.

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Selected

Poster Abstracts

Mesoscopic Insights into Ion Clustering and Transport in LHCEs Containing Heat Exchange Fluids

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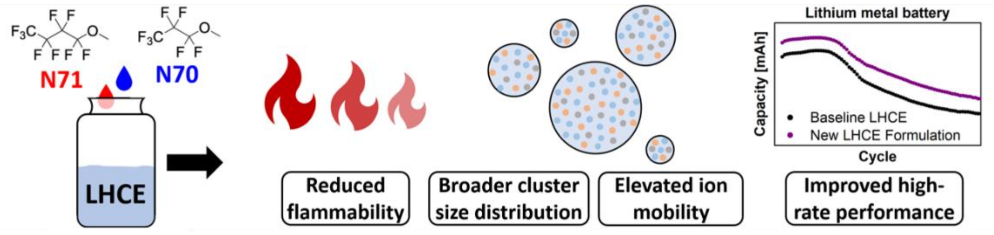
Localized high-concentration electrolytes (LHCEs) enable stable lithium metal cycling through anion-rich Li^+ solvation, yet their rate capability remains limited by sluggish ion transport. Here, industrial fluorinated heat-transfer fluids (N70, N71) are explored as intrinsically non-flammable co-diluents in LiFSI–DME-based LHCEs to enhance both safety and high-rate performance.

Density functional theory calculations show that the HOMO–LUMO energy levels of N70 and N71 lie within the same stability window as TTE, confirming their electrochemical compatibility. While experiments demonstrate extended cycle life and reduced overvoltages in ternary formulations, molecular dynamics simulations reveal the mechanistic origin of this improvement.

Across all systems, the primary Li^+ solvation shell remains unchanged. However, Voronoi-based interfacial analysis uncovers significant differences in mesoscopic salt-domain organization. TTE exhibits a stronger interfacial preference toward FSI^-, increasing salt–diluent contact area and preventing excessive agglomeration. In contrast, binary systems show sharper phase separation and a higher fraction of large (≥50 Li^+) clusters.

Importantly, enhanced transport does not correlate with reduced mean cluster size, as often suggested in previous studies. Instead, the ternary N70/N71/TTE formulation broadens the cluster-size distribution and suppresses poorly mobile aggregates, redistributing Li^+ into dynamically active, medium-sized clusters. This synergistic effect between N70 and N71 explains the improved ionic mobility and reduced concentration polarization observed experimentally.

These findings demonstrate that bulk transport—governed by mesoscopic ion clustering and interfacial structure—is the decisive factor controlling cycling performance in LHCEs. The work establishes a mechanistic framework for rational diluent selection and highlights heat-transfer fluids as promising, safe co-diluents for next-generation high-rate lithium metal batteries.



Investigation of Systematically Modified Xanthan Variants as Binders for Graphitic Negative Electrodes in Lithium-ion Batteries

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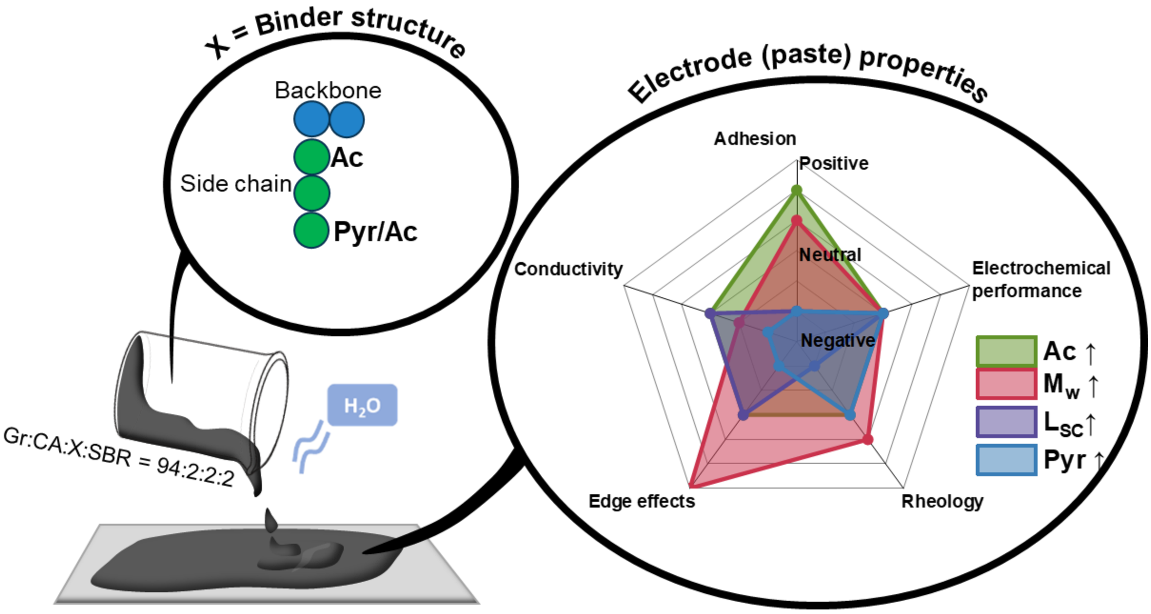
The present study investigates structure-property relationships in xanthan-based biopolymer binders for graphitic negative electrodes in lithium-ion batteries. Xanthan gum (XG) variants manifest well-defined molecular structures and stable shear-thinning behavior, rendering them optimal for systematic evaluation of binder structure effects. The present study analyzes the influence of side chain composition, degree of acetylation and pyruvylation, and polymer molecular weight on electrode and paste properties (i.e., adhesion, conductivity, rheology, and electrochemical performance). It has been demonstrated that an increased degree of acetylation enhances adhesion through improved interaction with the non-polar copper current collector. This effect occurs without any alteration in other properties. Conversely, an increase in pyruvylation has been observed to result in a reduction in adhesion and conductivity due to its poor compatibility with non-polar components, thereby promoting carbon-binder heterogeneity. The presence of larger side groups has been demonstrated to impede both adhesion and thixotropy. This phenomenon can be attributed to steric effects, which restrict polymer flexibility and prolong paste relaxation. Research has demonstrated a correlation between an increase in polymer molecular weight and enhanced shear-thinning behavior and thixotropy. This enhancement leads to a reduction in sedimentation and edge effects, although there is a concomitant decrease in conductivity. The findings indicate a discernible correlation between the molecular configuration of XG-based biopolymer binders and the performance of the electrodes. The insights provided in this study offer design guidelines for optimizing binder composition, with the objective of balancing rheological control, adhesion, and conductivity. This, in turn, contributes to more efficient electrode processing and improved performance in next-generation lithium-ion batteries.



Ac = (Degree of) acetylation; **Pyr** = (Degree of) pyruvylation
M_w = Polymer molecular weight; **L_{SC}** = Length of side chain

Activation and Phase Evolution Effects on the Performance of Low-Defects, Cubic KMnHCF for Zinc Metal Batteries

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Potassium manganese hexacyanoferrate (KMnHCF, Prussian White) is a promising cathode for aqueous Zn batteries due to its open framework, low cost, and environmental compatibility [1]. However, its performance is often limited by [$Fe(CN)_6$] vacancies and interstitial water, which destabilize the structure and promote Mn dissolution [2]. In this work, low-defect, low-water cubic KMnHCF was synthesized via controlled coprecipitation using sodium citrate and polyvinylpyrrolidone (PVP) chelating agents. Structural and compositional characterization (XRD, TGA, SEM, ICP-MS) confirmed the formation of a highly ordered framework with minimal structural water and well-defined cubic morphology. When evaluated in aqueous 1M $ZnSO_4$ + 0.1M $MnSO_4$ electrolyte against Zn metal, the material exhibits a pronounced electrochemical activation behavior, with the specific capacity increasing from 60 mAh.g^{-1} during initial cycles to a stable capacity of 120 mAh.g^{-1} at a current density of 100 mA.g^{-1}. This activation is accompanied by the gradual emergence of a secondary zinc hexacyanoferrate phase during cycling, as confirmed by ex-situ XRD. This activation process is currently under study by step potential electrochemical impedance spectroscopy (SPEIS) to probe the evolution of interfacial and transport properties during cycling. After activation, the electrochemical performance of the KMnHCF cathode was evaluated in both conventional aqueous electrolytes and agarose-based gel polymer electrolytes to assess the influence of electrolyte environment on cycling behavior and rate capability. Results provide insight into the interplay between structural evolution, electrochemical activation, and electrolyte environment in KMnHCF cathodes, highlighting their potential for stable operation in aqueous Zn-based battery systems aimed at sustainable large-scale energy storage.

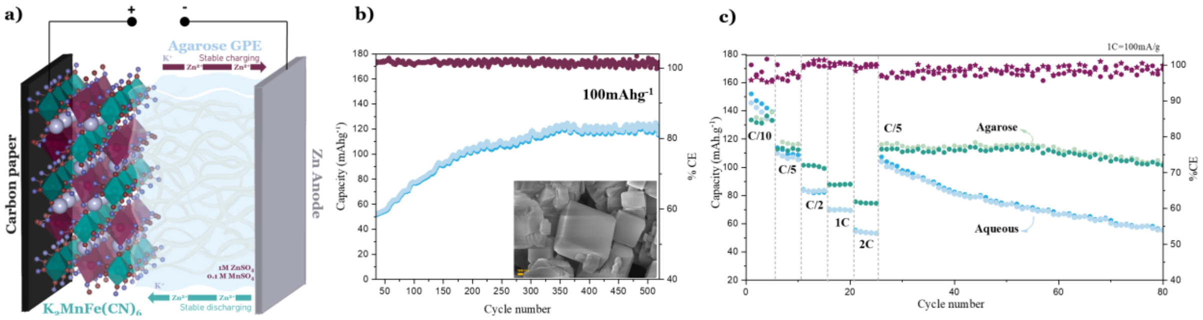

Figure 1. (a) schematic illustration of the KMnHCF-based system (b) Electrochemical activation behavior in aqueous electrolyte at 1C (c) Rate capability in aqueous and agarose-based electrolyte.

ACKNOWLEDGEMENT:
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Comparative Study of PVDF Removal from Black Mass-Derived Graphite: Atmospheric vs. Solvothermal Dissolution for Sustainable Recovery

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The recovery of graphite from lithium-ion battery (LIB) black mass is a fundamental pillar for the circularity of critical materials. The primary technical obstacle is the removal of the polyvinylidene fluoride (PVDF) binder (1). Industrially, this process is typically addressed via pyrolysis; however, technical literature warns that thermal treatments release hydrogen fluoride (HF) and phosphorus oxyfluoride (POF_3) gases, which are highly corrosive to infrastructure and cause systemic damage to filtration equipment (2). Given the toxicity of conventional solvents like NMP, this study investigated three low-environmental-impact routes: 1) Hot Ethyl Lactate (EtLac), 2) Hot DMSO, and 3) Solvothermal reaction with DMSO (180 °C, 3h). Experimental results demonstrated that the Hot EtLac method was ineffective, with fluorine content remaining nearly unchanged (from 12.30% to 11.93% wt), indicating poor thermodynamic affinity under atmospheric conditions. In contrast, both Hot DMSO and the solvothermal treatment were highly effective in binder removal, reducing fluorine content to 1.52% and 1.39% wt, respectively. Following filtration, the solvent was evaporated to obtain physical films of the extracted residues. FTIR analysis of these films confirmed the structural recovery of the PVDF polymer, while SEM/EDX analysis revealed a polymeric matrix enriched with carbon black and metallic traces (Ni, Mn, Co), correlating directly with the reduction of contaminants in the graphite determined by ICP-OES. The critical distinction between the effective methods lies in the energy cost: the solvothermal process achieves maximum purification within micropores via autogenous pressure, whereas Hot DMSO presents itself as a technically viable alternative with lower thermal demand. Finally, XRD analysis confirmed the crystalline integrity of graphite, as the (002) reflection and the interlayer spacing (d_{002}) remained constant. This route enables the effective elimination of PVDF without the harmful emissions or the deterioration of industrial assets associated with traditional thermal methods (3).

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GENERATION OF LITHIUM FROM DIRECT RECYCLING PROCESS OF THE END-OF-LIFE 18650 LITHIUM-ION CELLS

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This work describes the recovery of lithium during the process of direct recycling of spent lithium-ion battery cells. Two parts of the process are currently implemented at: American Energy Technologies Co.'s (AETC's) Wheeling, IL, USA plant (((A)-(B), Figure 1) and at ISPE in Ukraine ((C)-(D), Figure 1). For production of lithium, the team used a representative supply of 7000 end-of-life 18650 lithium-ion battery cells produced by Aspilsan Energy of Kayseri, Turkey. The bulk of lithium was recovered during filtration of cathode active material after the latter has been separated from aluminum foil current collectors in an ultrasonic-assisted water bath and subjected to centrifuge filtration and drying ((A), Figure 1). The powder that was collected on the filter became the precursor for recovery of nickel, cobalt, and manganese through means of selective electrowinning [1]. The underflow of filtration represented a dispersion of water with heavy concentrations of lithium salts produced during washing and ultrasonication of cathode active material. This cathode wash was recycled through an ultrasonic bath approximately ten times at which point the leachate became saturated with lithium salts. When it was no longer practical to reuse water from filtration, the leachate was evaporated and produced salt whose composition was determined to be 72 wt.% Li_2CO_3 and 28 wt.% LiF ((B), Figure 1, data: courtesy of Dr. Yuri Surace, AIT Austrian Institute of Technology, Vienna, Austria). Fluoride entered the system through the residue of PVDF binder and through presence of $LiPF_6$ salt that was part of the battery electrolyte. At this stage, as many as twelve grams of dry lithium salts were collected based on statistical analysis after processing of 4,000 18650 cells. The remaining lithium that was contained in cathode active material. It was electroplated by scientists at ISPE who recovered close to 3 grams of lithium per 18650 cell. The amount of electroplated metallic lithium obtained amounted to more than 62% of its remaining content of lithium in the cathode active material after leachate washing stage. The presence of impurities that are part of the composition of lithium-ion batteries (such as Al, Cu, Ni, Co, and Mn) was not detected in metallic lithium (D). The rate of Li deposition is shown by (E).

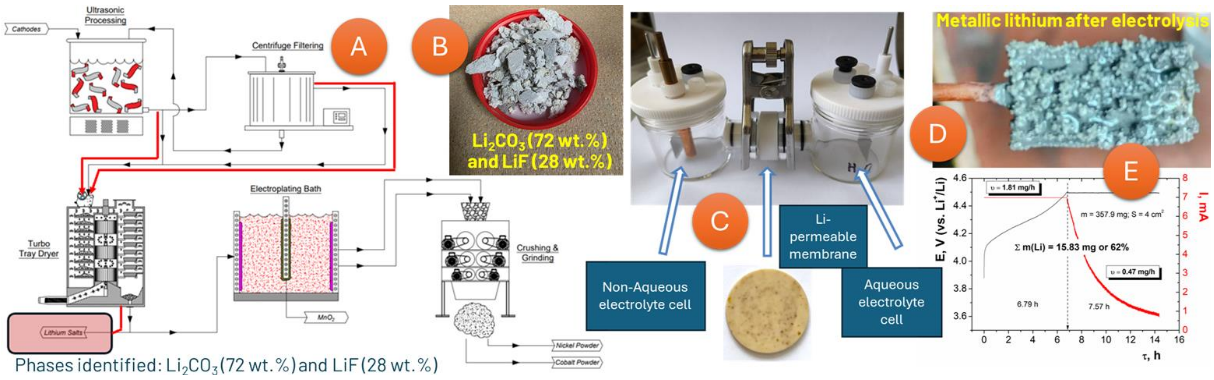

Figure 1. Recovery of lithium in the Direct Recycling process: (A) simplified Process Flow Diagram which shows recovery of Li2CO3 (LiF) dry salt precipitate (B) and dual-cell electrolysis (C); (D) Plated Li metal; (E) Change in the working electrode potential (black) and current (red) during electrolysis.

The above represents a significant yield of recovered lithium salts and metallic lithium considering that the overall weight of an 18650 cell is approximately 44 grams. Present work continues into the next phase as both lithium carbonate and metallic lithium dendrites will be purified and used for lithiation of co-precipitated Ni-Co and Mn compounds to form new, fully recycled, NMC811 cathode active material.

Work by ISPE was funded by the Horizon Europe Programme under Agreement No. 101137771, Action entitled "Sustainable Technologies for Reducing Europe's bAttery raw MaterialS dependence", or "STREAMS".

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LARGE SCALE DEMONSTRATION OF DIRECT RECYCLING OF END-OF-LIFE LITHIUM-ION BATTERIES WITH THE GOAL OF RECOVERY AND FULL REUSE OF SYNTHETIC GRAPHITE ANODES

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This work is a TRL8 demonstration of the ability to recover, “heal”, and fully reuse lithium-ion battery anode-grade graphite through means of Direct Recycling technology [1], which is implemented at American Energy Technologies Co. (AETC) in its Wheeling, IL, USA plant. AETC’s facility worked with a representative stockpile of 7,000 end-of-life 18650 size lithium-ion cells manufactured and supplied by ASPILSAN ENERJI Sanayi Ve Ticaret AS of Kayseri, Turkey. AETC’s technology utilizes AI-enabled precision machine shop equipment that is capable of opening diffused 18650 cells in quantities of thousands of cells per production lot. Multiple valuable materials are extracted in the process of recycling, yet this work focuses on the extraction of graphite anode.

Anode active materials coated on copper foil and held by SBR-CMC binder system on the metal substrate were seen to easily come off copper foil by simply immersing them into warm water. Nearly 100% of graphite is collected using this method. Water-graphite-binder solution is then filtered using vacuum-assisted technologies with graphite retained on top of the filter. Graphite active material is dried, calcined, rapidly re-spheroidized, re-purified, and re-surface coated at a fraction of cost of making new material so as to purify and heal its structure.

The resultant material has a tap density of 1.03 g/cm^3, purity of 99.99 wt.%C (LOI 950), and particle size of D50 of 12.7 um. We determined that this material required 2.5 wt.% addition of carbon pitch in order to fully heal its structure and bring its BET surface area to the desired target of 2.0 m^2/g. Electrochemical testing of recycled material by itself revealed reversible capacity on the order of 353 mAh/g with an ICL of 4.61%. Figure 1 summarized these impressive characteristics, noting that this material is 100% synthetic graphite.

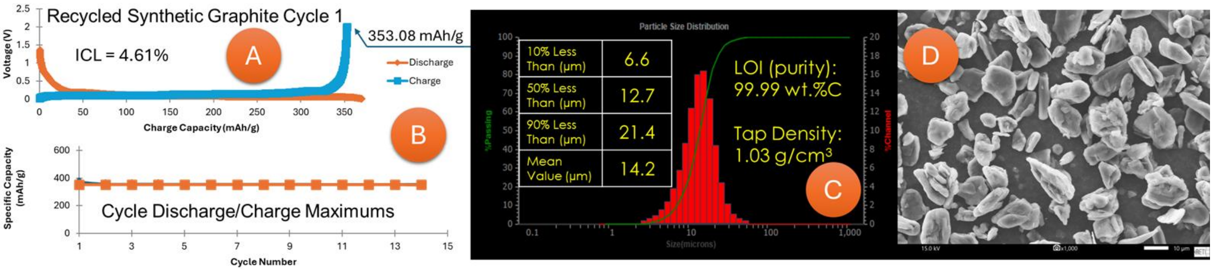

Figure 1. Recycled and healed synthetic graphite produced in AETC’s Direct Recycling process: (a) 1st charge-discharge cycle, C/10 v. Li/Li$^+$, CR2016; (b) 14-cycle summary; (c) Properties and SEM (d).

Based on its promising properties, this material was added in the amount of 5 wt.% to the newly made anode active material and supplied back to Aspilsan Energy to manufacture a production lot of nearly 25,000 new 18650 cells. This became the first known case in the worldwide battery industry practice where end-of-life anode active material was fully recycled, and its recycling & reuse concept circularity was demonstrated on a full gigafactory scale using Europe’s largest gigafactory that produces 18650 cylindrical cells. Thousands of cells containing this recycled material are on track for integration into the EV bus produced by BOZANKAYA OTOMOTIV Mak Imalat Ith Ve Ihr Anonim Sirketi of Sincan, Turkey. This work is currently unfolding.

This research was co-funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. The European Union cannot be held responsible for them. Specifically, research and development work of authors VB and ZZ received support through Horizon Europe Programme under Agreement No. 101147342, relating to the Action entitled: “**S**ecurely **A**dvancing **F**uture **E**Vs with **Li**-Ion batteries thr**o**ugh **O**ptimized **P**athways”, or **SAFELOOP** for short.

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THERMAL MODEL OF HIGH POWER 18650 NMC88-CELL-BASED LITHIUM-ION BATTERY MODULE FOR THE EV BUS POWERTRAIN

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This work presents results of development of a battery module that is designed to run powertrain of a 12-meter EV bus produced by BOZANKAYA Otomotiv Mak Imalat Ith Ve Ihr Anonim Sirketi of Sincan, Turkey. While typically EV buses run off of prismatic or pouch LFP cells, in this instance, a possibility for making a powertrain battery that is made of modules composed of high power 18650-sized NMC88 cells is demonstrated.

The development is done around ASPILSAN ENERJI Sanayi Ve Ticaret AS, Kayseri, Turkey 18650 battery cells that incorporate recycled graphite in the anode. Production of graphite for high power cells is enabled through application of innovative technologies to include deposition of high loadings of carbon pitch onto the surface of spherical composite carbon precursor. Cells are designed to operate at 4C rate which inevitably results in the generation of excessive amount of Joule-heat concurrently with the production of useful electrical energy.

The technical challenge addressed in this work focused on managing this excessive heat in a manner that the hottest cell located in the middle of the module would operate without exceeding critical temperature of up to 45℃. In order to enable safe operation of these cells, a stack of cylindrical cells was outfitted with custom made cooling tubes (A, Figure 1) that circulated (B, C) a 50/50 blend of water and ZEREX Valvoline G48 grade coolant which contains ethylene glycol. This coolant circulated through curved cooling tubes that came in contact with each individual cell of the module assembly. A technical challenge that needed to be solved was associated with the fact that in the instance of contacting two cylindrical bodies (e.g. an 18650 cell and a cooling tube of round cross section), the actual surface area of contact is negligible. Therefore, the proposed cooling tube is not very efficient. The solution that was found is filling the space between cells with a dielectric thermally conducting paste enhanced with nano-structured zinc oxide that has a thermal conductivity on the order of 14 W/(m·K). That enabled the operation of cells at the desired temperature. Another technical challenge solved in this work was the analysis of stability of cooling tubes against corrosion upon direct exposure to the coolant fluid. Corrosion experiments revealed that copper tubing cannot be used and it was ultimately replaced with aluminum.

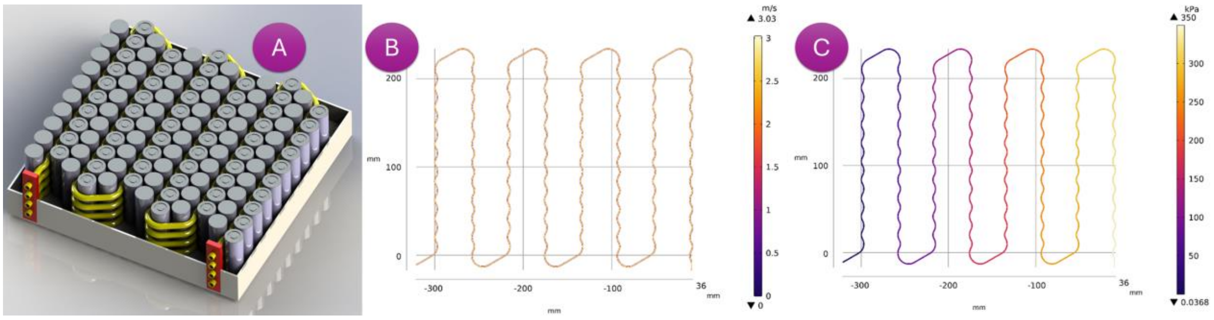

Figure 1. 3D model of an EV bus battery module (A), velocity (B), pressure (C) of cooling fluid supply.

The proposed solution represents an innovative approach to making cooling plates and should be considered an alternative to traditional cooling mantels that envelop each cell along its height in battery module designs originated in the South-East Asia. Also, the proposed solution made it possible to use cylindrical cells wrapped in shrink-wrap plastic for electrical insulation, making the module safer, lower cost and more practical for implementation. Work continues as the battery cooling plate undergoes continued optimization.

This research was co-funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. The European Union cannot be held responsible for them. Specifically, research and development work of authors AK and ES was supported through Horizon Europe Programme under Agreement No. 101103752, relating to the Action entitled "**G**raphite **R**esilience **F**or lithium-Ion ba**T**tery anodes through a sustainable **E**uropean **E**nd-to-**E**nd supply chain", or "**GR4FITE3**", while authors VB and ZZ received support through Horizon Europe Programme under Agreement No. 101147342, relating to the Action entitled: "**S**ecurely **A**dvancing **F**uture **E**Vs with **L**i-Ion batteries thr**o**ugh **O**ptimized **P**athways", or **SAFELOOP** for short. Authors dedicate this paper to the eternal memory of Prof. Dr. Borys I. Bondarenko, Academician of NASU and ex-Director of NASU's Gas Institute, a visionary and a mentor.

Cathode materials and electrolyte formulations for emerging potassium-sulfur batteries

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Potassium-sulfur batteries (KSBs) are emerging as a promising energy storage system due to the high natural abundance of the active materials and the high theoretical energy density [1]. This system (with the first room-temperature cell reported in 2014) exploits the same conversion mechanism as lithium-sulfur batteries (LSBs), which involves a two-electron transfer for each sulfur atom responsible for the high theoretical specific capacity of sulfur. Akin to LSBs, KSBs face challenges limiting their practical application, including cathodic volume expansion, sluggish reaction kinetics, shuttle effect, sulfur insulating nature, and potassium dendrite growth [2]. This work explores sulfur-hosting cathodes and compatible electrolytes, aiming at assembling a prototype KSB. Through extensive slurry optimization, we developed a stable and robust electrode formulation for use with glyme-based electrolytes, which are prone to co-intercalation causing active material detachment from the current collector [3].

The most promising cell configuration employs Ketjenblack (KJB) as sulfur host and tetraethylene glycol dimethyl ether (TEGDME) with 2 M Potasium bis(trifluoromethanesulfonyl)imide (KTFSI) as electrolyte. The corresponding electrochemical characterization is reported in Figure 1.

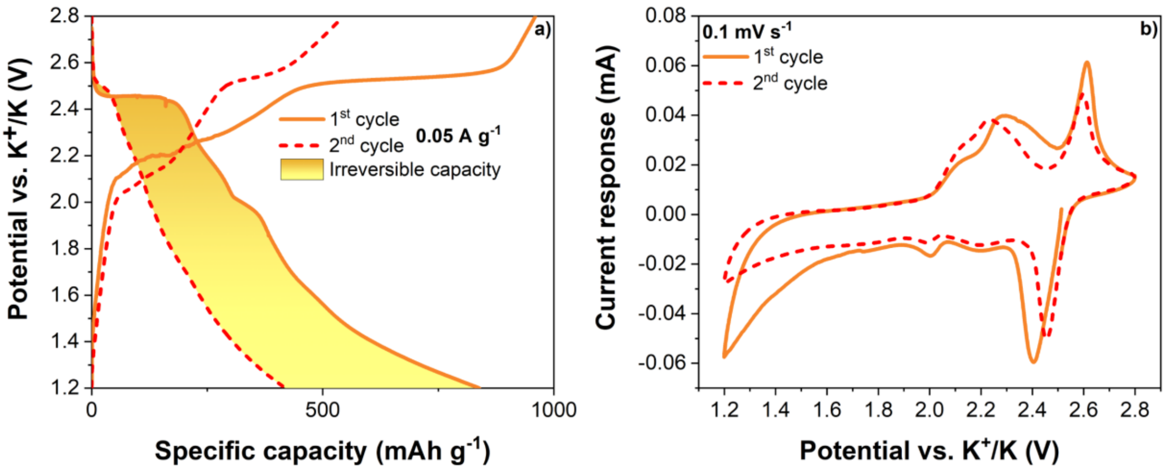

Figure 1. Figure 1. Electrochemical characterization of the first two cycles. (a) Charge and discharge profiles. (b) CV curves at a constant scan rate.

The optimized salt concentration effectively mitigates the shuttle effect, preventing the occurrence of apparent infinite charge states that hinder stable cycling. Moreover, this electrolyte formulation promotes the conversion of sulfur species, providing a promising basis for further optimization of the overall cell configuration.

Further research is required to optimize slurry and electrolyte formulations, using alternative solvents and exploring the localized high concentration electrolyte strategy. Moreover, the utilization of single-atom catalysts could be essential to improve reaction kinetics and system reversibility.

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Light-weight Multi-Particle Modelling approach for Cell-to-Cell and In-Cell Heterogeneity in Lithium-Ion Battery

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Understanding and characterizing degradation phenomena in lithium-ion batteries (LIBs) is essential to address the complexity of real-world aging, where non-uniform operating conditions induce heterogeneous degradation at both cell and module level. Such multi-scale heterogeneity leads to capacity unbalance, internal resistance mismatch, and accelerated performance decay, posing significant challenges for battery management and lifetime prediction [1]. This context requires fast and reliable diagnostic tools, such as Electrochemical Impedance Spectroscopy (EIS)[2], as well as lightweight yet reliable modelling approaches capable of describing internal operating conditions and ageing evolution while accounting for electrochemical and thermal inhomogeneities at both cell and module levels [3]. Although detailed Pseudo Two-Dimensional models are computationally expensive and equivalent circuit models lack physical interpretability, reduced-order physics-based approaches such as the Single Particle Model (SPM) offer a promising trade-off, preserving a strong physical foundation with reduced complexity [4]. However, existing lightweight models are not well suited to describe both in-cell particle heterogeneity and cell-to-cell imbalance in parallel configurations.

In this work, the classical SPM is extended through a Multi-Particle Model (MPM) structure, enabling the representation of real active material particle size distributions at the electrodes level. Additionally, second-order effects are integrated in the model, such as the Nernst-Planck equation for lithium transport in the electrolyte domain, double-layer capacitive behavior, and ageing modes, namely Loss of Lithium Inventory (LLI) and Loss of Active Material (LAM). This is further coupled with a 0D thermal model, enhancing its physical representativeness at a low computational cost. Moreover, an electrical system of parallel-connected cells is implemented in the framework, by means of Kirchhoff's current and voltage laws.

The model is calibrated through an extensive sensitivity analysis, allowing the simulation of both Constant Current and Constant Voltage protocols and EIS spectra of heterogeneous cells groups and thus enabling the prediction of current redistribution and thermal imbalance arising from uneven ageing in parallel-connected cells, a critical aspect for module-level diagnostics. This case is demonstrated with good accuracy against experimental data obtained from real-life aged samples from long-term (8 yrs, ≈500'000 km) automotive applications. Innovative FBG temperature sensors are used during the experimental campaign, allowing for accurate internal and external temperature measurements.

The proposed approach is demonstrated able to provide a computationally efficient and physically grounded tool for heterogeneity-aware diagnostics of real-world battery systems.

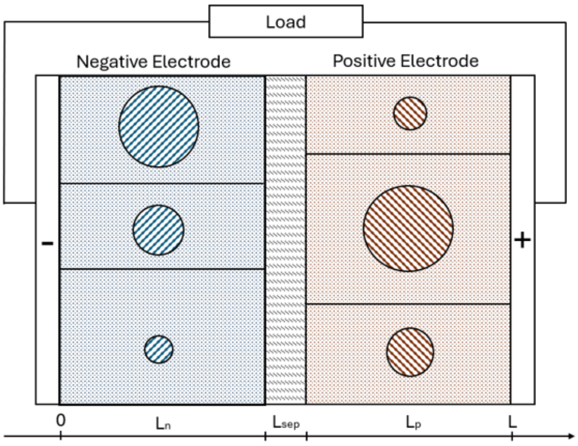

Figure 1. Schematic representation of MPM

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Sustainable chitosan-based binders for high-performance electrodes for lithium-ion batteries

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The growing demand for electric mobility calls for lithium-ion batteries with higher energy and power density, while complying with strict European sustainability regulations across the entire value chain. Balancing high electrochemical performance with environmental compatibility remains challenging: high-voltage cathodes can face electrolyte instability, whereas high-Ni materials enhance capacity but raise safety concerns and reliance on critical raw materials. Consequently, future battery development must integrate performance, safety, manufacturability, and sustainability in a unified strategy [1].

In this context, electrode manufacturing plays a key role. Although electrochemically inactive, the binder is essential for mechanical cohesion, adhesion, and interfacial stability. Its selection strongly affects processing routes, environmental impact, and recyclability. Replacing fluorinated binders processed in toxic organic solvents with water-based systems, preferably derived from renewable sources, represents a crucial step toward safer, more sustainable, and circular battery production [2].

In this context, we investigated a bio-derived binder based on chitosan, optimized for graphite anodes. Chitosan, obtained from the partial N-deacetylation of chitin, is abundant and biodegradable. To enable aqueous processing, chitosan is solubilized in acidic media, and different carboxylic acids were investigated not only to ensure dissolution but also to tailor mechanical integrity and interfacial properties. The formulation was optimized in terms of rheological behavior, adhesion/cohesion strength, wettability toward alkyl carbonate-based electrolytes, and electrochemical stability. Graphite electrodes prepared through a fully aqueous route were evaluated by galvanostatic cycling to assess rate capability and long-term stability, demonstrating the feasibility of sustainable binder systems without compromising performance [3].

We carried out parallel activities focused on high-voltage cathodes such as $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO), a cobalt-free material characterized by high operating voltage and reduced nickel content compared to layered high-Ni cathodes. Its Co-free composition contributes to lowering critical raw material dependency and improving sustainability. The development of water-processable binder systems for LNMO further enables fully aqueous cathode fabrication, minimizing the use of hazardous organic solvents. By combining sustainable binder design with intrinsically more responsible cathode chemistry demonstrates that environmental compatibility, material criticality reduction, and high electrochemical performance can be addressed synergistically in next-generation lithium-ion batteries [4].

ACKNOWLEDGEMENTS

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A Numerical Investigation of LNMO/LFP Blended Cathodes

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Blended cathodes combining different active materials have emerged as a promising strategy to exploit complementary electrochemical properties while mitigating the intrinsic limitations of individual components. In this context, cobalt-free systems based on lithium nickel manganese oxide (LNMO) and lithium iron phosphate (LFP) are particularly attractive, as they combine high operating voltage with enhanced safety and cycling stability. Based on a previous experimental study of Versaci et al. (2024) [1], this work presents a 4D multiscale numerical investigation of LNMO/LFP blended cathodes aimed at elucidating the role of material architecture and LFP content on electrochemical performance. Unlike homogenized or effective-medium descriptions, LNMO and LFP are treated as physically and electrochemically distinct phases throughout the modelling framework.

At the particle scale, the strong mismatch in characteristic dimensions between the two materials is explicitly accounted for by modelling a micrometric LNMO particle (10 µm) partially covered by nanometric LFP particles (≈200 nm). Separate transport and kinetic descriptions are retained for each phase, enabling the investigation of local lithium transport and potential lithium exchange between the two cathodic materials.

To bridge the gap between the detailed particle representation and the full electrode model, an intermediate equivalent geometry is introduced. In this step, the same LNMO particle used in the heterogeneous model is considered and coated with an LFP shell, defining a simplified core–shell configuration that preserves the key transport and kinetic interactions while reducing computational complexity. This reduced domain is used to analyse the numerical behaviour of the system and to calibrate the effective parameters associated with the shell description, ensuring consistency between the microscale physics and the upscaled representation.

The analysis is subsequently extended to the electrode scale through simulations of lithium-ion battery half-cells. The cathode is represented as a packed bed of spherical LNMO particles acting as active cores, each surrounded by a homogeneous porous shell whose solid phase corresponds to LFP. This core–shell architecture preserves the separation between the two active materials and avoids homogenization into an equivalent blended phase, while enabling a systematic assessment of the effect of LFP content on the macroscopic electrochemical response.

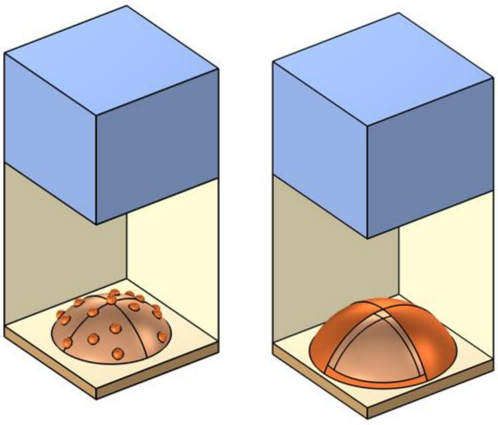

Figure 1: Heterogeneous and core-shell computational domains adopted for particle level simulations

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Functionalized SiO_2 Nanoparticles as HF Scavengers for Novel Separators in Li-ion Batteries

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The increasing demand for high-energy-density lithium-ion batteries has driven the development of advanced multifunctional separators capable of improving safety, electrochemical stability and ion transport. By tailoring their structure and composition, these separators can enhance electrolyte wettability, mechanical and thermal stability, and mitigate degradation processes during battery operation.[1] A key challenge in lithium-ion batteries is the leaching of transition metal ions (TM) from cathode materials, often triggered by hydrofluoric acid (HF) formed from the decomposition of $LiPF_6$-based electrolytes. HF promotes cathode degradation and metal dissolution; the dissolved ions can migrate to the anode, accelerating parasitic reactions and overall cell degradation.[2] In this work, a smart multifunctional separator is proposed by incorporating functionalized SiO_2 nanoparticles acting as chemical scavengers and ionic promoters. SiO_2 nanoparticles functionalized with N-(6-Aminohexyl)aminopropyltrimethoxysilane (SNP) were developed to neutralize acidic species and reduce transition metal dissolution. Their scavenging activity was evaluated by adding different SNP loadings to NMC-based cathodes in LP71 electrolyte and quantifying dissolved transition metals by ICP-OES after 5 days at 55 °C, conditions that accelerate HF formation and cathode degradation.

A second type of SiO_2 nanoparticles functionalized with 3-(Trihydroxysilyl)-1-propanesulfonic acid (SIP) was synthesized as an ionic promoter to enhance Li^+ diffusion. The separator was designed as a three-layer structure (PVdF-HFP|PEO|PVdF-HFP), where the outer layers contained 8wt% SIP to facilitate Li^+ transport, while the central PEO layer incorporated 5wt% SNP to capture acidic species and dissolved metals. A reference separator with the same architecture but without ionic promoter filler was also prepared. The multifunctional separator was characterized in terms of wettability, electrolyte uptake, thermal stability (TGA, DSC), mechanical properties (DMA) and morphology to assess the effect of membrane asymmetry. Electrochemical performance was evaluated through chronoamperometry to determine the Li^+ transference number (BEV method), ionic conductivity measurements at different temperatures, potentiodynamic electrochemical impedance spectroscopy (PEIS), and galvanostatic cycling (GCPL) in NMC811|separator|Li coin cells.

The separators were further tested in NMC532|Graphite full cells under CC–CV cycling, while accelerated rate calorimetry (ARC) was used to evaluate thermal stability. All results were compared with a commercial Celgard2500 separator. The developed separators exhibited superior mechanical properties, wettability, and electrolyte uptake compared to commercial benchmarks. The inclusion of an ionic promoter significantly enhanced lithium-ion transport, increasing the Li^+ transference number from 0.30 to 0.67 and boosting ionic conductivity. Notably, the realized smart separator also had beneficial effects on the electrochemical performance, leading to higher overall capacity and improved capacity retention over extended cycling. Moreover, the combined presence of nanoscavenger and ionic promoter mitigated transition metal dissolution, stabilized the cathode-electrolyte interface and hindered the formation of thermally unstable species generated in the presence of water traces

Overall, the proposed smart multifunctional separator represents a promising strategy to simultaneously enhance lithium-ion transport and suppress degradation mechanisms, contributing to safer and more durable high-energy lithium-ion batteries.

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Unraveling Structural and Redox Processes in P2-Layered Cathodes for Na-ion Batteries via *Operando* XRD and Advanced RIXS/XAS Experiment

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Sodium-ion batteries (SIBs) are emerging as promising alternatives to lithium-ion batteries due to the natural abundance of Na and the reduced reliance on critical raw materials (*e.g.* Co, Ni, graphite). Among various cathode materials, P2- and O3-type layered oxides are the most versatile and promising in terms of electrochemical performance. P2-type oxides exhibit the highest structural stability during cycling. However, their low initial Na content (x = 0.67) significantly limits their potential for large-scale production. Moreover, an irreversible phase transition occurs at high potentials (>4 V) during cycling, due to the partial collapse of the P2-layered structure into the so-called *Z-phase*,[1] which consists of a mixture of unstable layered phases such as P2- and OP4-type. To suppress this structural rearrangement, strategies such as doping with electrochemically inactive pillar ions, *e.g.*, Mg (II), or synthesizing oxides with mixed P2–O3 phases have been investigated and proven effective.[2]
In this work, we systematically evaluated the role of Mg (II) doping on the structural and electrochemical performance of P2-$Na_{0.67}Mn_{0.5}Fe_{0.5-x}Fe_xO_2$ (x = 0, 0,1, 0.2, 0.3) synthesized by solid-state synthesis. In addition to the conventional structural and electrochemical characterization techniques for the investigation of the cathodic properties, we also employed some other more advanced techniques. In particular, *operando* XRD and *ex-situ* RIXS/XAS analysis were conducted on the x = 0 and x = 0.2 materials. We selected these two compositions because electrochemical trends clearly indicated $x = 0.2$ as the best-performing material, while $x = 0$ was used as a reference, allowing a thorough assessment of the impact of Mg (II) substitution on P2-layered structural stabilization. At high potentials, several processes can simultaneously trigger structural degradation and phase transitions, making it difficult to unambiguously identify the dominant mechanism. Among these, the redox activity of oxygen remains one of the most challenging phenomena to fully understand. In addition, transition-metal migration into Na crystallographic sites, which leads to irreversible capacity loss, and the Jahn-Teller distortion associated with Mn (III) must also be considered.
Operando XRD experiments confirmed that Mg (II) effectively suppresses the partially irreversible phase transition from the pristine P2 structure to the previously mentioned *Z-phase* at low Na content. The evolution of the lattice parameters, particularly along the c-axis, during the first two cycles revealed that most irreversible structural changes occur during the initial charge-discharge cycle, whereas the second cycle exhibits a more symmetric and reversible electrochemical behavior. Motivated by these findings, *ex-situ* RIXS/XAS analyses were performed on electrodes quenched at six key potentials during the first two cycles. XAS spectra were collected in both Total Electron Yield (TEY) and inverse Partial Fluorescence Yield (i-PFY) modes to probe potential differences in transition-metal oxidation states between the electrode surface and the bulk. Notably, i-PFY proved particularly valuable, as it enables extraction of absorption spectra with a probing depth comparable to that of RIXS by integrating maps acquired at the transition-metal L-edges. RIXS maps at the O K-edge were also collected to investigate possible signatures of anionic redox activity,[3] such as oxygen dimer formation or molecular O_2 release, while Mn and Fe L-edge RIXS measurements were used to evaluate how Jahn-Teller distortions and transition-metal migration toward Na sites evolve with the voltage and how these processes are influenced by Mg (II) substitution. Collectively, these results demonstrate that the combination of *Operando* XRD with advanced spectroscopic techniques such as XAS and RIXS provides a powerful approach to unravel the complex structural and redox mechanisms governing high-voltage P2-layered cathodes.

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Unraveling Structural and Redox Processes in P2-Layered Cathodes for Na-ion Batteries via *Operando* XRD and Advanced RIXS/XAS Experiment

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Coat-Doping Strategies for Stabilizing Ni-rich Layered Cathodes

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$LiNiO_2$-based cathodes offer exceptionally high specific capacities for next-generation lithium-ion batteries, yet their practical deployment remains limited by structural and interfacial instabilities that emerge during electrochemical cycling. Oxygen loss, phase transitions, and surface reconstruction accelerate degradation in Ni-rich layered oxides, highlighting the need for materials design strategies that simultaneously stabilize both bulk structure and surface chemistry. This work, undertaken as part of the Horizon Europe INERRANT project, focuses on developing robust Ni-rich single-crystal cathodes through integrated synthetic control and targeted structural modification.

Optimized synthesis of single crystal Ni-rich $LiNiO_2$-based cathodes provides the foundation for developing a coat-doping strategy that simultaneously addresses bulk and surface degradation. In this approach, carefully selected substitution elements are introduced to stabilize the layered crystal structure while promoting the formation of a protective surface. Through judicious cation and anion substitution, structural pillaring within the bulk is combined with enhanced surface stability, supporting the formation of more robust cathodes with improved cycling stability.

Advanced characterization, including X-ray diffraction computed tomography and newly developed *operando* muon spectroscopy methods, provide insights into structural heterogeneity and lithium transport during cycling. These results contribute to the rational design of stable Ni-rich cathodes for next-generation Li-ion batteries.

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Correlating Optical Imaging and SERS/Raman Mapping for Chemical Characterisation of the Solid Electrolyte Interphase in Lithium-Ion Battery Graphite Anodes

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The solid electrolyte interphase (SEI) is a critical component in lithium-ion batteries, governing cell performance, lifetime, and safety. Despite its central role, a comprehensive understanding of SEI chemical composition and its spatial heterogeneity at the electrode surface remains a key challenge. Post-mortem analysis of cycled graphite anodes frequently reveals distinct visual features-including areas of different coloration and the presence of white spots-whose chemical identity and formation mechanism are the focus of the present investigation.

Within the BatWoMan project, this work investigates the SEI formed on graphite electrodes in NMC622||graphite pouch cells subjected to different formation protocols. Post-mortem characterisation was performed using Raman and surface-enhanced Raman scattering (SERS) spectroscopy in mapping mode, enabling spatially resolved chemical analysis at the micrometer scale. Spectral analysis in the 250–1400 cm^{-1} region allowed identification of key SEI components, including lithium carbonate (Li_2CO_3), lithium oxide (Li_2O), lithium hydroxide (LiOH), lithium phosphate species, and lithium acetate (CH_3COOLi). The SERS approach provided enhanced sensitivity for trace species at the electrode-electrolyte interface.

A central aim of this work is to establish a systematic correlation between the visual appearance of the harvested anodes and their chemical composition. Optical images of the electrodes reveal heterogeneous surface features, including regions of distinct coloration and localised white deposits. By co-registering these optical observations with Raman and SERS chemical maps, we seek to assign specific spectral signatures to the visually distinct zones, thereby linking macroscopic surface morphology to the underlying interfacial chemistry. This approach aims to provide new insight into the spatial distribution and nature of SEI components as a function of formation protocol, contributing to improved strategies for battery manufacturing and lifetime optimisation.

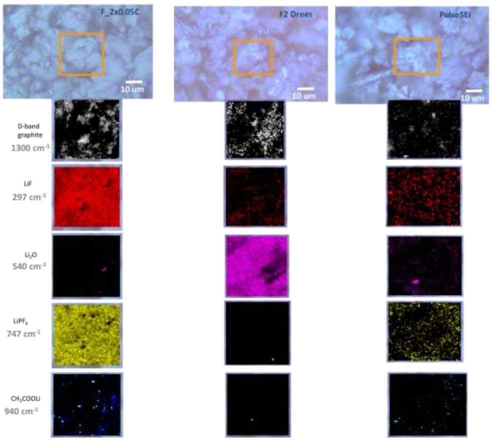

Figure 1. SEI micro-Raman mapping results.

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State estimation of commercial Na-Ion Batteries

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This work presents the state-of-charge (SoC) estimation of a commercial Na-Ion cell based on data extracted by laboratory experiments. The characterization of Na-Ion cells is done at three operating temperatures (10°C, 25°C, and 40°C), applying three experimental protocols: cycling tests to extract the cell capacity; pseudo-OCV tests for the computation of the SoC-OCV curve; and the Galvanostatic Intermittent Titration Technique (GITT) for the extraction of dynamic parameters. Despite the promising low-temperature performance reported in the literature for Na-Ion technology [1], the tested cell exhibits unexpected degradation at 10°C, suggesting that actual low-temperature behaviour may deviate significantly from theoretical expectations. The parameters extracted by the experimental data are suitable to model the battery with an equivalent circuit. Such a model is used inside a state observer to estimate the cell SoC[2]. A comparison with LFP chemistry is provided to highlight the intrinsic observability of Na-Ion cells, due to the OCV curve, which is not flat as the LFP one. This characteristic makes Na-Ion cells not directly suitable for integration into existing Li-ion BMS architectures.

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Fast-charging Li-ion battery modeling using electrode homogenization, parametrization, and experimental validation.

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Preventing lithium plating during fast charging of lithium-ion batteries requires dynamically adjusting the charging current to maintain the electrical potential of the negative electrode slightly above 0 V (vs. Li^+/Li) [1,2]. However, this potential cannot be directly measured in standard industrial Li-ion cells. To address this limitation, we developed a novel variant of the electrochemical pseudo–two-dimensional model that allows real-time estimation of the potential profile across the thickness of each electrode [3]. The non-linear state-space representation of the cell was derived from a set of coupled electrochemical partial differential equations using an electrode homogenization approach and a non-uniform discretization grid. The paper further details the model parameterization through experimental characterization conducted using a three-electrode assembly and presents its validation at 2C, 3C and 4C charging rates.

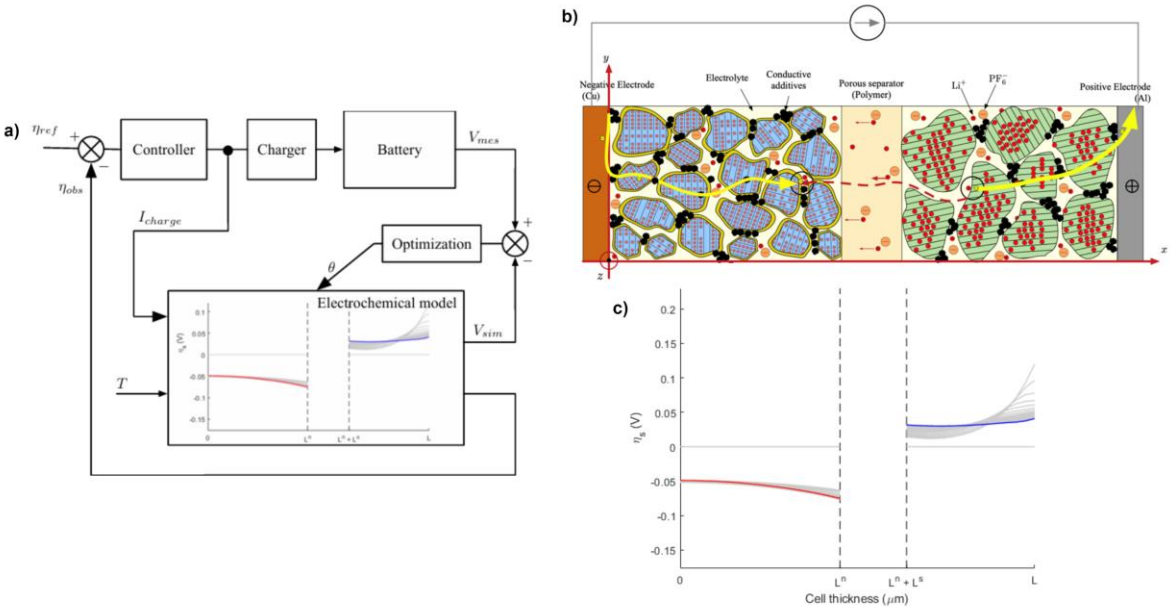

Figure 1. Block diagram of the proposed electrochemical state-space model (a). Illustration of a Li-ion battery during the charging process (b). Simulation result showing the overpotential distribution at the negative and positive electrode respectively.

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Insights into the pre-treatment of spent LFP ($LiFePO_4$) EV batteries for direct recycling purposes

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Recycling of Li-ion batteries (LIBs) is a hot research topic among both academic and industrial researchers and engineers. Especially for low-cost LIB chemistries, such as the LFP ($LiFePO_4$) chemistry, direct recycling has become a highly researched strategy for handling retired batteries due to its potential to recover active materials in their intact form, as compared to the more conventional recycling routes [1]. In terms of literature, there is already a vast number of publications reporting on novel methods of relithiation of spent LFP cathode active material (CAM), and the numbers are only rising. However, there is much less focus on the pre-treatment steps that must be taken before separating the CAM from the rest of the battery components. At the same time, the pre-treatment process can govern in what purity and chemical/mechanical integrity the CAM can be recovered, which in its turn can largely affect the electrochemical performance of the relithiated material.

In this work, we present our latest findings confined into two publications [2, 3] that deal with different parts of a pre-treatment process of spent LFP batteries from real-life EV applications, focusing solely on its impact on the purity and integrity of the recovered CAM. Specifically, we compare two methods of discharging the whole modules in terms of their impact on the recovered material, shedding new light on the choice of discharging method depending on the subsequent treatment strategy of the spent modules. Further, we explore methods of delamination of the CAM from the aluminum current collector foil, developing an existing but sparsely described method and demonstrating a fully novel one. We also compare the effects of different washing steps prior to the delamination to explore the possibilities of a greener approach to removing electrolyte residues from the CAM.

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Understanding aqueous processing of positive electrodes for lithium ion batteries: Investigation of the interaction mechanism of $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ with water via a D_2O treatment approach

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Aqueous processing of Ni-rich layered oxide active materials for positive electrodes, while attractive with regard to its ecological and economic footprint, possesses multiple obstacles not encountered when using state-of-the-art methods. One is found in the structural changes at the active materials' surface caused by the interaction with water. This study explores the mechanism of interaction of H_2O on such materials via use of D_2O in production and comparison to a state-of-the-art reference. The materials, electrode pastes, and positive electrodes were prepared with H_2O or D_2O and characterized with regard to their physical and chemical properties, combined with microscopy and thermal analysis. D_2O and H_2O exhibited similar behavior in most metrics, and expected differences were seen in others, e.g. concerning viscosity or pH/pD (higher for D_2O in both cases). EGA-MS indicated analogous decomposition of electrodes processed with H_2O and D_2O, with any water detected not stemming from processing in aqueous solution, but rather from surface residues of the active material, such as LiOH. Furthermore, the D_2O-processed sample showed a diverging signal from its H_2O-processed counterpart, indicating further penetration of deuterium into the layered active material's structure beyond surficial interactions. The findings offer a clear mechanistic insight into the effect; aqueous processing has on this class of positive electrode materials and thus contributes to greater understanding of the hurdles to be overcome to facilitate commercial viability for aqueously processed Ni-rich layered oxide material-based positive electrodes. Furthermore, they show the use of D_2O as a tracking agent when investigating the effect of water on active materials.

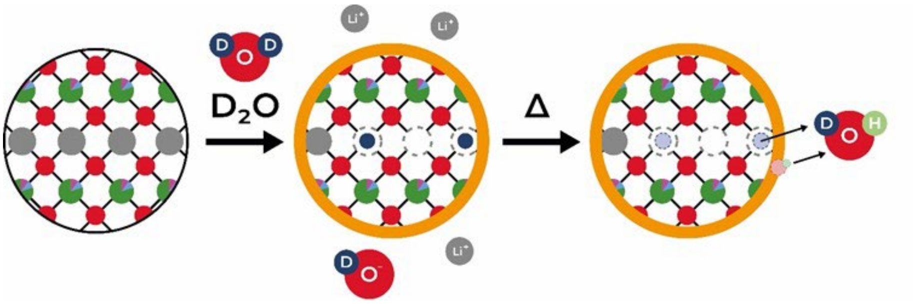

Figure 1: Schematic of the mechanism of lithium replacement by protons / deuterium atoms in NMC particles upon contact with water, showing the gaps in the lattice caused by water penetrating into the bulk material.

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Atomistic Insights into Electrolyte-Sodium Metal Interfaces

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Sodium metal batteries (SMBs) are gaining growing attention as promising alternatives to lithium-based energy storage technologies due to the natural abundance and low cost of sodium. Nevertheless, the practical implementation of Na metal anodes is critically limited by interfacial instability with the electrolyte, which results in uncontrolled solid electrolyte interphase (SEI) formation and rapid performance degradation [1,2]. Achieving an atomistic-level understanding of SEI formation mechanisms is therefore essential for the rational design of stable electrolyte systems.

In this work, we present a comparative atomistic study of SEI formation at the Na metal interface in two representative electrolyte systems: an ionic-liquid electrolyte (IL: NaFSI/PyrFSI) [3] and a polymer-based electrolyte, [Poly(ethylene oxide)Na][FSI] (PEO:Na) [4]. To overcome the limitations of first-principles simulations in accessing realistic system sizes and time scales, we develop a machine-learning interatomic potential (MLIP) within the MACE framework [5], trained on density-functional-theory data. Large-scale molecular dynamics simulations reveal FSI decomposition at the Na interface in both electrolyte environments. We also observe rapid formation of a NaF-rich passivation layer at the interface. These findings provide atomistic insight into electrolyte-dependent SEI formation in sodium metal batteries and demonstrate the potential of MLIP-based atomistic simulations as predictive tools for electrolyte-electrode interfaces.

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Temperature- and SoC-Dependent Resistance Behavior of LFP and NMC811 Cathodes for Application-Specific and Lifecycle-Aware Battery Chemistry Selection

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The transition towards more sustainable battery technologies requires not only improvements in energy density but also a deeper understanding of performance characteristics that influence lifetime, safety, and aging behavior. In the context of resource efficiency, lithium iron phosphate ($LiFePO_4$, LFP) has gained increasing attention as a positive electrode (cathode) active material due to its nickel- and cobalt-free composition compared to common high-energy alternatives such as $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811). In addition to its more abundant raw materials, LFP is known for enhanced safety and long cycle stability, making it particularly attractive for applications targeting advanced battery value chains and second-life applications, where cells are reused, for example, in stationary storage systems after their initial use to increase economic and environmental value [1], [2].

A key factor determining the suitability of battery chemistries for such sustainable use cases is the investigation of its aging behavior, (i.e., resistance evolution, capacity loss) over its expected operating conditions. However, conventional aging tests to assess these effects can take several months to complete and often allow comparisons only under specific operating conditions.
This study therefore investigates the internal resistance behavior of two cathode active materials, LFP and NMC811, at different states of charge (SoCs) and temperatures using a short constant current pulse test combined with electrochemical impedance spectroscopy (EIS). These methods allow the evaluation of resistance characteristics that can be used to infer the evolution of internal resistances over the cycle life depending on the intended application. A three-electrode cell setup with a lithium reference electrode was applied to analyze impedance and performance with a focus on the respective cathode. The instantaneous voltage drop after the current pulses was evaluated, and different resistance contributions were analyzed during EIS measurements at multiple SoC levels.
The results of this comparison enable the identification of optimal cathode chemistries for various operating conditions and use cases. Since increased internal resistance is closely correlated with electrochemical aging processes, the resistance characteristics obtained in this study can also be used to infer possible aging behavior under different operating conditions without the need for extended long-term cycling tests.

These insights help to evaluate typical real-world usage scenarios, such as operation at specific temperature ranges and commonly used SoC windows, enabling the selection of cell chemistries that maintain favorable performance not only during their first-life application but also after repurposing for second-life use.
Such knowledge contributes to more sustainable battery deployment by enabling improved matching between cell chemistry and application requirements, thereby facilitating longer first-life operation and more efficient second-life utilization in stationary energy storage systems. Ultimately, these insights support circular battery concepts by improving resource efficiency and extending the functional lifetime of lithium-ion batteries.

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The authors would like to acknowledge Horizon Europe for funding the project CIRCUBATT, a partner of the Battery 2030+ community.

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Degradation Mechanisms in Lithium-Ion Battery Electrodes: A Post-Mortem Structural and Chemical Characterization Approach

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The accelerated proliferation of electric vehicle manufacturing, in conjunction with the constrained longevity of lithium-ion batteries (LiBs), has given rise to substantial apprehensions concerning the sustainable utilization of critical raw materials and the management of end-of-life batteries. Consequently, the development of efficient recycling strategies and a comprehensive understanding of battery degradation mechanisms has become essential to extend battery lifetime and reduce reliance on critical raw materials. It is crucial to undertake detailed morphological and structural characterization of battery electrodes at different stages of their lifecycle to gain insight into degradation processes and the chemical state of valuable metals present in cathodes targeted for recycling.

In the present work, two distinct sets of LiB cathodes were extracted from a battery and subjected to advanced characterization to investigate the presence of degradation and the effect of it in the electrodes. Each set comprised one pristine electrode and one electrode that had undergone charge and discharge cycles. The first set originated from coin cells cycled under controlled laboratory conditions, while the second set was obtained from electric vehicle batteries. In this case, degradation occurred under uncontrolled real-world conditions, and the sample preparation was not controlled. Morphological characterization was performed using scanning electron microscopy (SEM), revealing clear differences between pristine and degraded electrodes, including surface damage, particle cracking, and structural heterogeneity. Energy-dispersive X-ray spectroscopy (EDS) was utilized to perform semi-quantitative elemental analysis. However, the presence of electrolyte-derived elements could not be conclusively assessed, particularly in the electrodes obtained from electric vehicle batteries, due to uncertainty regarding electrolyte removal during sample preparation. The detection and apparent concentration of elements originating from the electrolyte salt may be influenced by residual electrolyte or uneven drying on the electrode surface. Structural characterization was conducted using X-ray diffraction (XRD), which revealed a shift in the main diffraction peak in the degraded electrodes compared to pristine samples in both sets. This peak shift can be associated with lithium loss from the crystal structure, leading to changes in the lattice parameters. The loss of lithium is commonly related to irreversible processes such as the formation of within the solid electrolyte interphase (SEI) layer or deposited in the form of lithium dendrites.

X-ray photoelectron spectroscopy (XPS) was utilized to analyze the surface chemical composition and ascertain the chemical states of the elements, thus enabling the identification of surface degradation products and chemical modifications associated with electrode ageing. The combined use of SEM, SEM-EDS, XRD, and XPS enabled a comprehensive assessment of the morphological, structural, and chemical evolution of LiBs electrodes during degradation. Understanding these degradation mechanisms is essential for improving battery durability, optimizing recycling processes, and reducing the consumption of critical raw materials. The results of this study provide valuable insight into the structural and chemical changes occurring in cathodes from LiBs throughout their lifecycle, supporting the development of more sustainable battery technologies.

Assessing Maturity and Scalability of Li-metal cells

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Emerging battery technologies face a critical "Valley of Death" between laboratory research and industrial scale-up, since high technological risk and uncertainty about long-term returns discourage private investment and slow down commercialization [1]. This work proposes an integrated framework to simultaneously assess technical maturity and long-term cost competitiveness of next-generation battery cells. The methodology combines a quantitative Cell Readiness Level (CRL) with a component-level cost projection model based on engineering-constrained learning curves. The objective is to bridge development-stage risk assessment with the evaluation of long-term potential and scalability during deployment (Fig. 1a).

CRL is built on key scale-up parameters that strongly affect the reliability of results from lab tests: cathode mass loading (mg/cm2), N/P ratio, electrolyte loading (g/Ah), active area (cm2), and cycle life [1], [2]. Each parameter is converted into a normalized score from 1 to 9 using logarithmic or linear transfer functions, and the final CRL is calculated through a weighted product model. The model is validated on multiple Li-metal cell designs reported in the literature, showing that the resulting CRL remains consistent when the same design is tested under different experimental conditions, thus capturing intrinsic design readiness rather than tuned performance (Fig. 1b). Results from the combined analysis indicate that designs incorporating cathode coatings and protective interlayers achieve the highest CRL values.

Subsequently, the scalability of Li-metal cells employing sulfide solid electrolytes is assessed. Component-level material cost floors are estimated, highlighting the influence of Li_2CO_3 and Li_2S prices on the solid electrolyte and the impact of excess Li-metal thickness at the anode. Compared to LGPS that contain expensive Ge, LPSC exhibits significantly less prohibitive material constraints for large-scale deployment (Fig. 1c).

Assuming learning rates consistent with historical battery trends and the estimated material cost floors to constrain the learning curves, cost projections suggest that NMC||SSE||Li-metal cells could reach 70 $/kWh by 2045 (Fig. 1d). While this trajectory makes direct competition with LFP or Na-ion cells in mass-market applications challenging, it indicates potential entry into high-value segments such as premium electric vehicles, aviation, and advanced consumer electronics.

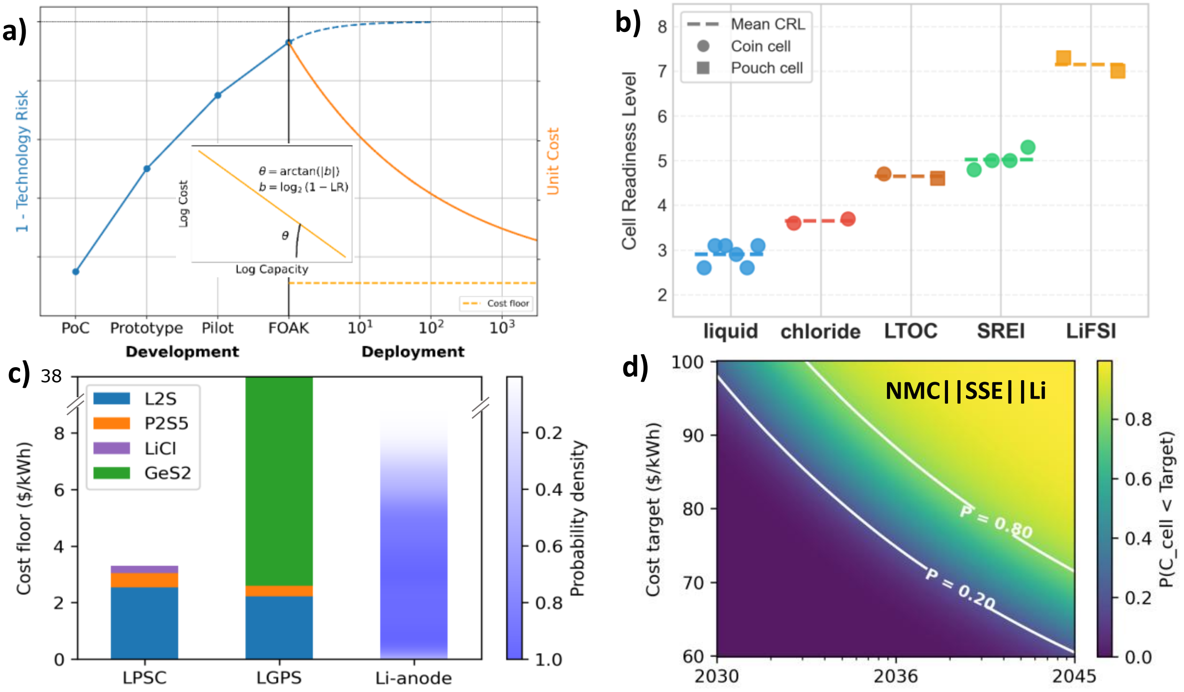

Figure 1. a) Methodological framework, b) model check, c) material cost floor estimation, d) cost projection

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Towards Sustainable Recycling of LFP Black Mass Using Deep Eutectic Solvent Leaching

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With the rapid growth of lithium iron phosphate (LFP) batteries in electric vehicles and energy storage applications, more sustainable recycling technologies are required. Current industry-standard pyrometallurgical and hydrometallurgical processes often generate significant waste streams or require high energy input. Deep eutectic solvents (DES) have emerged as promising green alternatives for metal recovery due to their low toxicity, tunable physicochemical properties, and potential for selective metal dissolution.

In this study, seven different organic acid-based DES systems were investigated for the leaching of lithium and iron from LFP waste material. Initial screening was conducted at 80 °C overnight and shows that several DES compositions selectively dissolved lithium while leaving the iron phosphate framework largely undissolved. Following an oxidative roasting pretreatment of the LFP material at 550 °C for 5 hours, one DES system enabled complete dissolution of the cathode material.

The proposed approach demonstrates a potential pathway for the separation of lithium, iron, and graphite from LFP black mass, contributing to the development of more environmentally sustainable battery recycling processes.

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Battery Parameter eXchange (BPX): a flexible standard for battery modelling

Carlos Garcia, Pete Keevill

www.**bpx**standard.com

Standardised definitions for Li-ion physics-based battery modelling

Battery Parameter eXchange (BPX) is an open standard for physics-based Li-ion battery models. BPX provides a standardised set of equations and parameters, and a JSON schema for expressing them. It is supported by parameter descriptions detailing how the parameters can be derived from physical battery cells. BPX aims to reduce fragmentation and support interoperability and data exchange. The standard makes it easier for established manufacturers, startups and innovators to access and leverage the insight provided by physics-based models across a broad range of development scenarios. The Faraday Institution supports BPX with the expectation that in the medium term it will become an independent industry standard maintained by its users.

Industrial relevance

- BPX has been developed to reduce costs and time-to-market through a common definition of physics-based battery models that can be used and shared widely across industry.
- As industrial interest increases, BPX has gained support from multiple simulators:
  - AVL CRUISE M
  - Gamma Technologies AutoLion
  - Ansys Fluent
  - PyBaMM
  - DandeLiion

An open standard

BPX is an open standard so <u>**you**</u> can engage with the development process:
- request changes to suit your needs
- report issues, share new ideas
- contribute new features

Come chat with us!

- *What models are **you** using? We'd love to know!*
- *How can BPX support **you**? Tell us your thoughts!*

Technical

BPX 1.1 provides:

Supported models (BPX 1.1)
DFN
SPM
SPM-e

- A standardised equation set
- A detailed description of the parameters
- A parameter-exchange format for physics-based battery modelling
- A human-readable JSON file format
  - containing the parameters
  - supporting the inclusion of validation data
- A python validator that ensures the parameter set in a BPX file is
  - correctly formatted and internally self-consistent
  - sufficient to compute a specific model

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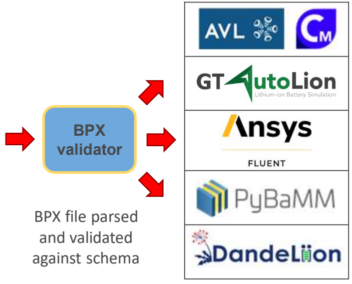


BPX file parsed and validated against schema

Supported simulators

<u>Some proposals for the future development of BPX include</u>:

- Best-practice parameterisation guide to accompany parameter descriptions
- Lightweight GUI app to create, edit, validate and visualise BPX files
- Public repository of parameter sets
- Improved hysteresis support for LFP
- Support for degradation models
- Support for 3D-DFN

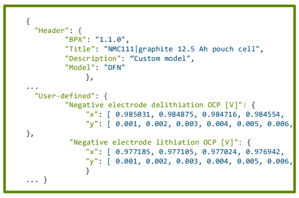
*What new feature would **you** like BPX to support?*

A flexible standard with optional, user-defined parameters

User-defined Parameters allow modellers to build on top of the well-defined core parameter set. Therefore,

BPX does <u>not</u> restrict the user to the models in the standard

- Miscellaneous, custom extensions are supported through user-defined parameters.



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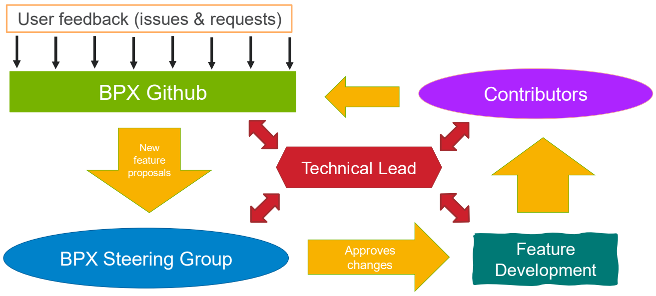
             "y": [ 0.001, 0.002, 0.003, 0.004, 0.005, 0.006,
             }
... }
```

Custom user-defined parameters

Contributors and governance

- BPX was conceived by Pete Keevill and brought to life by Dr Ivan Korotkin and Dr Rob Timms (Ionworks).
- With substantial contributions from Dr Edmund Dickinson (About:Energy) and support from Prof Jamie Foster (University of Southampton).
- The BPX Steering Group has an advisory role and meets periodically to make strategic decisions on the future of the BPX standard.
- As an open standard, BPX welcomes contributors and feedback from the community.



Learn more

- Watch the BPX Webinars

SCAN ME SCAN ME

- Download the latest BPX 1.1 standard

www.bpxstandard.com

- Get involved!

github.com/FaradayInstitution/BPX

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BPX Technical Lead

Dr Carlos Garcia supports the development of the BPX standard by making technical proposals, coordinating member's efforts, helping draft new version changes and representing BPX in public events. Carlos joined BPX after working for the MultiScale Modelling project and participating in several InnovateUK projects for a combined six years, focussing on electrochemical characterisation and rapid ageing of lithium-ion cells.

BPX Steering Group Chair

Pete Keevill had a 25-year career in Telecom R&D culminating in co-founding Ubiquisys in 2004, which was acquired by Cisco in 2013. Since leaving Cisco, Pete has supported innovation in sustainable technologies as an Entrepreneur in Residence at University of Bath and as a Commercialisation Consultant at the Faraday Institution.

THE FARADAY INSTITUTION BPX
BATTERY PARAMETER EXCHANGE
Faraday Battery Challenge
Delivered by Innovate UK

Strategies to Stabilize High-capacity Ni-rich Cathodes: Surface Modification and Electrolyte Additives

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Lithium-ion batteries are a vital part of the transition to renewable energies and electrified transportation. To achieve higher cell energy densities, Ni-rich layered oxides with capacities above 200 mAh g-1 and average voltages above 3.7 V are of particular interest. However, high nickel contents (above 80%) make the cathode active materials (CAM) susceptible to a variety of degradation phenomena, including phase transitions from the layered to a rock-salt structure, electrolyte decomposition at the electrode interface, particle cracking with subsequent contact loss, and transition metal dissolution followed by deposition on the anode.

Within Battery 2030+ umbrella project INERRANT, University College Dublin, Fraunhofer Institute for Silicate Research ISC and Julius-Maximilians-Universität Würzburg are bringing together multiple strategies to stabilize high-nickel cathode chemistries. Each partner addresses a different but synergetic aspect to improve the structural and surface stability (formation of a robust CEI) to minimize degradation of the CAM and to improve cell safety.

Fraunhofer ISC and the University of Würzburg are working together to design both surface modification/coatings based on phosphorus compounds which can be applied ex-situ to the CAM before electrode fabrication. Julius-Maximilians-Universität Würzburg is developed phosphorus-based electrolyte additives to stabilize the cathode-electrolyte interphase formation during cycling. This contribution will demonstrate the results of each strategy individually along which the first studies on potential synergetic effects derived from combining strategies.

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Knowledge integration and digital twin platform for battery manufacturing within the BatCAT project

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BatCAT is one of the battery manufacturability focused digital twin projects from the Horizon Europe research and innovation programme. The present contribution has a focus on two key aspects of a major upcoming project milestone: *Knowledge integration* by systematically ingesting data records to the data and knowledge management software (DKMS) and constructing the minimum viable product of the digital twin platform.

The main software component for the DKMS developed in BatCAT is LinkAhead, a database software supporting agile projects where data schemas can change over time. Data ingest forms and REST interfaces are automatically generated from the schemas for the different types of records, including experimental data, simulation data, simulation workflow descriptions, and models, with the latter covering physics-based (electronic, atomistic, mesoscopic, and continuum), data-driven, surrogate, and actionable models. In our architecture, the schema used within LinkAhead is mapped to a bespoke system of OWL ontologies, the lighweight BatCAT core ontologies (LBCO). The semantic architecture of the LBCO incorporates concepts from the battery value chain ontology (BVCO) and the relevant EMMO domain ontologies wherever possible and – among other reasons for making a mapping to other semantic artefacts and interoperability with external platforms easier – is also aligned with the EMMO and DOLCE foundational ontologies as well as the main interoperability layer for the ontologies developed from the VIMMP and MarketPlace projects (*i.e.*, earlier initiatives from Horizon 2020). Fragments of the LBCO are mapped to answer set programming, a type of logic programming. The DKMS is compliant with the specifications for dataspaces (*e.g.*, relevant to the Common European Dataspaces as advanced by the European Commission) and implements the dataspaces protocol.

The digital twin platform from BatCAT is based on physics-based modelling as part of its foundation, but completely relies on machine-learning (ML) models for its operation; these are either purely data-driven (e.g., ML directly from experimental data) or referred to as surrogate models – when, as their main or only purpose, they correlate simulation results – or as *actionable models*, when they contain a *real-time decision making* component for deployment within the manufacturing process. The ML models also include equations of state. The decision making is at this stage and technology readiness level (TRL) not meant to be fully autonomous (*i.e.*, a human will still need to take action); at higher TRLs and presupposing a thorough validation and documentation of its reliability, it is designed to make decisions autonomously. The consortium has decided to focus on optimizing charge-discharge patterns during cycling for solid-electrolyte interface formation in its coin-cell manufacturing pilot line as the main scenario for validating this technology to TRL 5. In addition to autonomous/assisted decision making, the minimum viable product of the digital twin will provide decision support in the form of an *interpretable industrial decision support system*, combining answer set programming with multicriteria optimization.

CATHODE-FREE Li-SULPHUR BATTERY

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Cathode-free lithium-sulphur (Li-S) batteries offer a promising route toward maximizing practical energy density by eliminating pre-fabricated sulphur/carbon composite cathodes, and reducing inactive mass. In this architecture, solution-based lithium polysulphides (typically Li_2S_6) serve as the active material and undergo reversible in-situ electrochemical conversion on inert conductive carbon substrates, removing the need for bulk sulphur host matrices, binders, and auxiliary additives, such as TiO_2, TiO_xN_y or $Li_4Ti_5O_{12}$ [1-4]. A practical embodiment previously reported involves catalytic carbon nanofibers containing Fe, Co, or Ni, synthesized via pyrolysis of filter paper impregnated with the corresponding metal chlorides at 800 °C under an Ar/H_2 atmosphere [5]. This so-called medium-entropy catalytic alloy is a variant of high-entropy oxychloride catalysts, which accelerate the redox reactions of polysulphides [6].

Here, we simplified this approach by employing commercial carbon buckypaper composed of multiwalled carbon nanotubes (BPMF 7525, Mainland Solutions LLC, USA) as the sulphur host. Even without any catalyst incorporation, our buckypaper substrate demonstrates promising electrochemical performance in the CR2032 coin cells assembled with a lithium metal anode, a glass fiber separator (Whatman CF/D), and a LiTFSI-based electrolyte containing 1.0 wt% $LiNO_3$. Polysulphide catholytes were prepared either via preparative electrolysis of the S/C composites or by prolonged vigorous stirring (typically overnight) of stoichiometric mixtures of Li_2S and S_8 in a 1:1 (v/v) mixture of 1,3-dioxolane and 1,2-dimethoxyethane. Advantages of the cathode-free design are demonstrated through comparison with conventional sulphur/carbon composite cathodes prepared either by mechanical milling or by melt-impregnation of mesoporous carbon (TOB-HPC) with elemental sulphur (S_8). An additional reference cathode material was Nanomyte BE-70 E (NEI Corporation). Cyclic voltammetry, galvanostatic charge/discharge cycling, and electrochemical impedance spectroscopy consistently confirm the reversible conversion of soluble polysulphides (Li_2S_6 or Li_2S_8) to Li_2S during discharge, followed by sulphur regeneration upon charging, without the necessity of a bulk sulphur composite cathode. While elimination of the traditional sulphur/carbon composite cathode reduces inactive mass and improves theoretical energy density, it also introduces challenges such as incomplete sulphur utilization, polysulphide shuttling, and limited cycle life.

Overall, cathode-free Li–S battery is a promising pathway toward high-energy-density storage systems for next-generation electric vehicles and grid-scale applications. However, achieving long-term cycling stability, high sulphur utilization, and scalable, cost-effective manufacturing remains essential for practical implementation.

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ANGeLiC

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TUNGSTEN OXIDE STABILIZATION INTERLAYER FOR IMPROVED CYCLING STABILITY OF CORE–SHELL STRUCTURED NI-RICH NMC CATHODES

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Lithium-ion batteries (LIBs) have established themselves as the leading technology for high energy density applications and cover a wide range – from consumer electronics, electromobility and stationary grid storage to specialized sectors such as aerospace, medical technology and industrial robotics. Nickel-rich layered transition metal oxides $LiNi_{1-x-y}Mn_xCo_yO_2$ (NMC) are currently among the most promising candidates for next-generation cathodes due to their high specific discharge capacity and the established scalability of their production. However, high-Ni NMCs such as $LiNi_{0.9}Mn_{0.05}Co_{0.05}O_2$ (NMC90) exhibit structural and chemical instabilities, leading to reduced cycle life and safety [1]. To mitigate these disadvantages, the design of core-shell architectures are thoroughly investigated. This design aims to combine the best properties of two different compositions: a nickel-rich core (e.g., NMC90) provides the necessary energy density, while a manganese-rich shell (e.g., NMC622) acts as a physical protective layer that isolates the reactive core from the electrolyte and suppresses aggressive surface chemistry [2]. However, the practical implementation of core–shell cathodes is often hindered by structural degradation caused by interdiffusion between the core and shell persists as a major challenge. This study investigates whether a tungsten oxide interlayer can act as a protective barrier that suppresses interdiffusion, stabilizes the crystal structure, and improves long-term electrochemical performance. Therefore, in frame of PHOENIX project, a $LiNi_{0.9}Mn_{0.05}Co_{0.05}O_2$ (NMC90) core and a $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622) shell, separated by a functional tungsten oxide interlayer, were synthesized via a one-pot oxalate co-precipitation route. Structural characterizations were conducted using SEM, EDX, XRD, XPS and ISS techniques. Electrochemical performance, including capacity retention, cycling stability, and internal resistance, was evaluated via GCD testing and EIS analysis on half-cell form fabricated with metallic lithium (Li) as anode, Glass Fiber-separators and EC/DMC = 50/50 (v/v) as an electrolyte. The long-term cycling stability of the core–shell samples, with and without a tungsten oxide coating, was evaluated over 50 cycles between 2.7 and 4.2 V at a rate of C/10 (Figure 1). The results demonstrate that the tungsten oxide-coated sample maintained a 80% state of health (SoH) until the 44th cycle, whereas the uncoated core–shell sample reached this degradation threshold by the 20th cycle. These results show that tungsten oxide effectively improves cycle stability by inhibiting core-shell interdiffusion, thus opening a promising path to longer-lasting high-Ni-NMC cathodes.

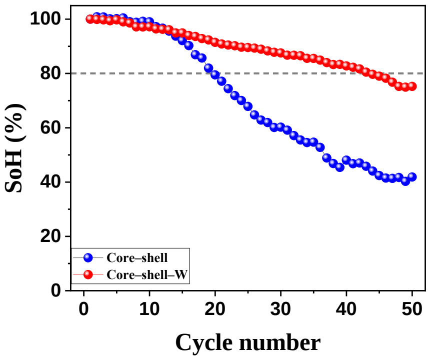

Figure 1. Long-term cycling stability of core–shell NMC cathode powders without (blue line) and with (red line) a tungsten oxide interlayer.

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Instrumentation design for real-time monitoring and triggered self-healing using micromachined sensor arrays

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Real-time monitoring of internal changes in parameters such as temperature, pressure, or gas evolution is crucial to detect degradation or failure onset in batteries with self-healing capabilities [1]. It allows for timely activation of self-healing mechanisms, preventing irreversible damage and extending battery lifespan.
This contribution presents means for integrating multi-sensor capabilities to monitor relevant parameters within battery environments. Additionally, it provides distributed heating control for self-healing activation either via a master Battery Management System (BMS).
To this end, a novel dual-function heating element circuit enables both thermal actuation for self-healing processes and resistive sensing capability. This is enabled by switching between constant-current heating mode and a Wheatstone bridge measurement mode employing precision amplification biased at mid-supply voltage. The core controller is a PIC18F25K80 microcontroller operating at 64 MHz with integrated SPI and UART interfaces for communication. Sensor inputs are processed through a 24-bit ADC connected via Zero Insertion Force connectors enabling direct in-situ measurements. The HealingBat sensor array [2] provides in-situ values of temperature, pressure, and hydrogen sulfide concentration.
Experimental validation confirms reliable operation across all modes with robust electrical protection and accurate sensor response. This integrated instrumentation platform demonstrates an effective approach toward intelligent battery monitoring systems capable of autonomous healing activation within next-generation Li–S energy storage technologies.

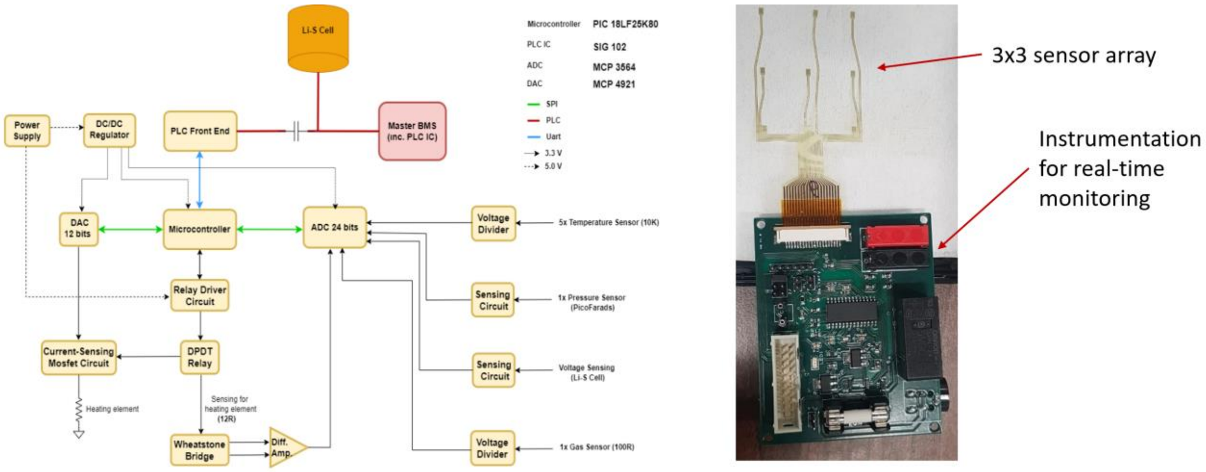

Figure 1. (left) System-level block diagram illustrating the integration of the instrumentation components to control and read-out one gas sensor, one pressure sensor, one voltage sensor, five temperature sensors, and one heating element. (right) The HealingBat sensor array platform connected to the instrumentation.

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RECOVERY AND PURIFICATION OF COBALT SULFATE HEPTAHYDRATE FROM PYRITE-DERIVED SECONDARY MATERIALS

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The rapid expansion of lithium-ion (Li-ion) battery technologies, driven by the global energy transition, has led to a significant increase in demand for critical cathode metals such as cobalt, lithium, manganese, and nickel. In this context, securing sustainable and reliable metal supplies from secondary raw material sources has become a strategic priority. Pyrite ore, commonly generated as a by-product of gold, copper, and nickel mining, represents a low-cost and abundant secondary resource with considerable potential for cobalt recovery and integration into the battery raw material supply chain.

The production of high-purity cobalt (II) sulfate heptahydrate ($CoSO_4 \cdot 7H_2O$), a key precursor for lithium-ion battery cathode materials, requires the efficient removal of metallic impurities prior to crystallization. In this study, a multi-step purification process combining ion exchange, solvent extraction, and controlled evaporation was developed to remove cadmium (Cd^{2+}) and manganese (Mn^{2+}) impurities from an acidic cobalt sulfate solution. Cadmium was selectively removed using ion exchange resin, while manganese was extracted using di-2-ethylhexylphosphoric acid (D2EHPA) at an optimized pH to ensure high selectivity.

Following purification, $CoSO_4 \cdot 7H_2O$ crystals were obtained through evaporation under controlled conditions, minimizing thermal degradation and undesired phase formation. The resulting crystals were characterized by ICP-OES and XRD analyses, confirming their high purity and structural integrity. The proposed approach demonstrates an effective route for producing battery-grade cobalt sulfate from secondary resources, supporting sustainable material supply for advanced energy storage applications.

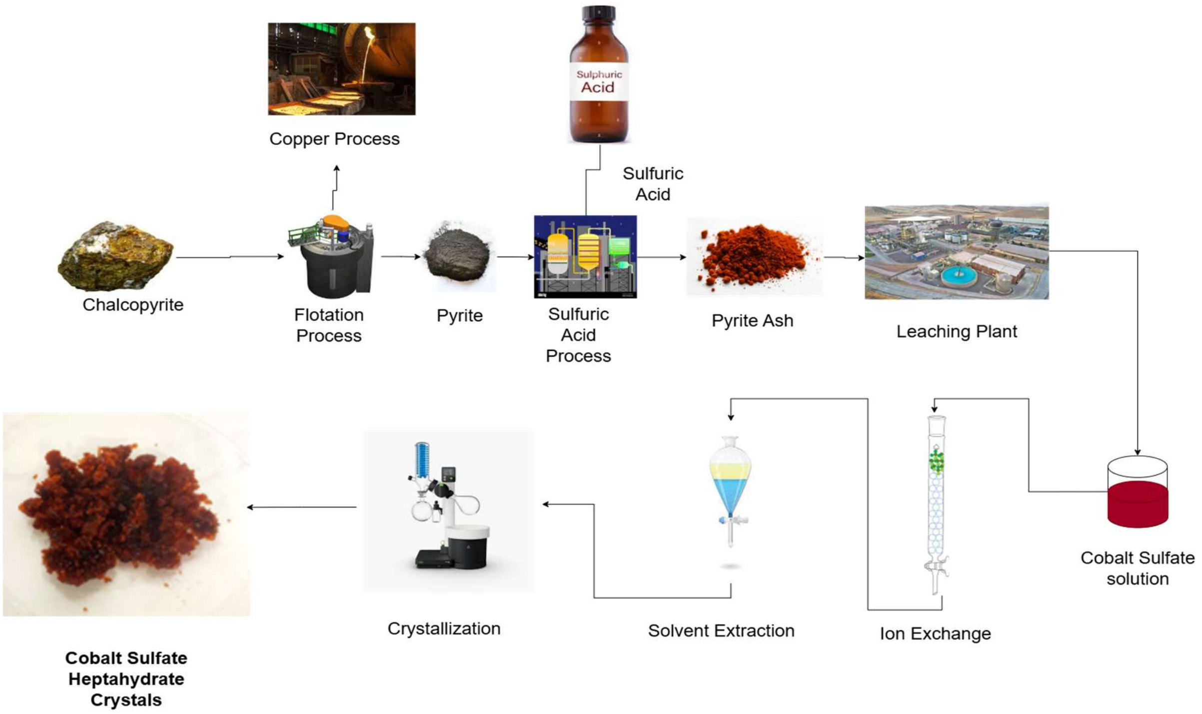

Figure 1. Block flow diagram of recovery and purification pathway to synthesis of cobalt sulfate heptahydrate crystals

This Study by Eti Gubre (Eti Bakır Inc) was funded by the Horizon Europe Programme under Agreement No. 101137771, Action entitled “Sustainable Technologies for Reducing Europe’s battery raw MaterialS dependence”, or “STREAMS”.

RECOVERY AND PURIFICATION OF NICKEL SULFATE HEXAHYDRATE FROM PYRITE-DERIVED SECONDARY MATERIALS

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The rapid expansion of lithium-ion (Li-ion) battery technologies, driven by the global energy transition, has significantly increased the demand for critical cathode metals such as nickel, cobalt, manganese, and lithium. Ensuring a sustainable and reliable supply of these materials from secondary raw resources has therefore become a strategic priority. Pyrite ore, commonly generated as waste or by-product of gold, copper, and nickel mining, represents an abundant and low-cost secondary resource with considerable potential for integration into the battery raw material supply chain.

In this study, a hydrometallurgical route was developed to produce high-purity nickel sulfate hexahydrate ($NiSO_4 \cdot 6H_2O$) from secondary cobalt–nickel-bearing materials. Cobalt and nickel present in a ZnCoSX solution were first recovered via a carbonation process, producing a Nickel-Cobalt carbonate precipitate (Ni-Co cake). The resulting Ni–Co carbonate intermediate was dissolved in sulfuric acid to generate an aqueous solution containing Ni^{2+} and Co^{2+} ions. Impurity removal was subsequently carried out using solvent extraction with di-(2-ethylhexyl) phosphoric acid (D2EHPA) to selectively eliminate divalent and trivalent impurities such as Ca^{2+}, Mg^{2+}, and Fe^{3+}.

Following purification, cobalt was selectively separated from nickel using Cobalt Extractant, yielding a nickel-rich sulfate solution. Nickel was then recovered as nickel hydroxide ($Ni(OH)_2$) through precipitation, followed by redissolution in sulfuric acid to form a purified nickel sulfate solution. Finally, controlled evaporation and cooling were employed to achieve the crystallization of nickel sulfate hexahydrate ($NiSO_4 \cdot 6H_2O$). The proposed process demonstrates an effective and sustainable pathway for producing battery-grade nickel sulfate from secondary resources, contributing to the circular economy of lithium-ion battery materials.

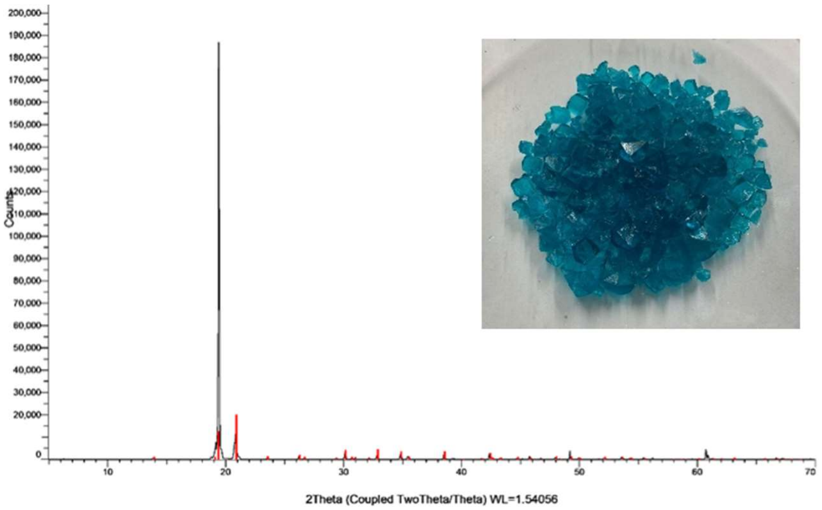

Figure 1. XRD analysis result of Nickel Sulfate Hexahydrate Crystals

This Study by Eti Gubre (Eti Bakır Inc) was funded by the Horizon Europe Programme under Agreement No. 101137771, Action entitled “Sustainable Technologies for Reducing Europe’s battery raw MaterialS dependence”, or “STREAMS”.

Nanoscale Imaging of Anode-Free Plating/Stripping

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K. Kataoka,[6] E. Vasco,[5] K. Nikolowski,[4] D. Rettenwander,[3] E.G. Michel,[2,7], M.A. Niño,[1] M. Foerster,[1] C. Polop[2,7]

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Achieving reversible anode-free solid-state batteries critically depends on controlling alkali-metal nucleation, growth, and dissolution at buried solid-electrolyte/current-collector interfaces. However, the nanoscale mechanisms governing plating and stripping remain largely inaccessible to conventional operando probes. Here, we introduce virtual-electrode low-energy electron microscopy (VE-LEEM), combined with photoemission electron microscopy (PEEM) and atomic force microscopy (AFM), to directly visualize anode formation and dissolution with nanoscale resolution (Fig.1a,b). Using this platform, we resolve the early stages of Li and Na plating (Fig.1c-f), showing that both systems converge toward common dynamic scaling regimes once a continuous metal layer is established, despite following distinct coarsening pathways governed by surface energetics. In contrast, stripping proceeds through asymmetric mechanisms dominated by grain-boundary unzipping and cluster decay, leaving behind a persistent interfacial residual layer. These observations reveal interfacial and cohesive energetics as fundamental constraints on reversibility in anode-free architectures [1].
Building on this approach, we discuss ongoing experiments exploring how ultrathin metallic interlayers and temperature modify the earliest stages of anode formation. VE-LEEM observations indicate that both parameters tune interfacial energetics and diffusion pathways, potentially reshaping nucleation density and early coalescence modes. Overall, this work establishes VE-LEEM as a versatile platform to resolve buried electrochemical interfaces at the nanoscale and provides an energetic framework to guide the rational design of durable, high-energy anode-free solid-state batteries.

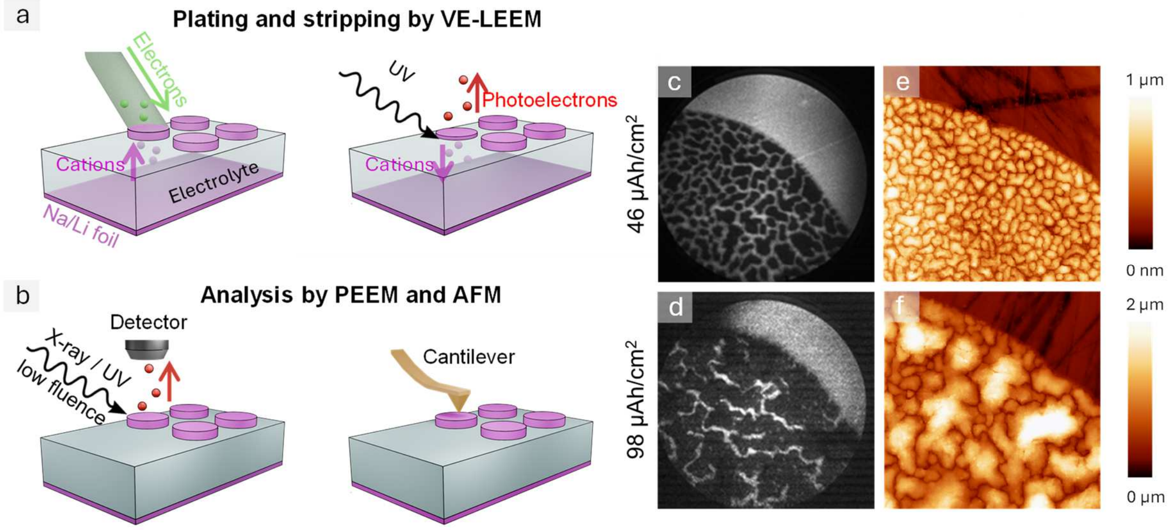

Fig. 1. Schematic of the VE-LEEM approach to study the anode growth at the nanoscale (a,b), XAS-PEEM images (c,d) and AFM topographies (e,f) revealing 3D cluster formation.

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Evaluation of Different (Quasi-)Reference Electrodes for Highly Concentrated Aqueous Electrolytes

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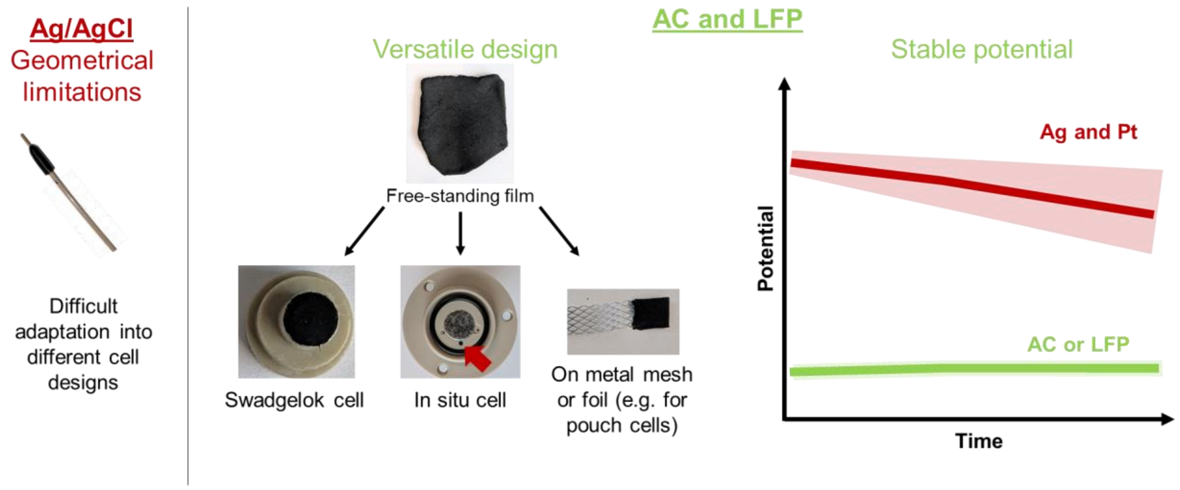
The choice of the reference electrode can be crucial for electrochemical measurements. Its main requirements are a stable half-cell potential as well as a low reactivity towards the electrolyte. While different approaches have been made for non-aqueous batteries including Li metal, but also partially delithiated $Li_4Ti_5O_{12}$ (LTO) and $LiFePO_4$ (LFP)[1], Ag|AgCl reference electrodes are mainly used for aqueous energy storage systems. While Ag|AgCl reference electrodes usually deliver a stable potential and leakless options for the use in organic or hybrid electrolytes are commercially available, their geometry is often designed for cells with large amounts of electrolyte and adaptation into other cell systems can be difficult and lead to lager error margins (e.g. up to ±20 mV for leakless Ag|AgCl reference electrodes were reported [2]). This can be especially relevant for *operando* cells, which often have limited variability regarding space, why in these cases often quasi-reference electrodes such as Ag wires are used[3], which can suffer from limited reproducibility[4].

In this study we focused on the evaluation of different alternative reference electrode materials which allow for a more versatile electrode setup and application in different cell types. Their suitability for aqueous imide-based electrolytes with different concentrations including highly concentrated electrolytes are tested using different internal redox couples. The tested materials include activated carbon (AC)[5], as well as partially delithiated LFP[6], showing a stable potential over time and a great versatility regarding shape, allowing their application in different cell formats.



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Scalable on-site direct recycling: returning LFP production scrap into functional active material

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Production scraps are currently a significant feedstock for battery recycling and as they have not undergone in-use degradation, they are ideal for nondestructive direct recycling [1]. However, reintegration of directly recycled scrap into new cells requires further validation [2]. This study evaluates strategies for on-site, low-temperature (200°C–600°C) direct recycling of lithium iron phosphate (LFP) production scrap in air and nitrogen environments. Optimal recycling conditions identified via technoeconomic analysis were used to recycle cathode scraps that were then comprehensively characterized. Coin cells were fabricated using 100%, 50%, and 30% recycled active material blended with virgin LFP. Material cost and environmental impacts for slurry production were assessed for each slurry formulation.

Results indicate that LFP production scrap recycled at 400°C in N_2 and 200°C in air can be directly reintegrated into new cells. Recycling at 400°C in N_2 maintained high capacity even at 100% recycled content, while recycling at 200°C in air delivered excellent performance at 30% blending, regardless of the residual PVDF in the recycled cathode structure (Figure 1A). Incorporation of recycled scrap also reduced the cost and environmental impact of slurry preparation for both conditions (Figure 1B).

Given the promising electrochemical performance and the associated economic and environmental benefits, the proposed direct recycling process demonstrates potential for industrial implementation.

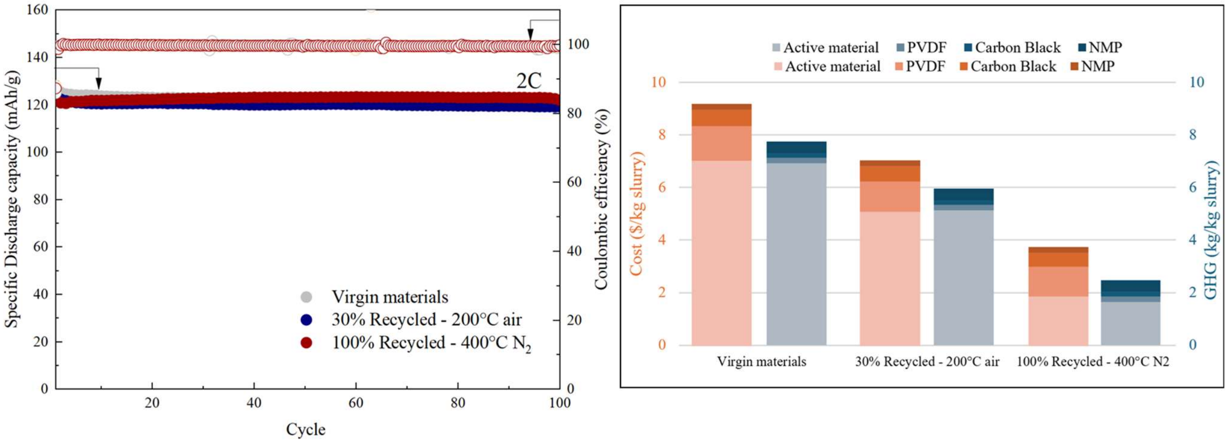

Figure 1. A) Cycling performance and B) economic and environmental analysis of 30% 200°C air and 100% 400°C N_2 recycled material compared to virgin materials.

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Degradation Pathways in High-Voltage Layered Sodium-Ion Cathodes

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High-voltage layered sodium-ion battery (SIB) cathodes are attractive for next-generation battery technologies because they can deliver high energy density through combined cationic and anionic redox activity. However, their degradation mechanisms remain controversial, which hinders the rational design of durable cathode materials. Here, we show that the dominant degradation pathway is not fixed, but strongly depends on the applied cycling current.

Using a compositionally controlled series of Sc-, Sc-Ti-, and Sc-Ti-B-doped O3-type layered oxides, we combine various advanced characterizations, such as operando X-ray diffraction, X-ray absorption spectroscopy, resonant inelastic X-ray scattering, electron microscopy, and theoretical calculations to identify two distinct degradation mechanisms. At low current, oxygen redox remains active and degradation is mainly associated with oxygen-loss-induced instability. At high current, oxygen redox becomes kinetically suppressed and degradation is governed primarily by structural evolution through simplified phase-transition pathways.

These results reconcile previously conflicting interpretations of degradation in high-voltage layered sodium cathodes by establishing a current-dependent mechanistic guideline. The work shows that degradation pathways must be evaluated under realistic operating conditions rather than inferred from a single cycling mode. These findings clarify how operating conditions influence cathode degradation and provide a basis for designing high-voltage sodium-ion cathodes with improved durability.

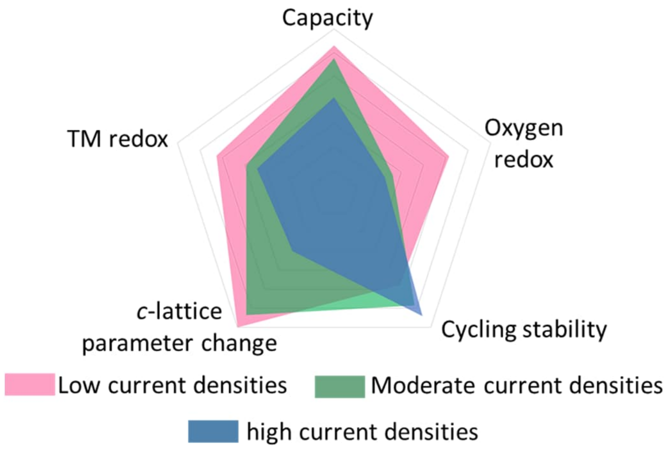

Figure 1. Schematic comparison of the relative contributions of structural evolution and oxygen-redox-related degradation in layered sodium-ion cathodes under different cycling conditions.

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Homogenization of LIBs: a fast model for state-of-charge in-line monitoring

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Lithium-ion batteries (LIBs) offer high energy density, low self-discharge, and decreasing production costs, but their performance and lifetime are often limited by local inhomogeneities, including non-uniform current distribution and concentration gradients. Electrode morphology strongly influences these effects, yet it is frequently oversimplified in conventional models because resolving realistic pore-scale geometries is computationally expensive.

This work builds a rigorous link between microscopic transport physics and macroscopic battery-scale modelling by applying homogenization via multiple-scale expansion to a lithium-ion cell [1]. Starting from pore-scale governing equations for mass and charge transport in the electrolyte and solid phases, we derive an upscaled macroscopic formulation in which the complex microstructure is replaced by effective transport properties. The approach exploits scale separation between a characteristic macroscopic length L (electrode/cell scale) and a microscopic length l (particle/pore scale). Under the common condition $L \gg l$, the homogenized model is significantly faster than pore-resolved simulations while introducing a controlled approximation error of order $O(l/L)$.

The equations are cast in dimensionless form to identify relevant Péclet and Damköhler regimes and to define conditions for homogenization. Effective parameters are then obtained by solving closure problems on a periodic unit cell representative of the electrode morphology, yielding effective diffusivity and electrical conductivity for both liquid and solid phases and naturally accounting for porosity and tortuosity. For graphitic anodes, where particle anisotropy can affect transport pathways, the microstructure can be generated using flattened ellipsoidal particles informed by experimental particle size distributions and SEM-derived aspect ratios, providing a more realistic alternative to spherical particles.

The resulting homogenized model is implemented and verified against a fully resolved 4D pore-scale simulation on the corresponding reconstructed microstructure. Figure 1 briefly illustrates the general workflow of this project. The homogenized formulation reproduces the main pore-scale trends with substantially reduced computational time and resources, enabling rapid parametric studies of morphology and operating conditions. Overall, homogenization provides a fast yet predictive framework for LIB simulations, supporting BMS implementation and fast in-line prediction for state-of-charge monitoring.

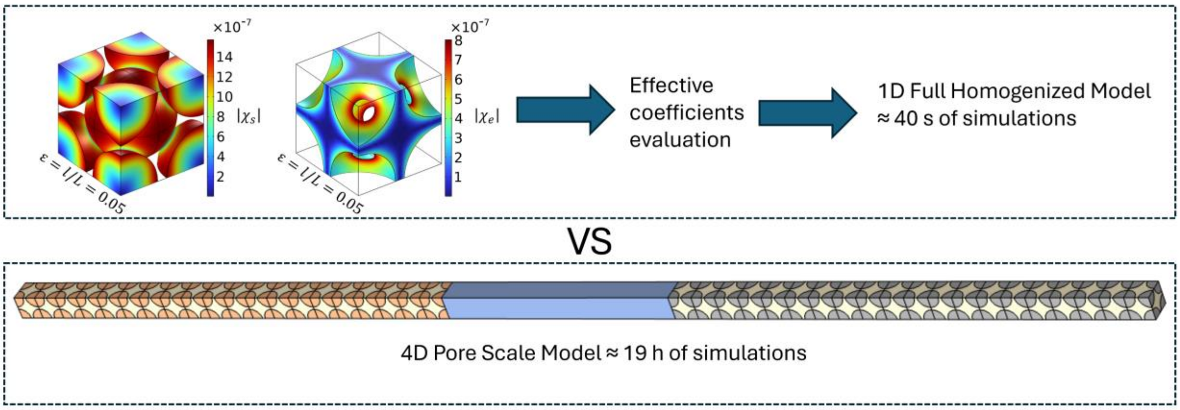

Figure 1. Workflow of the comparison between homogenized model and pore scale model.

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IN-SITU UV CURED DEEP EUTECTIC SOLVENT-BASED GEL POLYMER ELECTROLYTE FOR LI METAL BATTERIES

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The global rise in energy consumption has driven research towards safer, more efficient energy storage systems. The commonly employed Li-ion batteries are prone to safety risks due to flammable liquid organic solvents, which can evaporate or leak and pose hazards in case of a short circuit. Deep eutectic solvents (DES) are a relatively new family of solvents with room temperature molten salt behaviour and several advantageous characteristics in the context of Li-ion batteries electrolytes. Their low vapour pressure and non-flammability, as well as good electrochemical performances, render them interesting candidates for application in contact with Li metal [1]. In this work, a DES composed of trifluoroacetamide (TFA) and lithium bis(trifluoromethanesulfonyl) imide (LiTFSI) is prepared and thoroughly characterized. A gel polymer electrolyte (GPE) is subsequently developed with the focus on the up-scalability of the GPE production. The polymeric matrix, composed of polyethylene glycol diacrylate (PEGDA) and pentaerythritol tetrakis(3-mercaptopropionate) (T4), is crosslinked via thiol-ene polymerization directly in the DES solution, demonstrating a fast, cheap and easy reaction. The thiol-ene mechanism, moreover, avoids the sensitivity towards O_2 of the otherwise commonly employed UV-mediated radical polymerization and enables the crosslinking reaction to be carried out in a dryroom [2]. The precursor solution is deposited directly on the surface of the investigated cathodes and irradiated with 10 W UV light to obtain a GPE with excellent interfacial contact. The calendering of the cathodes is investigated to assess the dependence of the electrochemical performances of the crosslinked GPE on the different cathodes surface morphologies. Moreover, the addition of 10% of a mixture of ethylene carbonate and diethyl carbonate in the DES (DES10) considerably improves the electrochemical performances of the GPEs, increasing the ionic conductivity from $6.36 \cdot 10^{-4}$ S cm^{-1} to $1.25 \cdot 10^{-3}$ S cm^{-1} at room temperature and enabling a long lifetime of 220 cycles with a high specific capacity of 164 mAh g^{-1} when cycling in a Li||LFP cell at 1C and at room temperature.

This publication is part of the project PNRR-NGEU which has received funding from the MUR – DM 352/2022.

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Batteries as Key Enablers for Virtual Power Plants: Development of a Large-Scale VPP Framework in Portugal

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The increasing penetration of distributed renewable energy sources introduces new operational challenges for power systems, particularly regarding flexibility, stability, and efficient market participation. Virtual Power Plants (VPPs) have emerged as a promising approach to aggregate distributed energy resources such as generation, energy storage systems, and controllable loads, enabling their coordinated operation as a single flexible entity [1,2].

This work presents the development of a large-scale VPP framework in Portugal within the *Plano de Recuperação e Resiliência* (PRR) project, where batteries play a central role in enabling flexibility and market participation. The proposed architecture integrates photovoltaic generation assets, battery energy storage systems (BESS), and distributed monitoring infrastructure through an IoT-based communication platform and cloud computing environment. Real-time measurements from energy and environmental sensors are aggregated to support forecasting and optimization processes. Figure 1 illustrates the conceptual architecture of the VPP developed in the project, highlighting the interaction between distributed assets, communication infrastructure, and the centralized management system. The operational strategy of the VPP is formulated as a mixed-integer linear programming (MILP) optimization problem that schedules generation, consumption, and storage resources with a 15-minute granularity. The algorithm aims to minimize operational costs while enabling participation in the Iberian electricity market (MIBEL), particularly the day-ahead market.

Beyond the technological implementation, the project also addresses regulatory challenges associated with the deployment of VPPs in Portugal, where current legislation mainly focuses on energy communities. By demonstrating the technical and operational feasibility of geographically distributed VPPs, this work contributes to the discussion on regulatory evolution and highlights the role of battery systems as key enablers for future decentralized energy systems.

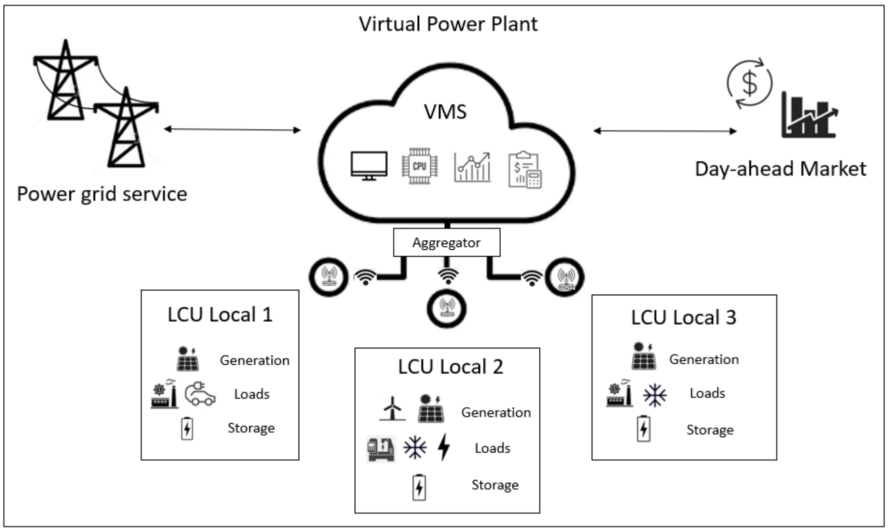

Figure 1. Conceptual architecture of the Virtual Power Plant

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Microwave-assisted synthesis of different metal sulphides for polysulphides anchoring and conversion in lithium-sulphur batteries

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Nowadays, lithium-ion batteries (LIBs) are the most widely used and reliable energy storage technology, but they also have drawbacks that hinder their ability to meet the rising demand for energy storage devices. Consequently, the study and development of alternative post-lithium-ion technologies is of crucial importance to make them commercially viable in the future. Among these systems, lithium-sulphur batteries (Li-S) are one of the most interesting due to the high theoretical specific capacity of sulphur (1672 mAh g^{-1}). However, the practical application of Li-S is still strongly limited by some issues, such as the sluggish sulphur redox kinetics and the so-called *shuttle effect*, which is caused by the diffusion of soluble lithium polysulphides formed during cell discharge. [1] To solve this problems, different materials capable of binding the soluble polysulphide species formed during cell discharge and catalysing their reduction reactions have been proposed as both sulphur host and catalytic additives. Among them, metal sulphides are a very promising class of materials thanks to their higher electronic conductivity as compared to oxides, together with their affinity and catalytic activity towards sulphurised species. [2]

The present work aims at studying metal sulphides as potential catalysts for sulphur reduction reactions, exploiting a microwave-assisted hydrothermal synthesis approach. Water is a green and eco-friendly solvent and can be easily separated from the obtained metal sulphides since they have very low solubility product constants and quickly precipitate in the reaction media once formed. The use of microwaves, instead, shortens the required reaction time by providing a homogeneous temperature distribution throughout the whole reaction media, which minimises the formation of thermal gradients, reduces the formation of unwanted phases, and enhances the process reproducibility. Moreover, the obtained products are characterised by high purity and crystallinity, and a fine control of their particle size and morphology is possible [3]. In particular, three different metal sulphides, tin, manganese and zinc-based, were synthesized using metal acetates or chlorides and thiourea as precursors and characterised by means of both physico-chemical and electrochemical techniques. The main objective was to study their structural and morphological properties together with their affinity, interaction and catalytic activity towards lithium polysulphide species. Then, the effect of these metal sulphides on cell performance was evaluated by implementing them in the cathode formulation at coin cell level. Different approaches have been evaluated, from the simple addition of the catalysts during the electrode preparation to their mixing with the carbon matrix used as sulphur host prior to sulphur infiltration.

The obtained results showed the different behaviours of the metal sulphides in polysulphides anchoring and conversion, and in Li_2S deposition process. In full cell studies, instead, the simple addition of the catalyst during electrode preparation led to poor performances due to their bad distribution within the carbon/sulphur composite and, thus, an insufficient interaction with the active material. In contrast, the sulphides mixing with carbonaceous phase before the melt diffusion of sulphur in the material revealed delivered good results in terms of rate capability tests and galvanostatic cycling, laying the foundations for further studies which include a better understanding of the catalytic mechanisms through *in operando* Raman spectroscopy, the direct synthesis of catalysts on sulphur host materials to enhance homogeneity and electronic conductivity and the tailoring of catalyst properties exploiting the peculiar features of different metals.

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MODELING THE LIMITED MASS TRASPORT OF POLYSULFIDES TO UNDERSTAND CAPACITY LOSS DURING CHARGE AND DISCHARGE

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In the latest years lithium–sulfur (Li–S) batteries have emerged as a promising alternative to conventional lithium-ion batteries due to their potential for significantly higher energy density and lower material costs[1]. However, despite their advantages, Li– S batteries face several challenges to be commercialized, especially rapid capacity fade and complex reaction mechanisms. To address these issues and optimize battery performance, continuum modeling has become an essential, enabling a deeper understanding of the key physicochemical processes occurring within the battery. Major concern have been placed on irreversible phenomena such as shuttling, however the intrinsic nature of lithium sulfur batteries leads also to reversible capacity loss that limits their performances, especially at higher current[2]. Polysulfides during cycling are constantly driven towards and backwards the porous cathode due to concentration gradient and migration. The kinetic mismatch between mass transport and electrochemical activity is responsible for the so called reversible losses. The electrochemical model presented is a 1D homogeneous model developed in COMSOL Multiphysics 6.2, based on the porous electrode theory, using Nernst-Plank equation to describe the mass transport of dissolved species. The purpose of the model is to understand the impact of Li+ diffusivity on both reversible and irreversible losses, and so in which direction we should look forward.

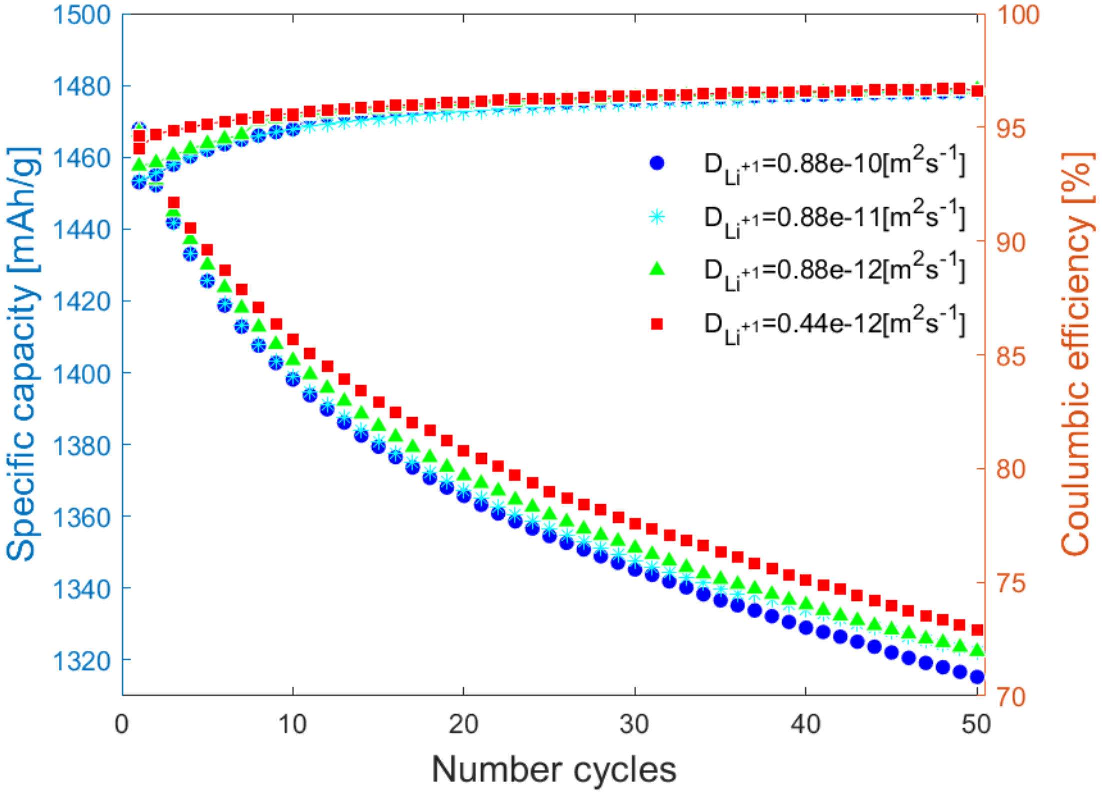

Figure 1. Specific capacity/Coulumbic efficiency vs number cycles.

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Understanding Precipitation of Iron Phosphate from Chloride Containing Battery Leachate

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Acid leaching of black mass is inevitably the first hydrometallurgical step in battery recycling, which in the case of LFP black mass, leads to highly acidic solutions containing the low value metal Fe^{3+}, in our case as chlorides. Treating such streams and recovering battery grade precursor materials is important to enable circular process. It will address the growing supply demand for battery materials amid Europe's push for domestic critical raw material. Iron phosphate ($FePO_4$) precipitation from this leachate is a key step for recycling $LiFePO_4$ (LFP) cathode materials, but obtaining it as a single, clean phase from leached solution is challenging as coprecipitation happens in presence of other cations. In this work, we studied the $FePO_4$ precipitation from chloride-based LFP leachates containing approx. 2000ppm Fe^{3+}, 150ppm Li^+, 70ppm Al^{3+}, and 5000ppm PO_4^{3-}, with a focus on how phosphate, lithium and aluminum concentrations influence impurity formation. We adjust the pH of leachate using LiOH, NaOH and NH_4OH solution added in a semi-continuous manner in the leachate in the range 1.0–2.0 and also diluted the leachate with water to change metal concentrations without adding extra cations. X-ray diffraction analysis shows that, in concentrated solutions, increasing pH leads to the co-precipitation of Lithium iron phosphate ($Li_3Fe_2(PO_4)_3$), sodium iron phosphate ($Na_3Fe_2(PO_4)_3$) and aluminum phosphate ($AlPO_4$) together with the desired $FePO_4$. Dilution with water, however, significantly suppresses these impurity phases and favors the formation of pure $FePO_4$. This approach creates a challenge, as it dilutes the Li^+ ions in the effluent stream, complicating its recovery in the downstream processing stages. These observations suggest that high Li^+ concentration stabilizes lithium-rich iron phosphate phases, while Al^{3+} strongly competes for phosphate to form $AlPO_4$. By systematically varying Li^+, Al^{3+} and PO_4^{3-} concentrations via controlled dilution and base addition, we aim to find concentration–pH range where impurity precipitation is minimized and $FePO_4$ purity is maximized. This work will provides an understanding that will help to select appropriate step after leaching, based on leachate composition for producing battery-grade $FePO_4$ from chloride-leached LFP stream without the impurities as part of EU-Revitalise project.

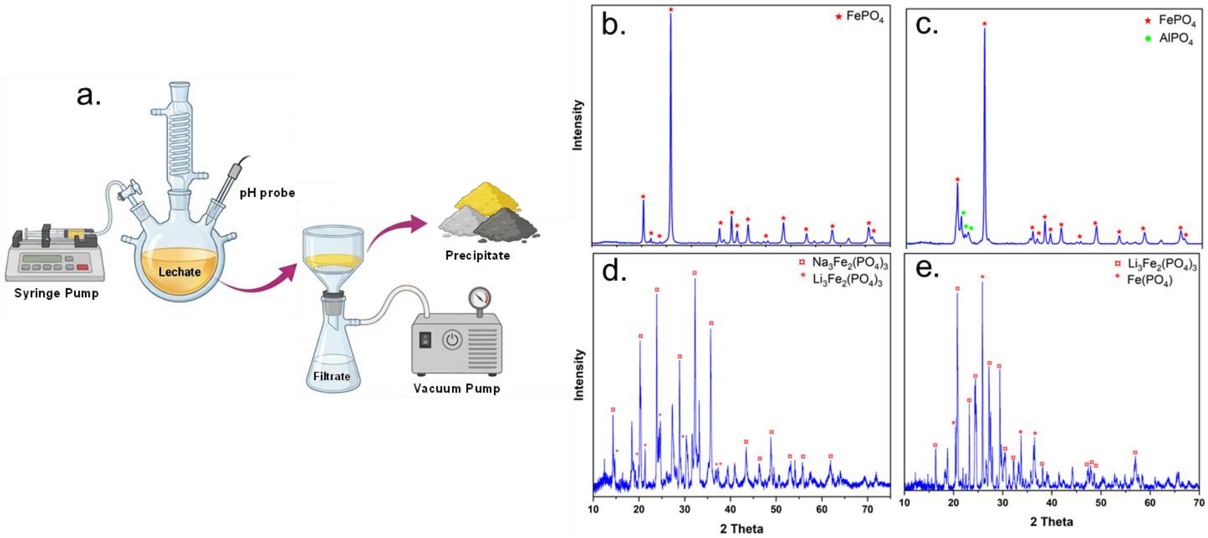

Figure 1. (a) Schematic of Process, XRD of (b) $FePO_4$ precipitate from water dilution (c) $AlPO_4$ (impurity) and $FePO_4$ precipitate from water dilution (d) $Na_3Fe_2(PO_4)_3$ and $Li_3Fe_2(PO_4)_3$ precipitate from NaOH addition (e) $Li_3Fe_2(PO_4)_3$, and $FePO_4$ precipitation by LiOH addition.

ON NEW STRATEGIES TO PUSH THE STORAGE PERFORMANCE OF SODIUM SALTS OF TEREPHTHALIC ACIDS

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One of the most promising technologies to support lithium-ion batteries (LIB) to follow the growing demand of electrochemical- storage devices, especially for stationary applications, are sodium-ion batteries (NIB). One of the limiting factors in the development of this new type of accumulator is the validation of a unique anode material that is capable of being synthesized in a sustainable and controlled way to assure an optimal microstructure and reproducible high storage performance over time. Hard Carbons are currently the most exploited solution as anodes for NIBs both on lab scale tests and in industrial products that are starting to become available on the market. The performance of these compounds is strongly linked to the precise control of the synthesis process as well as to the origin of carbonaceous precursors.

Another interesting family of organic materials for this application are those derived from the sodium salt of terephthalic acid (Na_2TP). This compound combines a good theoretical capacity (255 mAh/g) with a high global production of its precursor (≈100M tons/year), terephthalic acid (PTA), since it is used as a monomer in the production of widely used plastic materials. On one hand, the ease of preparation/handling and the low cost make Na_2TP an attractive option but, on the other hand, the difficulty to stabile its storage performance has always limited this compound like a good alternative.

Despite the extensive literature on the use of Na_2TP as a NIB anode, numerous strategies can still be explored to stabilize the performance, including: the effect of new functionalizations of the benzene ring and the development of composites with new conductive 2D materials. Specifically, this work investigates the effect induced both by the presence of –OH groups as functionalizing agents of the benzene ring (either single or double substitution) and by the possibility of using lamellar carbides Ti_3C_2–Tx, known as MXenes, to create a conductive network capable of stabilizing storage performance (see Figure 1).

From the preparation of the sodium salts of the substituted acids and their characterization, through various approaches to disperse MXenes to form homogeneous composite materials, the research activities were focused on validation of these strategies as functional and possibly synergistic approaches to stabilize storage performance. Supporting the interpretation of electrochemical cycling tests in half-cells vs. Na/Na^+ with in-operando measurements (e.g. Raman, XRD), as well as through post-mortem electrode analyses, made it possible to identify some optimal process parameters on which to focus attention for improving performance over time.

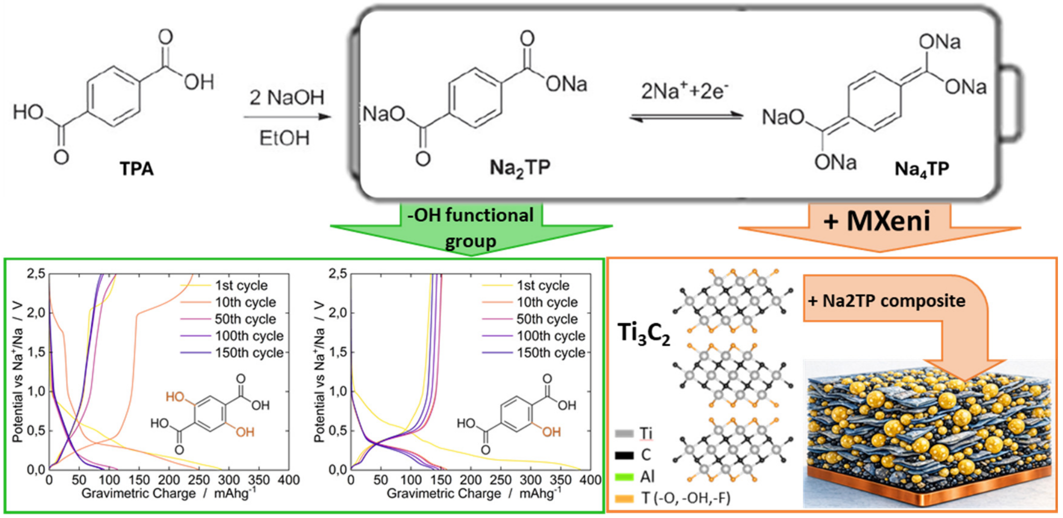

Figure 1. Na2TP electrochemical sodium ion storage mechanism and RSE's strategies to stabilize storage performance based on new functionalization or composite with MXenes.

Unlocking Accurate State Estimation in Silicon–Graphite Batteries through AI-Corrected OCV Modeling

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Degradation of silicon–graphite (SiG) composite anodes induce systematic drift in the open-circuit voltage (OCV) response of lithium-ion cells, thereby reducing the fidelity of equivalent-circuit-model (ECM)–based state estimation [1]. In SiG systems, the OCV–SOC relationship is inherently state-of-health dependent, as progressive loss of electrochemically active silicon and changes in lithiation pathways alter the effective anode thermodynamic potential and, consequently, the cell-level OCV profile [2].

In this work, an AI-corrected OCV modeling approach is proposed to enhance ECM-based state estimation in commercial SiG cells. Commercial cylindrical Li-ion cells (Molicel M35A, 3.5 Ah) with SiG anodes were subjected to a controlled degradation cycling study across defined SOC windows to induce differentiated silicon aging. OCV profiles were acquired under near-equilibrium conditions using minimal excitation current to suppress polarization effects. The results confirm that OCV evolution is predominantly governed by silicon-related degradation mechanisms within the composite anode. The resulting dataset was used to train an AI-based correction layer that adaptively updates the OCV characteristic employed by the ECM. The methodology was validated for SOC estimation, demonstrating a quantifiable improvement in estimation accuracy compared to a fixed-OCV implementation. The proposed framework provides a scalable pathway toward degradation-aware, high-accuracy battery management systems for silicon–graphite lithium-ion technologies.

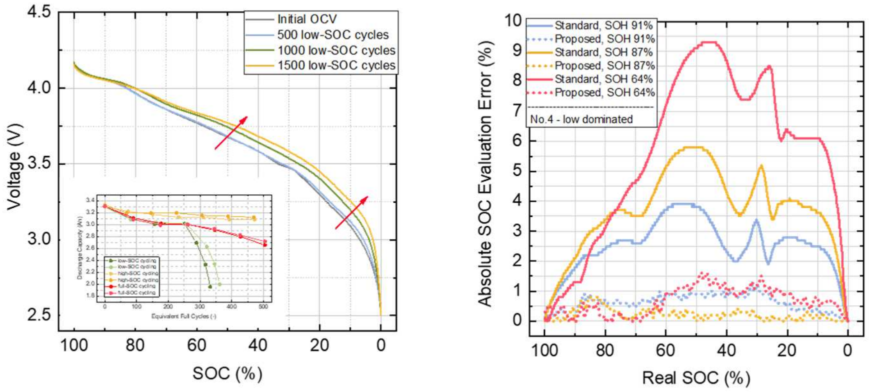

Figure 1: Evolution of OCV during cycling-induced degradation and reduction of SOC estimation error across different SOH levels using standard OCV and AI-generated proposed OCV curves

Acknowledgements

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Biopolymer-Based Gel Electrolytes for Stabilizing Zn Anodes in Aqueous Zn-Ion Batteries

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The Green Deal sets ambitious targets for climate neutrality by 2050, driving the need for safe, sustainable, and cost-effective electrochemical energy storage systems. Among emerging technologies, aqueous Zn-ion batteries are attracting growing interest due to their intrinsic safety, low cost, high ionic conductivity, and the natural abundance of zinc. However, their practical application is still limited by critical issues at the Zn anode, including limited plating/stripping reversibility, unstable interphases, non-uniform deposition and parasitic side reactions. In particular, the hydrogen evolution reaction (HER) is a major challenge in aqueous systems, as it lowers coulombic efficiency, alters the interfacial environment and accelerates anode degradation. In this context, gel polymer electrolytes (GPEs) represent a promising strategy to address these limitations [1]. By combining the high ionic conductivity of liquid electrolytes with the mechanical stability of polymer networks, GPEs can promote more homogeneous Zn deposition, mitigate interfacial instability, and suppress parasitic reactions such as HER. In particular, biopolymer-based GPEs, especially those based on agarose and prepared through simple and scalable routes, have shown strong potential in this field. Agarose-based GPEs containing simple $ZnSO_4$ electrolytes have demonstrated higher efficiencies than the corresponding liquid electrolyte even under severe operating conditions, together with a wider electrochemical stability window and markedly improved plating/stripping stability over extremely long cycling times, reaching thousands of hours[2]. In this framework, differential electrochemical mass spectrometry (DEMS) plays a key role, as it enables the direct and operando investigation of gas evolution phenomena during battery operation. In particular, DEMS provides a powerful tool to specifically identify and monitor HER, thus offering direct insight into one of the most detrimental parasitic reactions affecting Zn anodes[3]. Its application has highlighted the beneficial effect of agarose-based GPEs in mitigating hydrogen evolution, further supporting their potential for the development of more stable aqueous Zn-ion batteries.

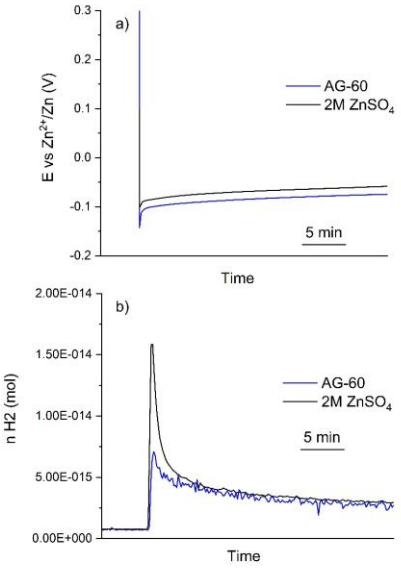

Figure 1. a) Potential vs time behavior during zinc deposition. b) H_2 evolution monitored by DEMS during zinc deposition.

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ENERGY-EFFICIENT FABRICATION OF GRAPHITE ANODES VIA SEMI-DRY COATING AND GREEN BINDER TECHNOLOGY

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Traditional wet-coating processes for lithium-ion battery electrodes typically rely on polymer binders such as polyvinylidene fluoride (PVdF) and toxic organic solvents like N-methyl-2-pyrrolidone (NMP), raising significant environmental and safety concerns. To address these issues, alternative fabrication strategies are being explored to enable more sustainable, energy-efficient, and scalable production routes. In this work, an eco-friendly binder system is introduced as a replacement for PVdF/NMP, combined with a semi-dry coating approach that minimizes solvent usage and significantly reduces drying requirements. The resulting graphite-based anode (S-G-Anode), fabricated from commercial graphite powder, exhibits improved mechanical flexibility, strong structural integrity, and enhanced adhesion. Material characterization using X-ray diffraction (XRD), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM) confirms the high-quality and uniform coating achieved through the semi-solventless process. Electrochemical performance was assessed via cyclic voltammetry and galvanostatic charge–discharge testing at various C-rates. The S-G-Anode delivers a high specific capacity of 371 mAh g^{-1} at C/20 in LP30 electrolyte and demonstrates good cycling stability, with only a 14.3% capacity loss as the rate increases to 2C. Notably, this work has been patented (ref. WO2025252882A1), highlighting its innovation and potential industrial relevance. Overall, the proposed approach represents a promising pathway toward greener and more sustainable lithium-ion battery manufacturing.

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THE NEXTCELL PROJECT: TOWARD THE NEXT GENERATION OF LITHIUM-ION BATTERY CELLS

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The increasing need for affordable, safe, and easy-to-use electric mobility solutions is creating strong pressure for breakthrough advancements in lithium-ion battery (LIB) materials and cell design.

The primary objective of NEXTCELL is to develop an innovative jellified LIB architecture that incorporates material-level improvements in all key cell components. By jellifying the electrodes and pairing them with a high-voltage-stable jellified electrolyte, the project aims to realize a fully jellified cell concept capable of operating up to 5 V vs. Li^+/Li, while preserving excellent electrochemical performance and enhanced safety standards. To achieve this, the project follows a multidisciplinary approach that integrates advanced materials engineering, physicochemical and electrochemical analysis, cell prototyping, modeling activities, and a thorough evaluation of safety, sustainability, and economic viability.

Through this strategy, NEXTCELL builds a strong and accelerated R&D framework dedicated to next-generation energy storage systems. The proposed technology streamlines manufacturing by removing the need for solvent evaporation and the electrolyte filling stage. In addition, the fully jellified configuration promotes intrinsic safety by eliminating low-boiling-point substances, thereby lowering flammability hazards. Moreover, the novel processing pathway is expected to cut production energy consumption by roughly 50%.

The consortium unites prominent industrial actors and research institutions spanning the entire battery value chain. Industrial partners provide know-how in large-scale manufacturing, automotive qualification, and advanced material production, while research organizations contribute high-level expertise in materials development, electrochemical testing, modeling, and sustainability analysis.

By integrating material innovation, optimized processing, inherent safety features, and sophisticated modeling tools, NEXTCELL strengthens Europe’s leadership in high-voltage, high-capacity, and sustainable lithium-ion battery production, fostering the rapid market uptake of next-generation energy storage technologies.

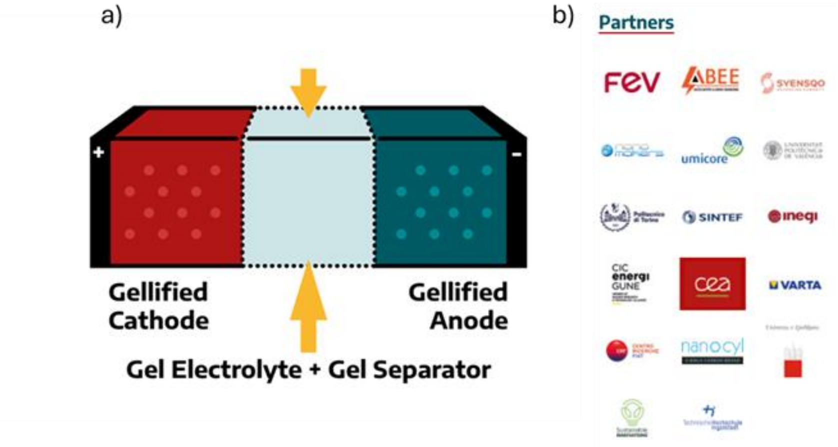

Figure 1. a) Jellified concept. b) NEXTCELL project partners

NEXTCELL project has received funding from the European Union. Project ID 101069910. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Climate, Infrastructure and Environment Executive Agency (CINEA) Neither the European Union nor CINEA can be held responsible for them.

A preliminary assessment of gel-polymer electrolytes for potassium-ion batteries

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The transition toward climate neutrality is accelerating the large-scale deployment of renewable energy systems and the electrification of transport, thereby intensifying the demand for sustainable, cost-effective, and high-performance energy storage technologies. Although lithium-ion batteries (LIBs) currently dominate the market, their long-term scalability is constrained by reliance on critical and geographically concentrated raw materials. In this context, potassium-ion batteries (PIBs) are emerging as a promising alternative, as they are based on earth-abundant and non-critical elements, thus offering improved resource sustainability and security.

A distinctive advantage of PIB technology lies in the compatibility of potassium with aluminium current collectors, as potassium does not form intermetallic alloy with aluminium. This enables the use of lightweight, low-cost aluminium collectors for both electrodes, simplifying cell design and reducing manufacturing costs. Furthermore PIBs, may exhibit enhanced rate capability, since K^+ ions display higher diffusion coefficients in liquid electrolytes compared to Li^+ and Na^+, attributed to their weaker Lewis acidity and reduced solvation strength. Graphite is capable of reversibly intercalating K^+, facilitating industrial scalability through compatibility with existing manufacturing infrastructure, while more sustainable carbon-based anode materials represent additional viable alternatives [1].

Despite these advantages, conventional PIB configurations typically rely on flammable liquid electrolytes, which raise significance safety concerns including leakage, volatility, thermal runaway, and dendrite-induced short circuits. Polymer-based electrolytes offer a safer alternative due to their reduced flammability, improved mechanical robustness, lightweight nature, and ease of processing into self-standing membranes. While solid polymer electrolytes mitigate many safety risks, their practical implementation is often hindered by limited ionic conductivity at ambient temperature [2]. Gel polymer electrolytes (GPEs) provide a promising compromise by combining the high ionic conductivity of liquid electrolytes with the mechanical stability of polymer networks, thereby enabling safer and high-performance PIB systems [3].

This work focuses on the development, physicochemical and electrochemical characterization of GPEs specifically tailored for potassium-ion batteries. The study aims to optimize ionic conductivity, electrochemical stability, and mechanical integrity while prioritizing material sustainability. By integrating abundant electrode materials with intrinsically safer electrolyte architectures, this research contributes to the development of next-generation PIBs aligned with the long-term sustainability and safety objectives.

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Acknowledgments

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Optimizing Waterborne LNMO Cathode Production: Evaluating Alternative Binders for Enhanced Electrochemical Performance and Processability

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Lithium-ion batteries (LIBs) play a key role in the global transition toward sustainable energy, particularly in electric transportation and large-scale energy storage. As demand for environmentally responsible technologies increases, improving the sustainability and scalability of cathode manufacturing processes has become a major challenge. Among next-generation cathode materials, Lithium Nickel Manganese Oxide (LNMO) represents a promising high-voltage alternative to conventional Nickel Manganese Cobalt (NMC) chemistries. Its cobalt-free composition enhances sustainability while eliminating reliance on cobalt-related economic and ethical constraints. In parallel with material development, increasing attention is being devoted to waterborne electrode manufacturing as a greener alternative to conventional organic solvent-based processes. Within this framework, the development of efficient water-compatible binders is essential to ensure both electrode processability and electrochemical stability. This study investigates the role of alternative binders in waterborne LNMO cathode fabrication, benchmarking their performance against the widely used Carboxymethyl Cellulose (CMC). Three candidates – Guar Gum (GG), Lithium Polyacrylate (Li-PAA), and Sodium Alginate (ALG) – are systematically evaluated, both as standalone binders and in blended formulations, to assess their potential for improving cathode performance. A Design of Experiments (DoE) methodology is adopted to optimize binder selection and formulation, targeting improved electrochemical stability while maintaining high slurry processability. The study integrates process characterization, through rheological analyses (shear rate, amplitude, and frequency sweeps), chemical and compositional investigation, using Fourier Transform Infrared Spectroscopy (FTIR), X-ray Fluorescence (XRF), and Inductively Coupled Plasma (ICP) techniques, and electrochemical evaluation, including galvanostatic cycling [Figure 1] and Potentiostatic Electrochemical Impedance Spectroscopy (PEIS). Preliminary results demonstrate that binder chemistry strongly affects both slurry behavior and electrochemical response. The findings highlight the potential of alternative binder systems and optimized formulations to enhance LNMO cathode performance within a fully waterborne processing route. These results contribute to the development of more sustainable and scalable lithium-ion battery manufacturing strategies.

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Funded by the European Union under grant agreement N° 101069707 (project GIGAGREEN) and N° 101135486 (project DIGICELL). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Climate, Infrastructure and Environment Executive Agency (CINEA) Neither the European Union nor CINEA can be held responsible for them.

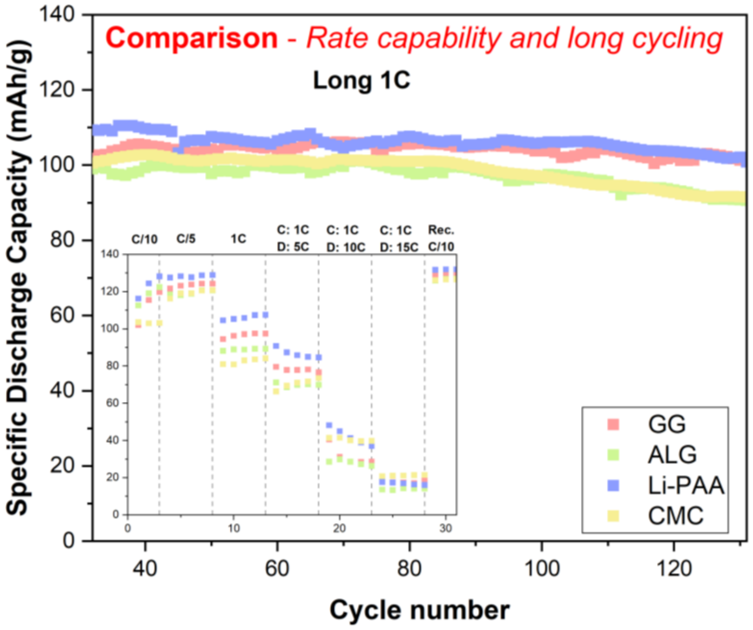

Figure 1. Brief comparison of the rate capability and long cycling tests carried out using different binders in a LNMO cathode formulation

Looking inside batteries: real-time fiber-optic pressure and temperature sensing during operation

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In response to the need for a compact technology capable of reducing the overall battery cost and determining with great accuracy the aforementioned factors, the Battery 2030+ Research Initiative, financed by the European Union, was created. An essential aspect of this mission is the development of sensors for the meticulous monitoring of internal battery parameters **[1]**. The INSTABAT project was a member of this initiative and aimed to research smart lithium-ion batteries (LiBs) and develop smart methodologies to sense critical parameters within the battery cells **[2]**. This work, developed in the scope of the INSTABAT project, represents a significant stride in enhancing the performance, safety, and understanding of this type of battery, ultimately contributing to the transition towards a more sustainable and secure energy future. The central focus of our study is the operando monitoring of commercial LiB internally by using highly sensitive optical fiber sensors (OFS). By employing an innovative hybrid sensing configuration based on fiber Bragg grating and intrinsic Fabry-Perot interferometer sensors, we have enabled the decoupling and tracking of critical safety parameters (such as temperature and pressure) inside a commercial LiB. Thereby, by correlating this data with electrochemical events during the battery operation, it was possible to evaluate their performance under several cycles at different environmental temperatures and operating conditions. Our findings challenge conventional wisdom, revealing that pressure dynamics within LiBs are associated with internal electrochemical events (such as the phase transitions of their materials) that occur during battery operation on the lithiation and delithiation processes and mainly behave as a "breathing profile" during the successive charge/discharge steps. Our work demonstrates the immense potential of advanced OFS technology in the field of LiB monitoring, marking a substantial contribution to the realm of sustainable energy solutions. It offers invaluable insights for enhancing LiB safety, reliability, and overall performance, ultimately advancing the integration of LiBs within our evolving sustainable energy landscape.

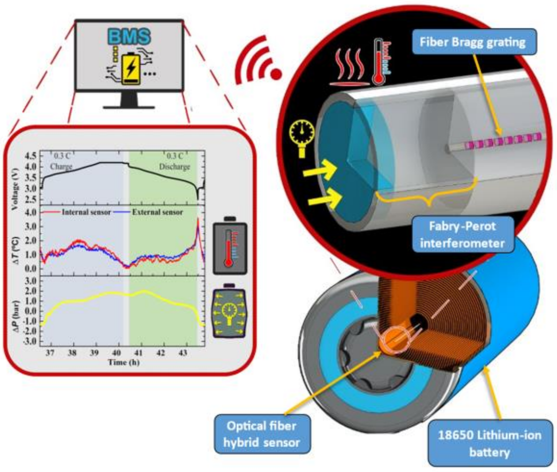

Figure 1. A hybrid optical fiber sensing configuration was proposed for highly sensitive detection of pressure and temperature inside a commercial lithium-ion battery operated under cycling tests.

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Structural and Electrochemical Screening of Layered Manganese Oxides for Potassium-Ion Batteries

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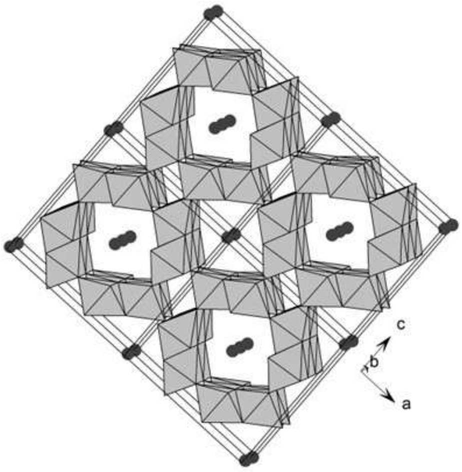
Lithium-ion batteries (LIBs) are currently the dominant electrochemical energy storage technology due to their long lifespan and high energy density. However, the relatively low abundance of lithium in the Earth crust, together with the uneven geographical distribution, has led to a growing interest in alternative battery technologies. In this frame, potassium represents a promising candidate as it is an abundant element on the Earth crust (a thousand times more than Li) and exhibits a standard electrode potential ($E(K^+/K) = -2.93$ V), which is only slightly lower than that of lithium ($E(Li^+/Li) = -3.04$ V) [1]. For these reasons potassium-ion batteries (KIBs) have emerged as potential low-cost and sustainable alternative to LIBs. Despite these advantages, KIBs are not yet commercially available, mainly due to the low stability of these systems and the sluggish K^+ intercalation/deintercalation kinetics at both electrodes [1]. In this context, the present study focuses on the development of novel cathode materials for KIBs, specifically layered manganese oxides containing intercalated potassium ions.

Layered manganese oxides are present in nature in various forms with different composition and morphological characteristics [2]. As a preliminary step, different manganese oxide phases were synthesized systematically investigating their morphology, structural stability, and electrochemical behavior. The successful formation of the material, including the dimensions of K^+ diffusion channels, was studied by X-ray diffraction. The thermal stability of the material has been analyzed through thermal gravimetric analysis. Preliminary electrochemical behavior has been evaluated by potentiostatic electrochemical impedance spectroscopy (PEIS) and cyclic voltammetry.

This initial screening is aimed at identifying the most promising materials, which will be subsequently engineered and optimized through transition-metal doping to mitigate intrinsic structural limitations, such as Jahn–Teller distortion effects and sluggish K^+ diffusion kinetics.



Representation of a 2x2 structure of cryptomelane, one of the investigated oxides. The black atoms represent K [3].

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COMPUTATIONAL SEARCH OF NA-ION HALIDE SOLID-STATE ELECTROLYTES

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Sodium-ion batteries (SIBs) have emerged as a compelling sustainable alternative to lithium-ion technologies, leveraging the earth-abundance of sodium to mitigate cost and supply chain constraints. [1] While the transition to solid-state electrolytes (SSEs) is pivotal for enhancing the safety and energy density of SIBs, the identification of materials exhibiting high ionic conductivity and broad electrochemical stability remains a significant bottleneck. Traditional experimental synthesis is often impeded by the vast chemical search space, necessitating accelerated discovery strategies. Consequently, high-throughput computational screening based on Density Functional Theory (DFT) has become indispensable for predicting thermodynamic stability and transport mechanisms, offering an efficient pathway to identify promising Na-ion SSE candidates prior to experimental validation. [2,3]

To find novel solid-state materials for battery applications, Density Functional Theory (DFT) based computational search were performed. Inspired by resent research that halide materials have improved their ionic conductivity, we investigated novel Na_3MX_6, $NaMX_4$, Na_5MX_8, $Na_3M_5X_{18}$, $Na_3M_7X_{24}$ and NaM_2X_7 stoichiometry (M=La, In; X=Cl, Br, I). Using computational utilities, including substitution and structural relaxation, more than 30 novel stable and metastable structures were found by placing all structures on the stability convex hull diagram. Among stable compounds are Na_3InCl_6 and Na_3LaI_6 monoclinic, $NaLaCl_4$ triclinic and $NaInCl_4$ orthorhombic, Na5LaI8 orthorhombic, $Na_3La_5Br_{18}$ and $Na_3La_7Br_{24}$ hexagonal structures. Using Machine Learned Interatomic potential, the ionic conductivity has been calculated. The results show that these compounds can achieve high values of ionic conductivity. In conclusion, our results support the candidacy of Na ion based halide materials as promising electrolytes for future advanced energy storage devices applications.

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Integrating life cycle thinking into the sustainable design of emerging battery technologies: insights from the TALISSMAN project

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TALISSMAN (Technologies for Advanced LIthium-Sulfur batteries toward Safe and Sustainable Mobility Applications) **[1]** is a Horizon Europe project developing a new generation of lithium-sulfur batteries (Li-S), integrating technological innovation with eco-design, circularity, and recyclability principles. To effectively address sustainability targets and support sustainable and circular design, environmental impacts should be assessed from the early stages of technology development. Life Cycle Assessment (LCA) **[2]** provides a standardized framework to quantify these impacts and can support informed decision-making during research and innovation processes. However, applying LCA to emerging technologies at low Technology Readiness Levels (TRLs) poses significant methodological challenges, including limited primary data availability and the absence of defined industrial-scale production routes.

This contribution explores the application of a Prospective LCA (pLCA) approach **[3]** to the TALISSMAN Li-S battery, currently at laboratory scale. The focus is on the methodological framework that can be adopted to meaningfully implement pLCA under the intrinsic uncertainty and data gaps typical of early-stage technologies **[3]**. The objective is to highlight the role of LCA as a sustainability-by-design tool, supporting material selection, cell design choices, and process development from the earliest research stages. From this perspective, LCA can act as a strategic instrument to steer innovation pathways and anticipate potential trade-offs among performance, safety, and environmental impacts before industrial deployment.

By reflecting on lessons learned from previous literature on prospective LCA of emerging energy technologies, particularly Li-S batteries, and applying them to the TALISSMAN case, this study aims to provide practical recommendations and good practices for integrating life cycle thinking into the design of emerging battery chemistries. This poster highlights the key role of LCA in supporting the transition toward sustainable, circular energy storage systems from the earliest stages of innovation.

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In Situ photopolymerized ionogels for safe high-Voltage lithium metal batteries

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The increasing demand for high-energy-density storage systems has accelerated research on lithium metal batteries (LMBs) coupled with high-voltage cathodes such as LMNO and LMFP. However, the practical implementation of these systems remains impeded from one side by the high reactivity of metallic lithium leading to uncontrolled dendrite growth, and to the other side from the limited oxidative stability of most common electrolytes. Two possible answers to these challenges are the use of a polymer based electrolyte to mechanically limit dendrite nucleation and growth and the addition of an ionic liquid to enhance the ionic conductivity and the interfacial contact, while taking advantage of the intrinsically high oxidative stability and low vapor pressure. Hence, we report a novel gel polymer electrolyte (GPE) synthesized via in situ UV-induced radical photopolymerization of butyl methacrylate (BMA) and poly(ethylene glycol) diacrylate (PEGDA) matrix incorporating the ionic liquid 1-ethyl-3-methylimidazolium bis(fluorosulfonyl)imide (EMIMFSI) and lithium bis(trifluoromethylsulfonyl)imide (LiTFSI). Electrochemical characterization demonstrates that the optimized GPE exhibits an electrochemical stability window exceeding 4.5 V vs. Li/Li^+, rendering it suitable for high-voltage operation. The GPE shows enhanced interfacial stability, slightly higher ionic conductivity compared to the neat ionic liquid electrolyte, and effective suppression of lithium dendrite growth during prolonged plating/stripping tests. Li/GPE/LMFP full cells deliver an initial discharge capacity of 120 mAh g^{-1} with a Coulombic efficiency of 90% over 50 cycles, and retain a capacity of 100 mAh g^{-1} after 100 cycles. These results highlight the potential of ionogel-based electrolytes as safe and stable candidates for next-generation lithium metal batteries.

Linking 3D Microstructure and Li Plating Homogeneity in a Grafted Al_2O_3-PCL Ceramic-in-Polymer Electrolyte

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Ceramic-in-polymer (CIP) hybrid electrolytes represent a promising class of materials for solid-state lithium metal batteries, combining the mechanical stability of ceramic particles with the interfacial wetting properties of polymer matrices. This work investigates the structure-property relationships in a grafted Al_2O_3-poly(caprolactone) CIP electrolyte through an integrated experimental and computational approach. Structural information was obtained via focused ion beam scanning electron microscopy (3D-PFIB-SEM) reconstruction revealing Al_2O_3 particles (8.2 vol.%) with a Gaussian size distribution centered around 350 nm diameter. Image analysis combined with TGA measurements identifies characteristic grafting domains between 150-250 nm.

The experimentally derived 3D microstructure was subsequently used as input for voxel-resolved GPU-accelerated finite-difference electrochemical transport simulations. Heterogeneous conductivity fields accounting for the enhanced transport properties of grafted polymer domains were constructed to match the observed ionic conductivity of the hybrid electrolyte (0.53 mS/cm).

This conductivity field was then used as input for transient migration-diffusion transport simulations under galvanostatic boundary conditions. Simulations reveal severe local current focusing induced by the heterogeneous microstructure, resulting in non-uniform salt concentration profiles and localized regions with elevated plating current during cell operation. Two mitigation strategies were investigated computationally. First, introducing a second ionically conductive layer at the anode that blocks grafted ceramic particles from entering the interfacial region can prevent inhomogeneous plating current. Second, if the ceramic particles near the anode are themselves ionically conductive, large particles cease to act as strong current blockers, thereby reducing current inhomogeneity.

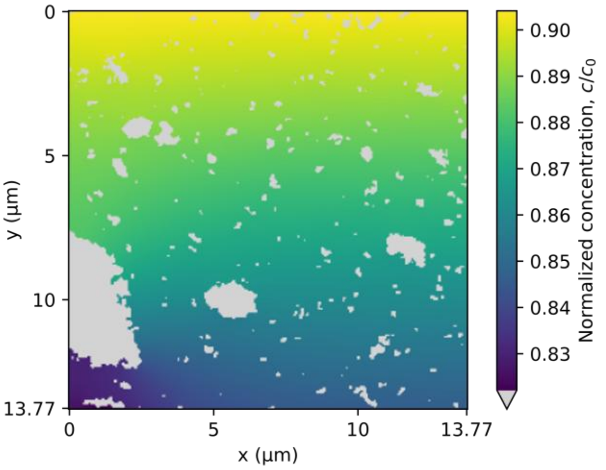

Figure 1. Derived salt concentration profile after reaching steady state. The area under the insulating particle in the bottom left shows a lower salt concentration than the rest of the Li-adjacent volume.

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A METHODOLOGY TO ACCELERATE DATASET GENERATION FOR RAPID STATE OF HEALTH ESTIMATION LOGICS

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In the current effort to fight climate change, transportation is a fundamental sector, as it generates around 20% of human-made CO_2 emissions[1]. As a result, the automotive sector is currently the main uptake of batteries in the world, overtaking production of consumer electronics such as smartphones and laptops[2]. High- voltage and power needed in EV applications requires the installation of large battery packs, consisting of hundreds or thousands of cells. Aging is expected to be heterogenous among the cells, with a portion displaying an end-of-life (EOL) capacity greater than 80%. Since battery disposal presents open issues related to land pollution and fire hazards, recycling of such cells for second-life application into stationary storage systems has the potential to turn waste into a resource[3].

For this reason, great research interest is present on the topic of rapid diagnostics for assessment of battery State of Health[4]. Methods based on artificial neural networks (ANNs) offer a good compromise between accuracy and complexity, allowing their deployment both on vehicle ECUs and on testing devices which can be employed in workshops or plants processing batteries retired from EV usage[5]. Data collected from voltage response to external current pulses is a common feature to describe battery SoH. A key requirement for these methods to be developed is the generation of datasets needed for ANN training, which requires controlled battery aging taking months or years.

To tackle this issue, the following abstract proposes a methodology for data collection and exploitation that eliminates the need for laboratory testing associated to aging. Instead, the proposal leverages the spread in degradation among cells inside an EOL battery pack. Given harsh usage conditions with fast transient and high peak power[6] that is evident in automotive applications, this sector lends itself to the purpose of data collection. Disassembly of two to three modules could provide enough cells to test with current pulses obtaining varying voltage responses. This would create a dataset sufficient for ANN training, accelerating the realization of SoH estimators and making it more efficient. Furthermore, a similar spread in quality can be observed at factory level, due to production tolerances and potential quality issues. The methodology presented here could therefore be applied by cellmakers as well, who would provide samples from production line to be characterized, in order to train a system that can rapidly assess the quality of each cell right at the end of its production.

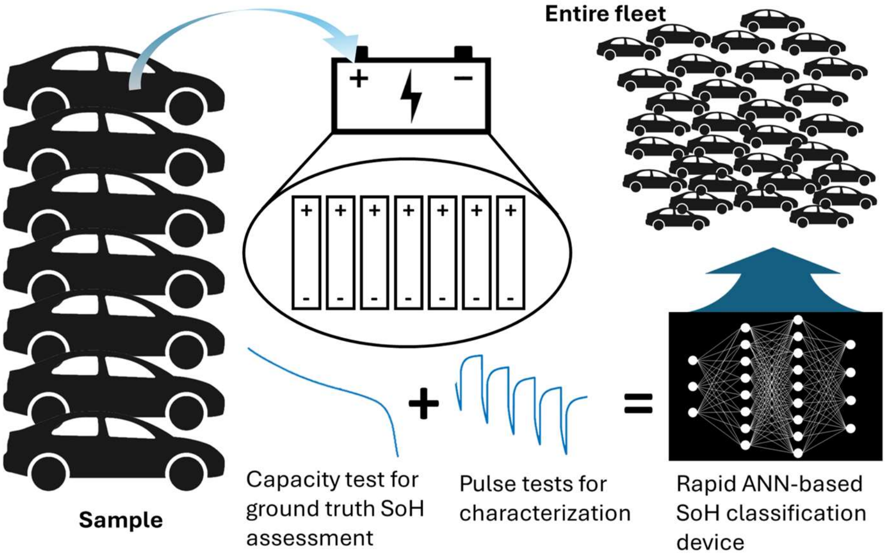

Figure 1. Process flow from characterization of a small sample to entire fleet testing capability

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Graphite Matters: Reassessing the Impacts of Graphite on the Carbon Footprints of LIB Cell Production

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Background: The central focus of existing life cycle assessment (LCA) studies on lithium-ion battery (LIB) cell production has been around cell manufacturing energy, different cathode chemistries, and the supply chain of cathode active materials (1-5). In contrast, the crucial role of graphite as the anode active material on the carbon footprint (CF) of LIB cell production has remained largely underexplored (6,7). Particularly the differences between synthetic graphite (SG) and natural graphite (NG), and their varying compositions in LIB anodes and sourcing are not considered. Moreover, the usage of outdated databases for NG and SG in the last 10-15 years led to a lower than actual CF of cell production (6,7).

Results: This gap is addressed by conducting an LCA on LIB cell production using latest industrial primary LCA data for both graphite types. The results show that the CF of LIB cell production is substantially higher than LIB cell with older graphite datasets, with graphite emerging as a key hotspot. Moreover, the results highlight that the choice and proportion of the graphite types in the anode strongly influence the CF of LIB cell production. The findings further reveal the importance of relative proportions of the two graphite types in benchmarking where different ratios of graphite types may lead to different benchmarking results. The results are representative of the current global graphite supply chains, where China controls more than 92% of the global supply chains- more than any other LIB minerals. However, large scale deployment of emerging technologies such as continuous graphitization and close-loop furnace technology for graphite production in future have the potential to decrease the graphite's CF.

Implications: The ongoing efforts for localizing the graphite supply chains to derisk the battery production in EU are taken into consideration (8), and show that the graphite sourced from EU- a higher proportion of renewable energy in their electricity mix- significantly reduces the CF of cell production compared to graphite sourced from northern and eastern regions of China. However, China's aggressive expansion of graphite supply chains to the southwest region (9,10), where the grid has high share of renewable energy than the national average grid, suggests a need of further push to increase the renewables at EU level for a long-term environmental competitiveness with China. Overall, the study provides important insights for multiple stakeholders such as LCA practitioners, battery researchers and manufacturers, and policy makers by highlighting the pivotal role of graphite, its types, and sourcing in determining the environmental performance of LIB cell and benchmarking against other cell chemistries such as NIBs and other post LIBs systems.

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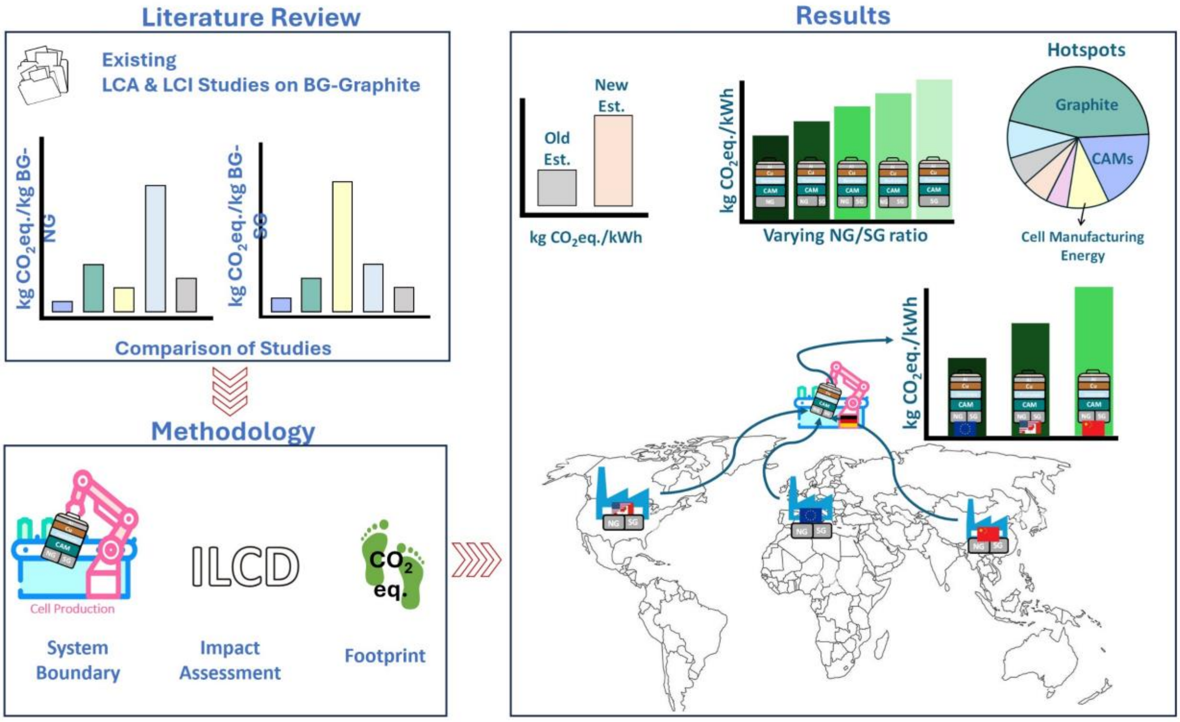

Figure 1. Graphical abstract for **Graphite Matters: Reassessing the impacts of graphite on the carbon footprints of LIB cell production**

4D computational characterization of lithium-sulfur cathode via CFD and PBM simulation

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As the global demand for electric batteries continues to rise in several fields, such as automotive, energy storage and electric portable devices, lithium-sulfur (LiS) batteries have emerged as a promising alternative to conventional lithium-ion batteries (LiB) thanks to their potential for significantly higher energy density and lower material costs. However, the commercialization of this technology is still limited due to the large capacity fade, which is strictly related to phenomena such as polysulfide shuttling and uncontrolled lithium-sulfide (Li_2S) deposition. A deeper understanding of the mechanisms governing these phenomena is crucial to develop and produce cells with high specific energy density and long cycle life. Computational models have become a useful tool for better understanding the nature and mechanisms of these physical and chemical processes, which normally can be characterized by very complex techniques such as X-ray tomography and synchrotron-based ones.

In this work, we present a computational framework that describes the evolution in time of the complex geometry of LiS cathode active material, considering the physical and electrochemical reactions that characterize this technology. We have modified the model developed by *Zhang et al.* **[1]**, by geometrically describing the sulfur contained within the cathode, adopting a heterogeneous approach. The realistic description of the electrode structure will provide great benefits, both on the accuracy of the modelling predictions and on the understanding of the physical and chemical phenomena that occur during the charge and discharge processes. Therefore, we added a computational tool that illustrates the physical evolution in time of the sulfur domain due to its dissolution in the electrolyte and, at the same time, characterizes the precipitation of Li_2S and tracks its particle size distribution (PSD). Moreover, the nucleation and growth of Li_2S particles, were formulated based on a set of empirical parameters, providing the possibility to develop a universal computational model that works with different operating conditions and material properties, making it more flexible and adaptable to different technologies.

In Figure 1 are shown some of the results obtained with the heterogeneous model coupled with PBM, comparing the predictions obtained with the ones of the homogeneous model.

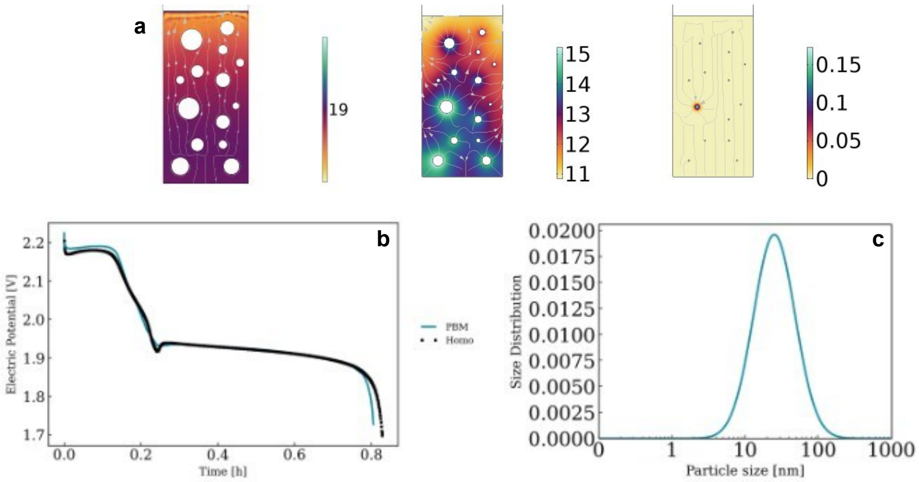

Figure 1. Contour plots of S_8 concentration at different states of discharge (a), comparison of the discharge profile between the predictions of the heterogeneous model coupled with PBM and homogeneous model (b) and an example of PSD obtained (c).

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Reducing the Environmental Impact of Lithium-Ion Batteries through High-Silicon Anodes: A Life Cycle Assessment

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Lithium-ion batteries (LIBs) play a central role in electrification and energy storage, however, their environmental sustainability remains a critical challenge, particularly as higher energy density materials are introduced. In this work, laboratory-based life cycle assessment (LCA) was performed on three different anode chemistries: conventional graphite, silicon composite (10 wt% Si), and silicon-dominant (80 wt% Si, capacity limited to ≈1000 mAh g^{-1}), to quantify and compare their cradle-to-gate environmental impacts using the ReCiPe 2016 Midpoint (H) and Endpoint (H) methods. Two functional units were adopted: a mass-based approach (per kg of anode produced) and a performance-based approach (per Ah of practical electrode capacity), enabling a direct comparison between material intensity and delivered electrochemical output.

Although silicon production is more energy intensive than synthetic graphite, results show that increasing silicon content can significantly reduce environmental impacts when normalized to practical electrode capacity. In terms of climate change, the carbon footprint, expressed in kg CO_2-Eq, decreases by approximately 40% for the silicon composite compared to graphite and up to around 97% for the silicon-dominant formulation, highlighting the potential of high-silicon formulations to lower environmental impacts under laboratory-scale production conditions (Figure 1). A sensitivity analysis further underscores the importance of supply-chain conditions, comparing a European supply chain scenario with a global baseline. The adoption of a lower-carbon European electricity mix and shorter transportation distances provides additional impact reductions. Monte Carlo simulations were used to assess uncertainty, strengthening the robustness of the comparative results.

Overall, this study emphasizes that emerging silicon-based anode technologies can offer environmental advantages over conventional graphite, when assessed under realistic production and supply-chain conditions. The results underline the importance of assessing emerging materials on a performance-normalized basis, where environmental impacts are related to the practical capacity delivered by the electrode, demonstrating that electrochemical performance and environmental sustainability must be evaluated in an integrated framework.

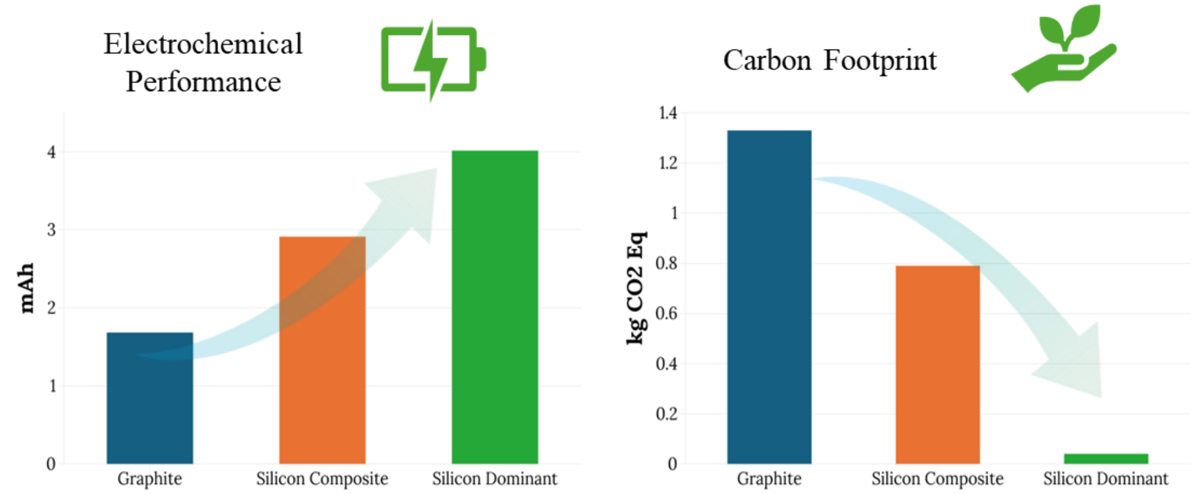

Figure 1. Enhanced electrochemical performance and reduced CO_2 emissions of silicon-dominant anodes compared to graphite and silicon composite formulations.

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Exploration of Various Catalyst Materials for Green Ammonia Production for Chemical Energy Storage

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Ammonia (NH_3) serves as a critical fertilizers precursor and carbon free energy carrier for electrochemical storage systems, yet Haber-Bosch process (HBP) synthesis consumes 2% of global energy with high CO_2 emissions [1-3]. Electrochemical nitrate reduction reaction (ENO$_3$RR) enables sustainable NH_3 production from wastewater nitrates using renewable electricity [4-5]. This study investigates Fe- and Mn-based perovskites ($LaMnO_3$ and $LaFeO_3$) as electrocatalysts for ENO$_3$RR in a flow cell with gas diffusion electrodes. Catalysts were air-brushed onto electrodes; performance was evaluated via Faradaic efficiency, NH_3 yield (UV-Vis, IC), and overpotential dependence under various electrolytes and pH values. The hydrogen evolution reaction (HER) was identified as the primary competing side reaction reducing NH_3 selectivity [6]. The experimental optimizations suppressed HER, achieving high ENO$_3$RR selectivity and exhibiting high Faradaic efficiency of > 90% with significant yield of around 3000 μg h^{-1} (mg cm^{-2})$^{-1}$ for -Fe based perovskite catalysts. These results reveal perovskite stability against wastewater interferents, advancing electrochemical energy conversion from waste nitrates.

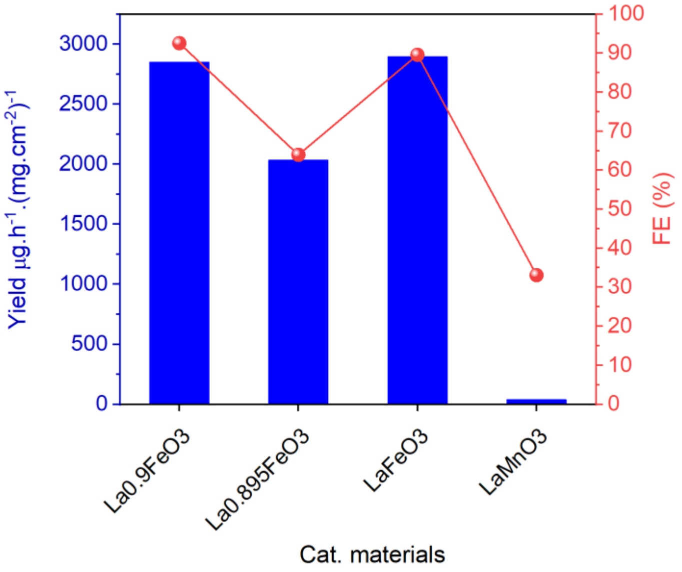

Figure 1. Performance metrics of perovskite catalysts.

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Ni-MOF-INTEGRATED FUNCTIONAL SEPARATORS FOR LITHIUM-ION BATTERIES

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In recent years, Metal–organic frameworks (MOFs) have emerged as promising advanced materials for electrochemical energy storage and conversion systems due to their highly ordered and tunable compositions, excellent thermal stability, ultra-high specific surface area, adjustable porosity and structures [1]. In the field of electrochemical energy storage devices, rechargeable lithium-ion batteries (LIBs) have become the most popular and widely used in portable electronics, electric vehicles, aerospace and many other applications due to their remarkable performance. However, with the advancement and demand of modern energy technologies, LIBs are facing several challenges in meeting the expectations of current customers [2]. Along with the cathode, anode and electrolyte, the separator is one of the most important components for LIBs which prevents the physical contact between the cathode and anode while facilitating the movements of Li+ ions. However, typical polymer separators suffer from poor electrolyte wettability, inhomogeneous pore distribution and insufficient thermal stability, which stimulates the need for novel functional separators [3]. In this work, Ni-MOF-74 nanomaterials have been synthesized by hydrothermal process and integrated with glass fiber (GF) separator for LIB applications in the framework of PHOENIX project (grant agreement no. 101103702). Microstructural and morphological analysis have been performed using sophisticated XRD, SEM and EDX studies. Afterwards, the electrochemical LIB performance of this Ni-MOF integrated GF-separators have been initially conducted using CR2032 type half–coin cells composed of synthesized $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ (NMC622) active cathode material, pure Li-anode and 1 M $LiPF_6$ in EC/DMC (50/50) (v/v) electrolyte. The Ni-MOF integrated GF-separators have been fabricated using different wt% such as 5 wt%, 10 wt% and 15 wt% of Ni-MOF. The capacity retention, cycling stability and internal resistance have been evaluated via galvanostatic charge-discharge (GCD) testing in the voltage range of 2.7 V to 4.2 V at C/10 and electrochemical impedance spectroscopy (EIS) analysis. Ni-MOF-74 (5 wt%) integrated GF-separator based LIB shows excellent capacity retention after 50 cycles offering capacity of 96.6 mAh/g in the 1st cycle and reduced to 94.1 mAh/g after 50 cycles, which indicates the stable performance of Ni-MOF-integrated separator-based LIBs compared to pure GF-based LIBs (Figure 1). Finally, the Ni-MOF integrated GF separator also improves the cyclic stability and electrochemical performance of the full cell LIB composed of NMC811 cathode and Gr/SiO_x anode over 200 cycles at C/3. Overall, this work demonstrates the potential future of MOF-integrated functional separators in battery technologies and energy storage systems.

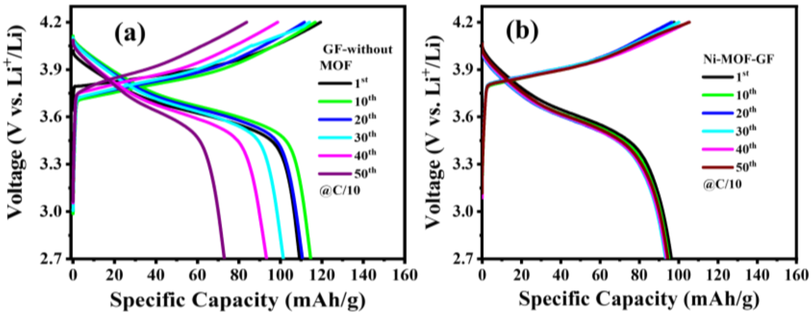

Figure 1 Long-term cycling stability of LIBs composed of (a) bare GF and (b)5 wt% Ni-MOF integrated GF separator, NMC622 cathode and Li anode.

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Model-Free Capacitance Extraction from a Single EIS Spectrum Enables Real-Time Identification of Intercalation and Interfacial Processes in a Commercial LCO Battery

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Electrochemical Impedance Spectroscopy (EIS) presents several unique advantages. Among them, the ability to relate voltage and current in both time and frequency domains, enabling the extraction of kinetic parameters associated with internal processes in lithium-ion batteries (LIBs). In addition, it is a non-destructive technique applicable to in situ and operando studies, and it can play an important role in monitoring the state of health of a battery during operation [1]. Although, under ideal conditions EIS can distinguish different electrochemical processes, such as electron transfer, ionic diffusion, double-layer charging, and insertion processes, in practice these phenomena can overlap. Consequently, the analysis becomes highly model-dependent, hindering the reliable extraction of internal parameters and preventing a physically self-consistent interpretation of the data. Traditional EIS analysis methods are generally based on predefined models, such as equivalent electrical circuits. This approach may introduce ambiguities in the interpretation of fitted parameters and limit the direct identification of physical properties associated with electrochemical interfaces [2]. In this context, the present work proposes the application of an innovative EIS data analysis methodology, termed the Generalized Phase Element (GPE) method. This approach enables the direct extraction of capacitance values in electrochemical systems without the need to employ predefined models such as equivalent electrical circuits [3]. Furthermore, the method allows real-time monitoring of the evolution of reactive electrochemical systems, in contrast to traditional approaches. The methodology was validated using simulated circuits and a dummy cell to assess its accuracy in the direct determination of capacitance. Quantitative agreement was observed between the obtained values, the simulated values, and the parameters provided by the manufacturer, with lower deviation compared to traditional methods. These results indicate that the proposed approach provides a more faithful representation of the intrinsic capacitance of the electrochemical system. Subsequently, the method was applied to a real system consisting of commercial LCO batteries under operando conditions. From a single EIS spectrum, it was possible to deconvolute and quantify capacitances associated with different processes: (i) pseudocapacitance related to lithium-ion intercalation into the active material matrix; (ii) capacitance associated with the Solid Electrolyte Interphase (SEI) layer; and (iii) double-layer capacitance. The results indicate that the proposed approach enables the quantitative identification of distinct interfacial contributions from a single EIS measurement, contributing to the advancement of diagnostic methodologies for lithium-ion batteries.

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Selective Nickel Recovery via Amine-Assisted Mineral Carbonation and Electromediated Regeneration

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The sustainable recovery of transition metals from end-of-life lithium-ion batteries remains a central challenge for circular energy technologies, largely due to the reliance of current hydrometallurgical routes on mineral acids, inorganic bases and solvent extraction.[1] Here we report a separation strategy that combines amine-assisted mineral carbonation with electromediated stripping and regeneration (EMR), enabling the selective recovery of nickel while avoiding acid-based stripping steps. The process relies on the contrasted coordination thermodynamics and kinetic lability of ethylenediamine complexes,[2] and on the use of copper as a reversible redox mediator to induce nickel decomplexation under electrochemical control. Fundamental thermodynamic analysis and spectroscopic validation demonstrate selective nickel stripping in the presence of kinetically inert cobalt complexes, followed by nickel recovery as carbonate. Integration of this technological brick into a multi-step recycling flowsheet starting from NMC 811 blackmass highlights a projected 60–75% reduction in acid-derived effluents and a 50–65% reduction in total saline waste compared to solvent extraction-based processes.[3] While demonstrated here at proof-of-concept scale, this work establishes a mechanistically grounded framework for replacing stoichiometric acid–base operations by redox-mediated control, opening new perspectives for greener hydrometallurgical separations.

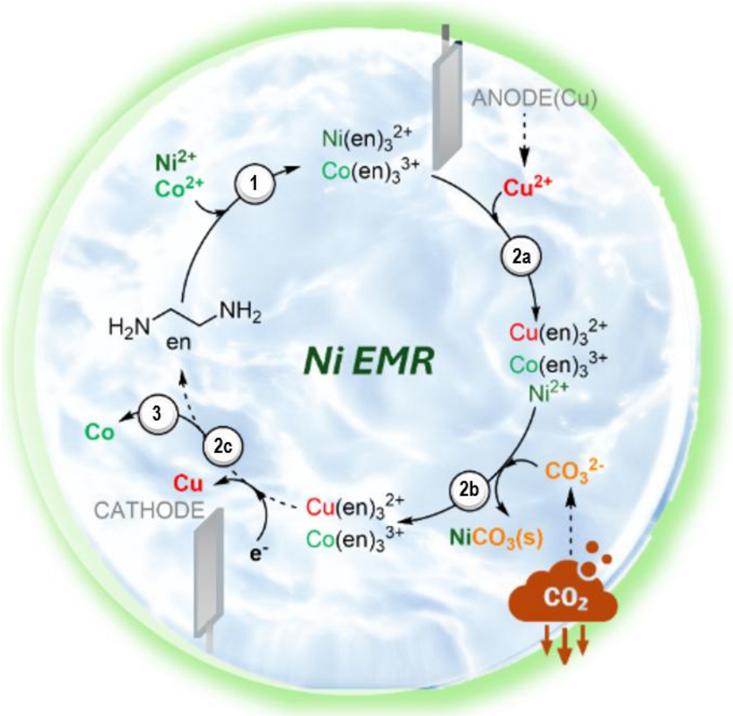

Figure 1. Schematic representation of the electromediated nickel stripping and regeneration (Ni EMR) developed in this work, which aims at overcoming the key drawbacks of conventional hydrometallurgy by exploiting thermodynamic lability of nickel-amine complexes upon electrochemical addition of copper.

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Solderless Connection Design For Pounch Cells

Presenting Author[1], Second Author[2], Third Author[3]…

This study presents the development and electrical validation of a solderless high-voltage (HV) module connection for lithium-ion battery applications. The proposed solution is based on a mechanically compressed busbar system positioned between two plates, enabling electrical contact without welding. The objective is to evaluate contact resistivity and thermal behavior under controlled mechanical compression by varying screw-tightening torque. The initial implementation focuses on a 2-cell 2P tab-to-tab connection, considering the geometrical and material differences between aluminum positive tabs (0.4 mm) and nickel-plated copper negative tabs (0.3 mm). A customized lower plate design compensates for the 0.1 mm height difference to ensure uniform pressure distribution across both terminals. The design is subsequently extended to a 4-cell 2P configuration for module-level integration.

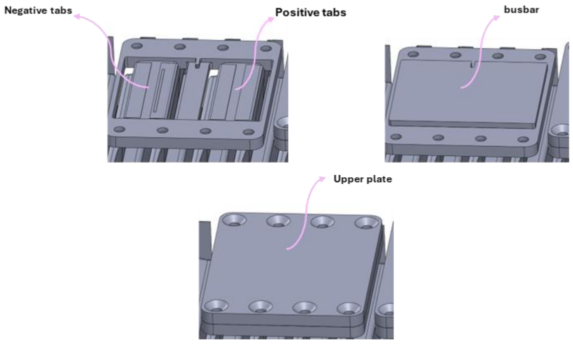

Figure 1. Cad of the 4P-configuration

To experimentally assess performance, a dedicated test bench was developed. Due to welding incompatibility between aluminum and nickel-plated copper tabs with the available laser welding system, a clamping method using aluminum interface plates was adopted. Additive manufacturing was used to produce electrically insulating structural components. Initial prototypes made from PLA exhibited excessive deformation under compression, leading to unstable contact resistance. Therefore, a high-stiffness Formlabs 10K resin was selected. Mechanical limitations of the resin required increasing plate thickness from 5 mm to 10 mm, enabling a maximum applicable tightening torque of 0.5 N·m without fracture.

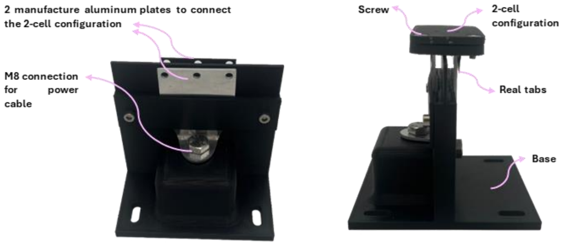

Figure 2. 3D print base for the test bench

Electrical tests at 76 A and 152 A (30 min) showed a voltage drop of 24.8 mV at 76 A with an 8 °C temperature rise, and 32 mV at 152 A with a 30–40 °C increase. Although the voltage drop remains below the 0.1 V target at both currents, thermal behavior becomes limiting at higher current levels.

The results confirm that mechanical stiffness and compression strongly affect contact resistance and thermal stability. The concept is feasible for module integration, provided thermal and mechanical optimization is improved.

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Solderless Connection Design for Prismatics Cells

Presenting Author[1], Second Author[2], Third Author[3]…

This study evaluates multiple solder-free electrical connection solutions for a low-voltage (LV) battery module integrating prismatic cells with threaded terminals. The objective is to establish robust, removable, and electrically efficient connections between the cell terminals and a PCB-based busbar, while preserving second-life usability of the cells and minimizing additional hardware. Special attention is given to long-term reliability, mixed copper/aluminum interfaces, cost, and tolerance to potential terminal misalignment. Seven connection concepts were analyzed: a reference screw with Belleville washers, a clamp-on printed bracket, a removable rivet, cam-lock levers, Molex press-fit sockets, Molex floating sockets, and Radsok sockets. Solutions were first assessed based on mechanical feasibility and cost, then experimentally characterized using a high-current test bench capable of delivering up to 600 A. Voltage drop (contact resistance) and temperature rise were measured at 1C (72 A), 100 A, and up to 2C (144 A). The reference screw solution demonstrated excellent electrical performance (<1 mV at 1C) with stable torque-dependent behavior, serving as a baseline. The rivet solution proved non-repeatable and unreliable, exhibiting large variability in voltage drop (up to 500 mV) and significant temperature rise, leading to its rejection. Cam-lock levers showed very low voltage drops comparable to the reference solution but presented integration constraints due to bulkiness. Connector-based solutions demonstrated strong performance. The Molex press-fit configuration achieved low voltage drops (≈4 mV at 1C) and excellent thermal stability, remaining well below the 20 mV per connection limit even at 2C. The Molex floating socket, designed to accommodate 1 mm terminal misalignment, showed slightly higher but compliant voltage drops (≈10–14 mV at 1C). The Radsok solution also performed reliably, maintaining voltage drops below specification limits, though without misalignment tolerance. Cost analysis revealed that simple mechanical fasteners are the most economical (<€1), whereas connector-based systems range from €8 to €17 per connection. Despite higher cost, connector solutions offer superior modularity, repeatability, and controlled contact interfaces. Based on electrical performance, thermal behavior, mechanical robustness, and integration considerations, the Molex-based connection was selected in agreement with EVE System. Real-world validation on uncleaned second-life cell terminals confirmed compliance with the 20 mV limit at 1C, although contact resistance increased by 10 % compared to controlled laboratory conditions due to surface oxidation. Thermal rise remained limited (<3 °C), confirming operational safety.

Overall, the study demonstrates that properly engineered solder-free connector solutions can meet electrical, mechanical, and second-life requirements for LV battery modules, with Molex-based architectures representing the most balanced solution between performance, robustness, and integration flexibility.

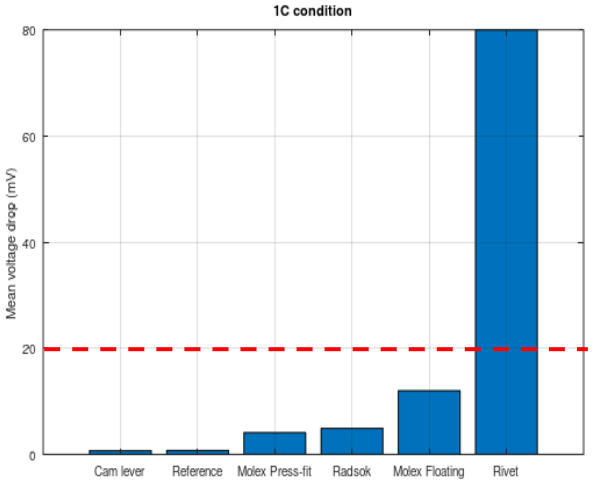

Figure 1. Voltage drop for each of the tested solutions as a function of current at 1C [1]

REFERENCES

[1] REBORN deliverable 5.1

ACCELERATING BATTERY DEVELOPMENT USING AUTONOMOUS WORKFLOWS

Jagdeep Sagu[1], Adam Todd[1], Jack Maxfield[1], Lauren Horn[1], Lilly Gill[1], Liyuan Liu[1], Danya Senthilkumar[1], Alexander Chaudhary[1], Aakifah Amjad[1], Catrin Jones[1], Ian Manfren[1], Nicole Fleck[1], Robert Mitchell[1], Keri Goodwin[1]

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A primary bottleneck in lab-scale battery R&D is the manual and iterative nature of slurry formulation, electrode coating and cell building **[1]**. As part of the FULL-MAP project, this work demonstrates the development and usage of an autonomous R&D workflow, which is ideal for rapid screening and optimization of new battery materials. This powder-to-cell workflow (Figure 1) at CPI forms a crucial part of the chemistry-neutral materials acceleration platform, which aims to achieve at least a five-fold acceleration in the development of new battery chemistries. The FULL-MAP platform will combine high-throughput automated experimentation with AI/ML tools and physics-based modelling to realize this target **[2]**. The platform will be validated by testing on nine different use cases.

To date, we have successfully tested our automated workflow to execute an extensive Design of Experiments campaign to optimize lithium iron phosphate (LFP) and graphite active materials to serve as a benchmark. We have been able to rapidly determine the limits for maximizing solid and active material content in the slurry, whilst still maintaining suitable rheology, coating adhesion, electrode conductivity, and electrochemical performance. We have also investigated how changing the electrode specification (coat weight and porosity) effects the aforementioned properties. Going forward, this data stream will be used to parameterize cell-level performance models, which will ultimately enable the platform to down-select optimal configurations for the desired applications, ranging from high-power delivery to maximized cycle life.

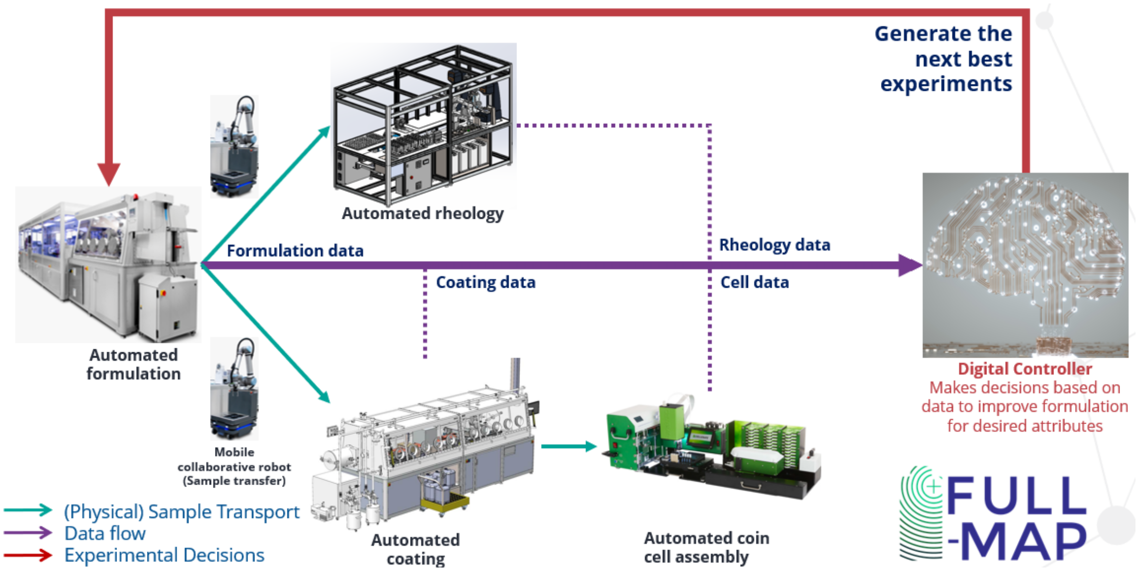

Figure 1. CPI's automated high-throughput workflow

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Clustering of Battery Projects: How to Maximise Impact and Sustainability in Europe's Battery Ecosystem[1]

Since early 2023, six Horizon Europe projects (GIGAGREEN, NoVOC, greenSPEED, BatWoMan, GigaBat, BATMACHINE) have joined forces under the *Battery Heroes* cluster to advance sustainable battery manufacturing in Europe. What started as a collaboration focused on joint dissemination (shared branding, events, outreach) has progressively evolved into a more structured and strategic platform, including technical exchange, alignment of approaches, and policy-oriented dialogue with the European Commission. A key outcome is the joint work on sustainability and LCA, leading to a first common paper and an abstract submitted to the Battery 2030+ conference (https://papers.ssrn.com/sol3/papers.cfm?abstract_id=6417503).

In December 2025, together with the COLLABAT cluster, Battery Heroes co-organised a cross-cluster workshop in Graz, gathering representatives from six clusters and key stakeholders (European Commission, BEPA, LiPLANET, Battery 2030+). Discussions confirmed that, while clustering is increasingly widespread, important challenges remain: moving beyond short-term, project-based collaboration, strengthening existing clusters rather than creating parallel structures, and ensuring continuity and effective knowledge transfer across funding cycles.

Figure 2. The Battery Heroes Cross-Cluster Workshop on Dec 1, 2025 in Graz

A joint white paper is currently under development and will be presented at the Battery 2030+ conference. It aims to provide concrete, actionable recommendations to enhance long-term impact, coordination, and sustainability of clustering activities within the European battery innovation ecosystem.

Figure 1. The Battery Heroes booth at the Battery Innovation Days 2025 in Graz

[1] For any interaction you can contact Silvia Bodoardo (GigaGreen) or Nicole Schmidt (NoVOC) during the annual conference (silvia.bodoardo@polito.it, schmidt@eutema-research.eu)

Lithium Iron Phosphate (LFP) battery recycling focused on the recovery of high-purity chemical precursors

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The Lithium Iron Phosphate ($LiFePO_4$, LFP) battery market is expected to grow to USD 77.07 billion by 2034 [1]. The reasons are that this type of battery offers excellent thermal stability, non-toxicity, cost-effectiveness, and competent cycling performance [2]. Therefore, many efforts are underway to contribute to the future production of LFP batteries using recycled raw materials. Therefore, this work presents a suitable approach for LFP battery recycling. A hydrometallurgical methodology for processing a batch of LFP black mass is proposed. The process consists of a leaching stage and a chemical precipitation phase. The first leaching stage focused on selectively extracting lithium. To dissolve lithium, sodium hydroxide (NaOH) was used as a leaching agent. It has been determined that this chemical system selectively dissolves lithium, achieving leaching yields ≥90% [3].

In the proposed methodology, the experimental conditions: 2 M NaOH, 25°C, 300 rpm, and 20 g/L allowed to extract 98% lithium and 96 %; however, aluminum was also dissolved (90%). Afterwards, the solutions rich in lithium and phosphorus ions were heated at 90 °C for 3 h, and a white salt was formed. The solid was dried in an oven at 60 °C for 24 h, and then the compound was analyzed by X-ray diffraction (XRD). The XRD technique confirmed the presence of lithium phosphate (Li_3PO_4). Moreover, the precipitate was chemically analyzed to determine its purity. The results showed a purity of 98.15% and, without aluminum content.

Finally, this work presents a feasible methodology for recovering salts as potential precursors for the production of new lithium-ion batteries. Also, it was demonstrated that hydrometallurgical methodologies, combined with recovery stages, allow the production of high-purity compounds.

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Nanoconfined complex hydride electrolytes for solid-state lithium batteries

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Solid-state lithium-metal batteries (SSBs) are emerging as a pivotal solution to meet the growing demand for safe, high-energy-density storage systems, particularly for electric mobility and stationary grid applications. However, conventional solid-state electrolytes (SSEs), such as sulfides and oxides, often suffer from limited interfacial stability, dependence on critical raw materials, and safety concerns.

In this contribution, a novel class of SSEs based on lithium borohydride ($LiBH_4$) nanoconfined within porous hosts, including zeolites and ion-conducting oxides[1], is presented. This architecture enhances ionic mobility by reducing the coordination environment of Li^+ ions at the interface with the porous support and improves electrode–electrolyte compatibility, thereby overcoming key limitations of traditional SSEs. The materials were synthesized using scalable procedures and characterized by impedance spectroscopy, X-ray diffraction, and electrochemical stability analysis. The most promising composites were selected for half- and full-cell testing to evaluate electrolyte stability in contact with electrode active materials.

This work demonstrates the feasibility of engineering next-generation SSEs based on abundant and non-toxic elements through nano-structuring strategies, providing a compelling alternative to sulfide-based systems. The proposed materials and methods are compatible with industrial prototyping, thereby bridging academic innovation and technological deployment.

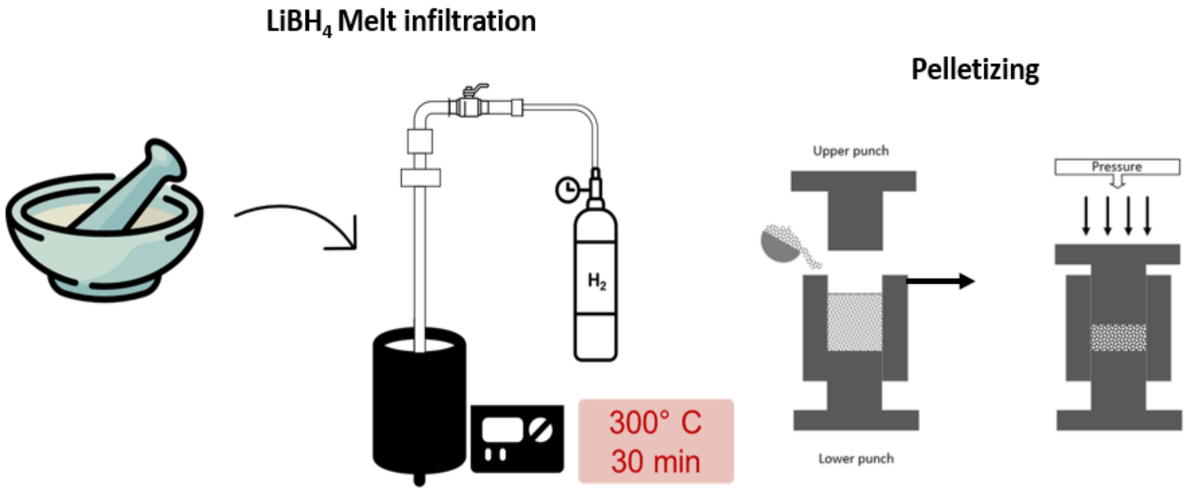

Figure 1. Preparation procedure of the nanoconfined solid state electrolytes.

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Hybrid Alucone Coatings via Molecular Layer Deposition for improved Performance of $LiCoO_2$ cathode

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The practical capacity of $LiCoO_2$ (LCO) cathodes is limited by the upper cut-off voltage due to surface degradation and electrolyte instability at high potentials. To enable stable operation above 4.5 V vs. Li/Li^+, we developed a facile Molecular Layer Deposition (MLD) process for hybrid organic–inorganic alucone coatings on LCO particles. Alucone thin films were deposited using trimethylaluminum (TMA) with either ethylene glycol (EG) or hydroquinone (HQ), forming conformal Al/EG and Al/HQ coatings with controlled thickness.

Both coated electrodes demonstrated significantly improved electrochemical performance compared to pristine LCO, including enhanced cycling stability, higher specific capacity, and improved capacity retention. The coatings effectively mitigated surface degradation and suppressed phase instability at elevated voltages. Notably, the Al/EG coating showed superior performance, achieving ~94% capacity retention at C/3 and 92% after 100 cycles at 1C (4.45 V cut-off), with substantial improvements also observed at 4.52–4.55 V. These results demonstrate the strong potential of MLD alucone coatings for stabilizing high-voltage LCO cathodes.

These results demonstrate a highly innovative strategy for stabilizing high-voltage cathodes through ultrathin hybrid organic–inorganic coatings deposited by MLD. The ability to precisely tailor conformal alucone layers opens a new pathway for interfacial engineering without compromising ionic transport. Importantly, this approach enables the broader application of hybrid ultrathin films to other electrode chemistries and battery systems, providing a versatile platform for next-generation high-energy materials.

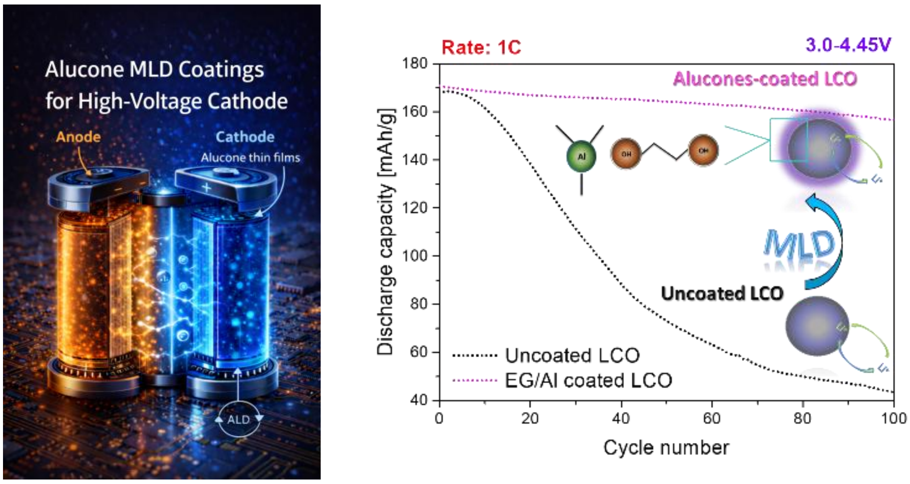

Figure 1: (a) Schematic description of the work, (b) Cycling performance of Alucone coated LCO versus pristine evaluated over 200 charge/discharge cycles.

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Atomic-Scale Insights into Anti-Perovskite Electrolytes for Structural Solid-State Batteries

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All-solid-state batteries (ASSBs) offer safer, more energy-dense alternatives to traditional Li-ion systems, yet their widespread adoption remains challenging by limited understanding of ion transport and interfacial stability in solid electrolytes (SE). Li_3ClO, a glassy antiperovskite SE, exhibits exceptionally high ionic conductivity (10^{-2}–10^{-1} S cm^{-1}) and a wide electrochemical stability window (> 6 V vs Li/Li^+), positioning it as a promising candidate for next-generation structural batteries [1,2]. However, its extreme sensitivity to moisture and electron beam irradiation has made direct atomic-scale investigation difficult, leaving the mechanisms behind its fast-ion conduction unclear [3].

In this work, we performed cryogenic electron microscopy (Cryo-EM) with strict air-free transfer protocols to stabilize and preserve Li_3ClO's native structure and chemistry during imaging [4]. Low dose cryo-Scanning Transmission Electron Microscopy (STEM) imaging enabled the first high-resolution visualization of the cubic $Pm\bar{3}m$ antiperovskite framework, revealing lattice distortions and strain fields. Cryo 4D-STEM highlighted regions linked to Li^+ mobility and local polarization phenomena. Selected area electron diffraction (SAED) confirmed a mixed of polycrystalline microstructure with embedded single-crystal domains, while some other regions appeared amorphous. Cryo-Electron Energy Loss Spectroscopy (EELS) mapping showed oxygen loss and vacancy formation within the Li–O–Cl lattice, affecting its local electronic structure.

This study demonstrates how Cryo-EM overcomes radiation and environmental degradation limitations, enabling nano-scale analysis of beam- and moisture- sensitive fast-ion conductors [5,6]. The results provide direct structural evidence linking local polarization effects to ion-transport pathways in Li_3ClO, offering critical insights for the rational design and optimization of solid electrolytes for lightweight structural solid-state batteries.

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Tuning the Defect Structure of NiO to Improve Electrocatalytic Nitrate-to-Ammonia Conversion

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Ammonia plays a pivotal role in sustaining global agriculture; however, its conventional production via the Haber–Bosch process remains highly energy intensive and environmentally impactful, accounting for approximately 2% of global CO_2 emissions.[1] At the same time, the widespread application of ammonia based fertilizers has resulted in significant nitrate contamination of aquatic systems. The electrochemical nitrate reduction reaction (E-NO_3RR) represents a promising strategy to address both challenges, offering the possibility of nitrate remediation alongside decentralized and sustainable ammonia synthesis. [2]
In this work, nickel oxide (NiO) nanoparticles are investigated as cost effective and earth abundant electrocatalysts for E-NO_3RR, leveraging their intrinsic ability to suppress the competing hydrogen evolution reaction.[3] NiO materials were synthesized through a scalable precipitation approach, employing varying ethanol/water solvent ratios to systematically tune defect density, porosity and crystallinity. The resulting samples were comprehensively characterized using thermal analysis, structural techniques and spectroscopic methods to elucidate structure-property relationships.
Electrochemical evaluation demonstrates that increasing the ethanol fraction during synthesis promotes higher defect density, which correlates with enhanced Faradaic efficiency and ammonia production rates. These findings highlight the decisive influence of synthetic parameters on catalytic behavior and identify defect engineered NiO as a promising platform for sustainable ammonia generation via electrochemical nitrate reduction.

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Kinetically Controlled Rotary Bed Pyrolysis for Enhanced Lithium Recovery from Lithium Iron Phosphate (LFP) Black Mass

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The industrial adoption of lithium iron phosphate (LFP) batteries recycling strategies demands pre-treatments specifically tailored to their thermodynamically stable olivine structure. In contrast to layered oxides, $LiFePO_4$ exhibits low lithium solubility and strong structural integrity, limiting lithium recovery efficiency in direct hydrometallurgical processing. A controlled thermal activation step is therefore essential to modify phase stability and enhance lithium accessibility.

This work investigates rotary bed pyrolysis as a scalable and kinetically controlled pre-treatment for LFP black mass. Unlike static furnace systems, the rotating bed configuration ensures continuous particle agitation, improved heat transfer uniformity, and enhanced gas-solid interaction, thereby minimizing thermal gradients and diffusion limitations. Pyrolysis was conducted in the temperature range of 400-800 °C under controlled inert and mildly oxidative atmospheres with defined residence times.

Phase changes was characterized by X-ray diffraction and thermodynamic modelling, while lithium redistribution and extractability were quantified via selective aqueous leaching coupled with ICP analysis. The results demonstrate that controlled thermal treatment induces partial phase transformation and surface restructuring without complete phosphate breakdown. The extent of structural modification strongly depends on temperature, oxygen partial pressure, and holding time, directly controlling subsequent lithium leaching efficiency.

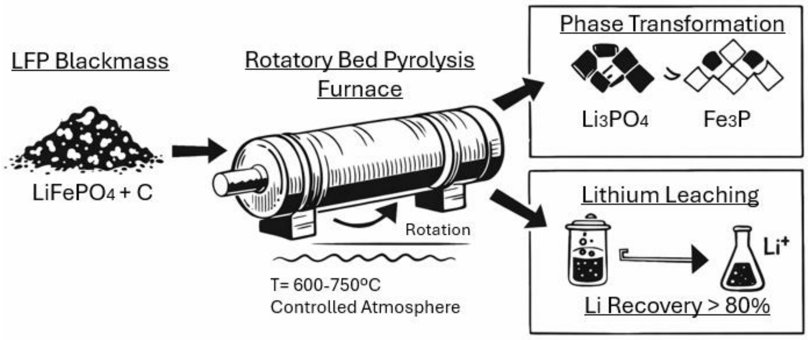

Figure 1. LFP Pyrolysis for Lithium Recovery.

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Redesigning Zinc-Metal Batteries through Tailored Electrode Coatings and Electrolyte Engineering

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The transition toward a renewable energy economy necessitates the integration of robust energy storage systems to stabilize the grid against the inherent fluctuations of solar and wind power. While Lithium-ion batteries currently dominate the market, their long-term viability is challenged by high costs and a reliance on critical raw materials. Aqueous zinc-ion batteries (AZIBs) offer a promising alternative, offering a safe, low-cost, and environmentally friendly solution with an established recycling infrastructure and a global warming potential significantly lower than traditional systems. Furthermore, the abundance of zinc is approximately ten times higher than that of lithium, and with projected costs as low as 40-50 €/kWh by 2030, there is a unique strategic window for European players to lead the industrialization of this technology [1]. Despite this potential, the transition from primary cells to high-performance secondary AZIBs is currently hindered by significant material challenges, including cathode dissolution, zinc dendrite growth, and parasitic hydrogen evolution, which limits both operating voltage and efficiency [2]. This doctoral research addresses these bottlenecks through an innovative material redesign of the cell architecture, optimizing the critical electrode-electrolyte interfaces to enhance longevity and efficiency. To stabilize the cathode, the investigation focuses on high-entropy oxides, utilizing their high configurational entropy to stabilize the host lattice and suppress the cation dissolution. This structural stabilization is synergistically coupled with the development of zinc-alloys via sputtering techniques for the anode to regulate zinc plating and suppress dendrite-induced short circuits. To further enhance performance, a specialized polymer-gel electrolyte is integrated to widen the electrochemical stability window and minimize hydrogen evolution. By combining these improvements, this work aims to contribute to the development of AZIBs as a sustainable addition to the energy storage landscape, offering a safe, low-cost, and non-flammable alternative to traditional systems.

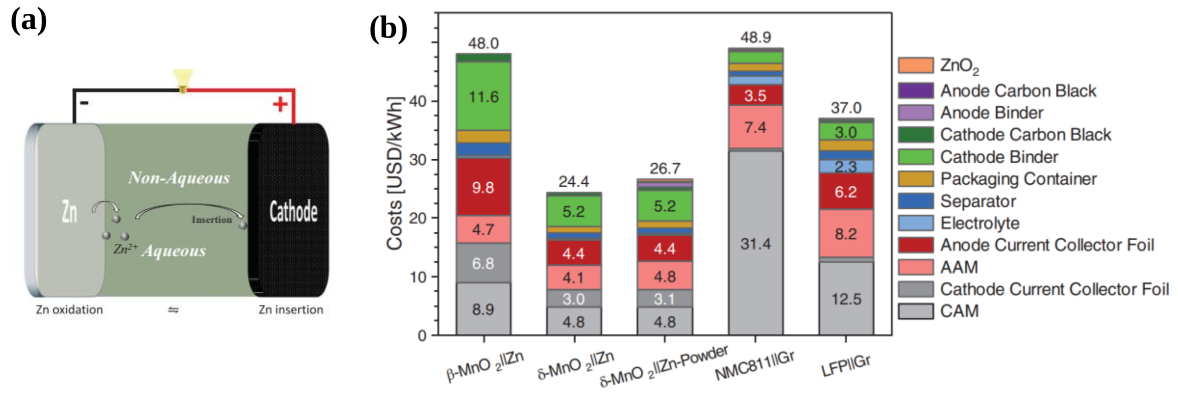

Figure 1: (a) Schematic diagram of zinc-metal battery and (b) comparison of material costs for zinc-metal batteries, NMC811 and LFP cell [2]

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Impact of Cathode–Electrolyte Interfacial Degradation on the Direct Recycling of Solid Electrolyte Li_6PS_5Cl from Spent Batteries

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Lithium solid-state batteries (LSSBs) represent a promising next-generation energy storage technology thanks to their potential for high energy density and improved safety relative to lithium-ion batteries [1]. As LSSBs are dependent on multiple critical elements, the development of viable recycling approaches is important for their long-term sustainability. Despite rapid progress of LSSB technology, recycling strategies for LSSBs remain at an early proof-of-concept stage [2-4]. In particular, the recoverability of functional materials from electrochemically aged cells is not yet well understood. Here, we studied how different aging conditions of LSSBs influence the structural, transport, and electrochemical characteristics of directly recycled Li_6PS_5Cl (LPSCl), a benchmark solid electrolyte material. LSSB cells employing composite $LiNi_{0.83}Co_{0.11}Mn_{0.06}O_2$ (NCM83)–LPSCl cathode were subjected to mild and severe calendar aging prior to ethanol-based recycling of LPSCl. The recycled solid electrolytes were analyzed by X-ray diffraction, neutron powder diffraction, Raman spectroscopy, solid-state nuclear magnetic resonance (ssNMR) spectroscopy, and *operando* electrochemical impedance spectroscopy. While the argyrodite framework was largely retained after recycling, prior degradation at the NCM83–LPSCl interface markedly affected material structure, ionic transport, and electrochemical properties of the recovered solid electrolytes. Notably, despite comparable ionic conductivity at 25 °C, solid electrolytes recycled from different aging conditions show considerable discrepancies in cell performance and interfacial stability. Our findings underline the significant impact of cathode–electrolyte interfacial degradation during cell operation and the necessity of accounting for battery aging when designing direct recycling strategies for sulfide-based LSSBs.

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Advancing Direct Recycling of ILE-Based Li-ion Batteries through Interface-Focused Delamination

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Ionic liquid electrolytes (ILEs) offer a safer and more sustainable alternative to conventional organic electrolytes in lithium-ion (Li-ion) batteries. Their low flammability, high electrochemical stability above 4.2 V, and resistance to thermal decomposition make them suitable for applications that require high safety and long-term durability [1]. Conventional electrolytes are highly volatile, which limits their recovery during recycling and often leads to material loss [2]. In contrast, ILEs are less volatile and more thermally stable, creating opportunities for improved electrolyte recovery. Despite these advantages, recycling methods tailored to ILE-based Li-ion batteries remain limited.

This work introduces an interface-focused delamination technique for the direct recycling of electrodes from used ILE-based lithium-ion batteries. Instead of relying on binder decomposition, the method targets the adhesion between the current collector and the active material layer. The process induces controlled interfacial oxidation and volume expansion at the current collector–active material interface, weakening adhesion and enabling clean separation of the CAM or AAM from aluminium or copper foils with minimal structural damage. This approach preserves both the active material and the current collector in a state closer to their original form, reducing the need for harsh chemical treatments and lowering material loss during recycling. The study examines the mechanism and key parameters that control this interface-driven separation, as well as post-separation cleaning, purification, and validation of the recovered materials. The technique provides a scalable route for direct recycling of ILE-based cells and helps retain active materials and current collectors during electrode recovery.

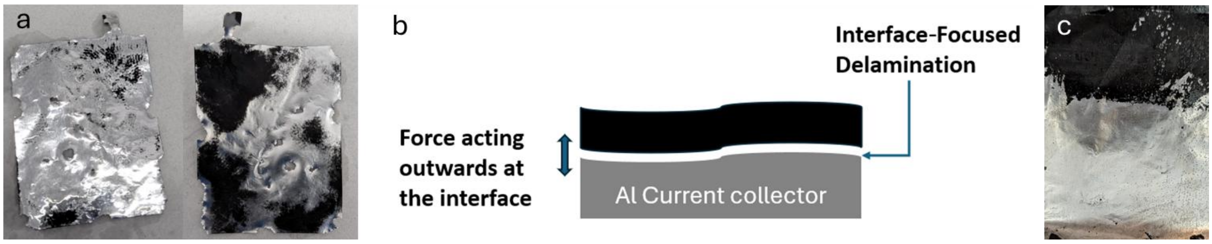

Figure 1 a) Sonication-based delamination of used electrodes. At low frequencies, strong cavitation leads to pitting and tearing of the aluminium current collector. At higher frequencies, delamination remains incomplete and residual CAM stays adhered to the foil. b) Schematic of the interface-focused delamination mechanism. The method targets the current collector–CAM interface by inducing controlled interfacial oxidation and volume expansion. This weakens adhesion and generates an outward force that lifts the CAM layer from the foil. In contrast, sonication concentrates mechanical energy at the current collector surface. c) Cathode recovered using the interface-focused process, showing clean separation of the CAM from the current collector with minimal mechanical damage.

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Coupled LLZTO–Succinonitrile Effects in PEO Solid-State Electrolytes: A Synergistic Pathway to Enhanced Performance

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All solid-state lithium metal batteries are emerging as a promising energy storage technology due to their high energy density compared to conventional lithium-ion systems. Their performance relies on the development of a solid-state electrolyte (SSE), which must combine high ionic conductivity with interfacial stability, mechanical strength and long-term electrochemical durability [1,2]. Among polymer-based SSEs, polyethylene oxide (PEO) is widely investigated for its strong lithium salt solvation and good Li-ion transport. However, its high crystallinity, arising from linear chain structure, limits room temperature ionic conductivity [3,4]. To enhance the performance without compromising flexibility, passive or active inorganic fillers are added in the polymeric matrix. $Li_{6.75}La_3Zr_{1.75}Ta_{0.25}O_{12}$ (LLZTO) is an active ceramic oxide, which can work as a conductive phase within polymer matrix, improving ionic conductivity, electrochemical stability window and mechanical stability. However, LLZTO nanoparticles are difficult to disperse homogeneously and are susceptible to air exposure, leading to the formation of a resistive surface layer [1,5]. An alternative solution to promote PEO performances involves solid plasticizers, such as succinonitrile (SN). SN is a non-ionic plastic crystal that undergoes a solid–solid phase transition near −40 °C, resulting in increased structural disorder and molecular mobility, which in turn enables high ionic conductivity at room temperature. However, SN-based electrolytes suffer from poor mechanical strength, high sublimation tendency of SN and chemical reactivity with lithium [2,6].

The present work investigates the preparation and characterization of hybrid polymer-ceramic SSEs based on a reference PEO/LiTFSI system, incorporating LLZTO and SN, with the aim of achieving an optimal balance between high ionic conductivity, adequate mechanical strength and good interfacial stability. SSEs were characterized chemically (SEM, FTIR, XRD), thermically (TGA, DSC) and electrochemically (IC, LSV, IS). Compared to PEO/LiTFSI-based electrolyte, the introduction of SN enhances the cycling performance of Li|electrolyte|LFP cells, maintaining high retentions even at high C-rates. However, symmetric Li|electrolyte|Li cells containing SN exhibit unstable plating and stripping behaviour and increasing interfacial resistance. Conversely, the addition of LLZTO improves interfacial stability, resulting in higher long-term stability, despite relatively modest cycling performance. The combined addition of LLZTO and SN provides enhanced battery performance in terms of both capacity retention in half cell configuration (> 90 % at C/5 and C/2) and plating/stripping durability (above 1700 h at 0.1 $mA\ cm^{-2}$), indicating the hybrid electrolyte benefits from good ionic conductivity and interfacial stability.

The experimental results collected in this work enable a clear differentiation and comparison of the effects of the two additives, while also highlighting the benefits of their combined use in a mixed formulation, which offers a promising route toward improved performance in solid-state lithium metal batteries.

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Benchmarking Composition-Based Machine Learning for the Accelerated Discovery of Battery Electrode Materials

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The rapid development of next-generation battery technologies requires a transition from traditional experimental trial and error to accelerated, data-driven discovery workflows. While machine learning (ML) has emerged as a powerful tool for predicting material properties, most current models rely on structural descriptors that necessitate prior knowledge of crystal geometries, thereby limiting their utility in initial high-throughput composition screening [1].

This study presents a systematic benchmark of state-of-the-art compositional ML models (MODNet, CrabNet, and Random Forest) using the Materials Project (MP) Battery dataset [2]. By utilizing exclusively composition-based features, we demonstrate that CrabNet achieves predictive accuracy for gravimetric capacity that is comparable to, or exceeds, established structural models. Our methodology employs non-linear dimensionality reduction (t-SNE and UMAP) and Density-Based Spatial Clustering (DBSCAN) to map the chemical space of over 5,000 electrode materials, revealing clear clustering based on working ions and electrochemical potential [3].

To ensure the reliability of these predictions for future battery chemistries, we evaluate model robustness through Leave-One-Cluster-Out (LOCO) and stratified 5-fold cross-validation. These results highlight the ability of composition-only architectures to generalize across diverse chemical regimes, including multivalent systems like Mg and Ca. This work establishes a rigorous performance baseline and provides open-source model weights, offering a computationally efficient first-stage screening tool to accelerate the identification of high-performance cathodes for sustainable energy storage.

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AMMONIA AS ENERGY VECTOR AND LITHIUM MEDIATED AMMONIA ELECTROSYNTHESIS

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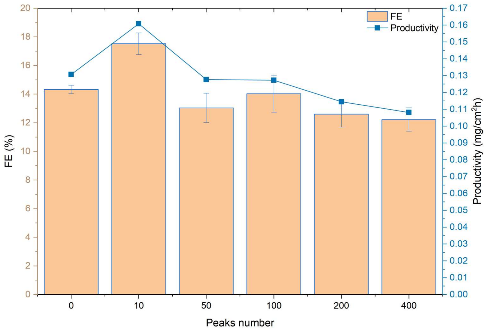
As a fundamental chemical with diverse applications, ammonia (NH_3) has emerged as a promising energy carrier for hydrogen transport and power generation via internal combustion engines and gas turbines, making it a pivotal energy vector for reducing global emissions and achieving net-zero targets by 2050 [1, 2]. The primary drawback related to the use of ammonia is its production process, the Haber-Bosch, which is extremely energy-intensive and contributes significantly to global CO_2 emissions [3, 4]. To mitigate this environmental impact and achieve independence from fossil fuels, alternative green ammonia synthesis methods are being developed. Among these, lithium-mediated electrochemical nitrogen reduction (Li-NRR) is currently considered one of the most viable pathways [5].

This study focuses on optimizing the electrochemical protocol for a Li-mediated system. Initially, a batch configuration was employed using two consecutive current regimes: (i) a pulsed- high current regime to promote the Li-plating and the formation of the solid electrolyte interphase (SEI) layer, followed by (ii) a steady- lower current regime where the nitrogen reduction reaction primarily occurs. To ensure a consistent comparison, the duration of the steady-current step was adjusted to maintain a fixed total charge of 20 C. The objective was to evaluate how the number of pulsed- high current peaks influences SEI formation, composition, ammonia yield, and overall system efficiency. Faradaic efficiency (FE) and ammonia productivity were used as the main performance descriptor. Ammonia quantification was performed via Berthelot reaction and UV-Vis spectrophotometry. Moreover, the SEI-layers corresponding to the conditions that yielded the best and worst results were analyzed using air-free X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM). The maximum Faradaic efficiency obtained was approximately 18%, while the highest productivity reached was 0.16 mg/cm^{2}h. Both were obtained when 10 current pulses at 25 mA cm^{-2} were applied. FESEM micrographs revealed a more homogeneous and compact SEI layer under these conditions, while XRD analysis indicated the presence of LiF.

The study subsequently transitioned to a flow system to investigate the effect of the same electrochemical protocol on ammonia production and SEI formation. The set-up of this electrochemical cell is characterized by two countercurrent flows of electrolyte and nitrogen. The effect of the electrochemical protocol remained consistent with the batch setup. Therefore, the best results are obtained imposing 10 current pulses at 25 mA cm^{-2}, in this case the total charge was fixed at 100 C to match the test duration of the batch experiments. Although the obtained results are still far from the performance of Haber-Bosch process, further research is necessary to better understand SEI dynamics, improve the investigated system, and explore more innovative solutions.



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DIRECT RECYCLING OF BATTERIES WITH THE FOCUS ON RECOVERY AND REUSE OF NICKEL, COLBALT AND MANGANESE METALS FROM NMC811-BASED END-OF-LIFE LITHIUM ION CELLS

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This work highlights recent advances with the development and scale-up of TRL7 technology of Direct Recycling of 18650-sized end-of-life lithium-ion battery cells implemented at American Energy Technologies Co.'s (AETC's) Wheeling IL, USA plant. Spent cells were supplied by Europe's largest gigafactory producing 18650 cells, ASPILSAN ENERJI Sanayi Ve Ticaret AS of Kayseri, Turkey and were processed through a unique Direct Recycling flow sheet that defuses residual charge from the cell, uses precision machine shop equipment to open cylindrical cells, and retrieve cathode, anode, and separator as three separate streams of recoverable feedstocks.

NMC811-based cathodes that are tape cast on aluminum foil are first heat-treated in air at a temperature of 450˚C to loosen the bond between active material and current collectors. In the next step, heat treated electrodes in bulk are subjected to ultrasonic treatment in a water tank which causes approximately 95% of cathode active material to fall into solution. Next, the solution is processed through vacuum filtration and subsequently is sent to downstream processors at ISPE. ISPE dissolves active material into a mixed salt solution which is then subjected to selective electrowinning in the plating bath with moving anode. The deposit that forms on the anode is manganese dioxide which takes the form of EMD or ɤ-MnO_2. The deposit on the cathode is a solid alloy whose concentration can be fine-tuned based on a desired voltage, tied to a RedOx potential. In this particular work, Ni-Co alloy with a composition of 85.1wt.% nickel and 14.9wt.% cobalt was deposited (Figure 1).

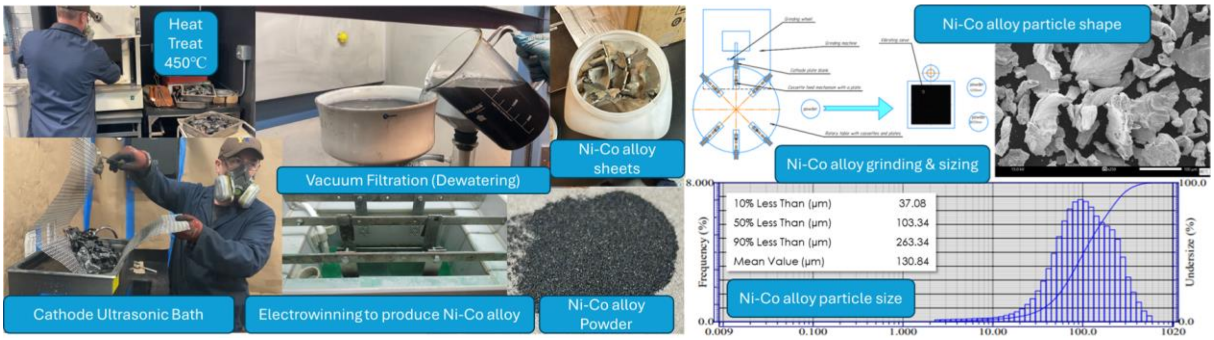

Figure 1. Processing of the end-of-life battery grade NMC811 and its properties prior to full recycling.

It was determined that dissolving the alloy from ingot or foil form is difficult and therefore technology was developed jointly between AETC and UNE for pulverizing Ni-Co blocks into fine powder. The powder has magnetic properties, and its composition did not change during grinding and sizing, which indicates that the original metal plated as an alloy and not as a multi-layer deposit. Powders are now ready for continued processing through co-precipitation to form recycled NMC811. This work will be reported in future publications.

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INFLUENCE OF ADDITIVES AND CELL DESIGN ON THE ELECTROCHEMICAL PERFORMANCE OF Li–S COIN CELL BATTERIES

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Lithium–sulfur (Li–S) batteries are promising energy-storage systems thanks to their exceptional theoretical capacity of 1675 mAh/g, the abundance and low cost of raw materials, and their overall environmental friendliness. Despite significant advances in recent years, the key challenge limiting the practical use of Li–S technology is the gradual capacity decline during long-term cycling. This deterioration is mainly driven by the high reactivity of lithium polysulfides, which leads to the so-called *shuttle effect*—a process in which less reduced polysulfides oxidize the more reduced ones, resulting in energy loss and reduced efficiency.

In our research, we investigated how the morphology of cathode additives [1-3] (porous carbon materials that facilitate sulfur reduction and accommodate substantial volume changes during electrochemical reactions), affects the charge capacity and cycling stability of Li–S coin cells. Alongside commercially available additives, we also examined a macroporous carbon synthesized via glucose pyrolysis using silica spheres as a templating agent. The Li–S cell with a cathode based on this macroporous carbon delivered an initial capacity exceeding 700 mAh/g of sulfur. After 120 cycles at 0.1C, the capacity loss remained below 10%. Furthermore, the impact of the electrolyte-to-sulfur ratio, the geometry of the specific coin cell, and the presence of the electrocatalyst was investigated, and their influence on the electrochemical performance of Li–S coin cells was evaluated.

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The Path of Lithium During Pyrometallurgical LFP Recycling

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The pyrometallurgical recycling of lithium-ion batteries is a robust and efficient process for the recycling of end-of-life lithium-ion batteries. Nevertheless, the significant challenge lies in the recovery of lithium. Recovering lithium is crucial, not only due to its economic value but also the limited availability of primary sources. Therefore, this study investigates the fate of lithium during pyrometallurgical recycling from LFP batteries. It is known that during this process, Li forms a slag compound which is difficult to treat further. Moreover, by adjusting the flux system, it is possible to suppress Li slagging and Li can be collected from the flue dust in a soluble form. [1, 2] The present study investigates the impact of various flux systems on Li volatilization by means of a simulation tool provided by HSC Chemistry.

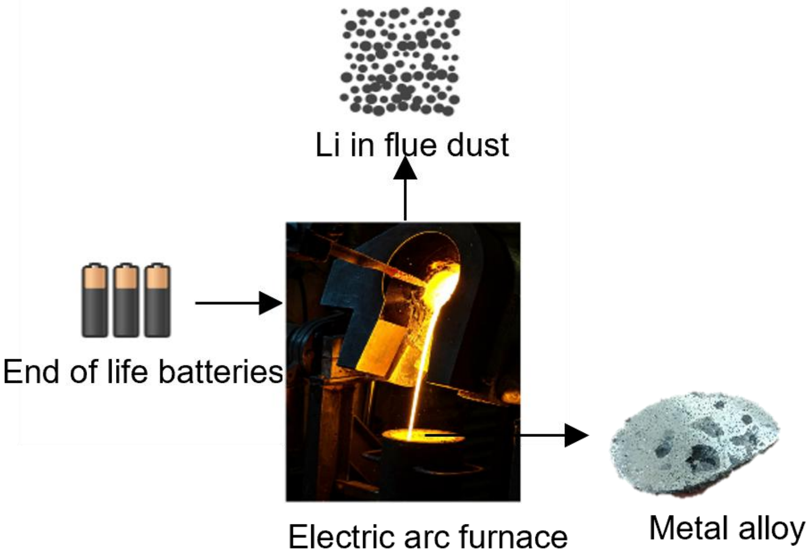

Figure 1. Process flow chart for lithium volatilization from end-of-life batteries in an electric arc furnace

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